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The Vacuum State in Hybrid Loop Quantum Cosmology

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It was a question, she remembered, how to connect this mass on the right hand with that on the left. She might do it by bringing the line of the branch across so; or break the vacancy in the foreground by an object. But the danger was that by doing that the unity of the whole might me broken.

Virginia Woolf

Para Natalia, que la va a leer pero no la va a entender

Para Enrique, que la hubiera entendido

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[1] El Inge
[2] Lench
[3] Kents

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Abstract

In generic curved spacetimes, the absence of a natural vacuum state introduces an ambiguity that can undermine the physical relevance of predictions from any field quantization. In the context of inhomogeneous fields propagating in homogeneous, isotropic, but otherwise general cosmological spacetimes, this problem obstructs the extraction of robust predictions. This obstruction is aggravated in applications to cosmology of candidates to a quantum theory of gravity, where even the cosmological background where the fields propagate is treated as a quantum entity, or at most as an effective spacetime. One example is provided by the hybrid approach to quantum cosmology, in which a quantum mechanical description of the cosmological degrees of freedom, usually within Loop Quantum Cosmology (LQC), is combined with a more conventional Fock quantization of the infinite number of degrees of freedom that account for the inhomogeneities. In this context, we investigate in this thesis physical criteria to successfully remove the ambiguity of choice of vacuum state for two different types of fields in hybrid LQC: fermionic fields treated as perturbations, and primordial scalar and tensor perturbations leading to non-oscillating (NO) power spectra. For fermions, we first restrict ourselves to a family of vacua which leads to a unitarily implementable quantum Heisenberg evolution. Then, we manage to further restrict this choice by considering the asymptotic limit of large Fourier wavenumbers in the mode decomposition of the Dirac field and demanding there a convergent quantum backreaction. Further restrictions in this limit also guarantee that the fermionic contribution to the Hamiltonian be a well defined quantum operator on the dense subset of the fermionic Fock space which is spanned by the n-particle/antiparticle states. Finally, we use the entire available asymptotic freedom in what respects the definition of a vacuum state to eliminate from the fermionic Hamiltonian any term which creates or annihilates pairs of particles, at any given order in the asymptotic limit. We compare the vacuum selected by these physical criteria with fermionic adiabatic states, which had previously been proposed as potential vacua in cosmology. Actually, we prove that all adiabatic states allow a unitarily implementable quantum evolution. Furthermore, all of them but the zeroth order adiabatic state give rise to a finite backreaction. To finish our study of the fermionic vacuum, we apply the suggested asymptotic diagonalization procedure in a de Sitter Universe, showing that it picks out a unique vacuum state, which in fact coincides with the well-known Bunch-davies vacuum. In addition to the problem of fermions in cosmology, we also discuss the possible choice of a vacuum state for scalar and tensor cosmological perturbations in LQC by demanding an NO power spectrum. This type of NO vacuum was originally introduced by numeric means to avoid the rapid oscillations in the spectrum found in the literature for other states of the perturbations, oscillations that could result in an amplification of power when averaged over bins of Fourier wavenumbers. We provide some analytic insights into why these oscillations may in fact be an artifact of the choice of vacuum state and how they can blur the actual quantum geometry effects in observational predictions if they are not avoided. We also give some analytical conditions that are necessary on a vacuum state if it is of NO type, and prove that in the ultraviolet asymptotic limit this class of vacua satisfy the asymptotic diagonalization proposal. Finally, we compare these necessary NO conditions with a construction for the vacuum put forward recently by Ashtekar and Gupt. This construction should select the state which is maximally classic at the end of inflation from a ball of

states that is picked out by the so-called Quantum Homogeneity and Isotropy Hypothesis (QHIH). However, we find a loose step in the proposed construction which allows that the Ashtekar-Gupt vacuum to exist outside of the QHIH ball. In fact, we prove numerically that, in a kinetically dominated short-lived inflationary scenario typically considered in LQC, the Ashtekar-Gupt vacuum lies outside of the QHIH ball. Nonetheless, we show that the NO necessary conditions and the QHIH are mutually non-exclusive in this scenario.

Resumen

En espaciostiempos curvos genéricos, la ausencia de un estado de vacío natural introduce una ambigüedad que puede minar la relevancia física de las predicciones de cualquier cuantización de campos. En el contexto de campos inhomogéneos que se propagan en espaciostiempos cosmológicos homogéneos e isótropos, pero por lo demás generales, este problema obstruye la extracción de predicciones robustas. Esta obstrucción se agrava en las aplicaciones a cosmología de los candidatos a una teoría cuántica de la gravedad, donde incluso el fondo cosmológico sobre el que se propagan los campos se trata como una entidad cuántica, o como mucho como un espaciotiempo efectivo. Un ejemplo de esto se da en el enfoque híbrido a la cosmología cuántica, en el que se combina cierta descripción cuántica de los grados de libertad cosmológicos, normalmente aquella dada por la Cosmología Cuántica de Lazos (CCL), con una cuantización de Fock más convencional del número infinito de grados de libertad que describen las inhomogeneidades. En este contexto, en esta tesis investigamos criterios físicos para eliminar con éxito la ambigüedad en la elección del estado del vacío para dos tipos diferentes de campos en CCL híbrida: campos fermiónicos tratados como perturbaciones, y fluctuaciones primordiales de tipo escalar y tensorial que conducen a espectros de potencia no oscilantes (NO). Para tratar los fermiones, primero nos restringimos a una familia de vacíos que conduce a una evolución cuántica en imagen de Heisenberg que es unitariamente implementable. A partir de ahí, restringimos aún más esta elección considerando el límite asintótico de números de onda de Fourier infinitamente grandes en la descomposición de modos del campo de Dirac y exigiendo allí una *backreaction* cuántica convergente. Otras restricciones en este límite también garantizan que la contribución fermiónica al hamiltoniano sea un operador cuántico bien definido en el subespacio denso del espacio de Fock fermiónico generado por los estados de n partículas/antipartículas. Por último, utilizamos toda la libertad asintótica disponible en lo que respecta a la definición del estado de vacío para eliminar del hamiltoniano fermiónico cualquier término que cree o aniquile pares de partículas, para cualquier orden dado en el límite asintótico. Comparamos el vacío seleccionado por estos criterios físicos con los estados adiabáticos fermiónicos, que habían sido propuestos previamente como posibles vacíos en cosmología. De hecho, demostramos que todos los estados adiabáticos permiten una evolución cuántica unitariamente implementable. Además, todos ellos, excepto el estado adiabático de orden cero, dan lugar a una *backreaction* finita. Para terminar nuestro estudio del vacío fermiónico, aplicamos el procedimiento de diagonalización asintótica sugerido en un universo de tipo de Sitter, mostrando que permite seleccionar un único estado de vacío que coincide con el bien conocido vacío de Bunch-Davies. Además del estudio de fermiones en la cosmología, también discutimos la posible elección de un estado de vacío para las perturbaciones cosmológicas de tipo escalar y tensorial en CCL, exigiendo un espectro de potencia NO. Este tipo de vacío NO fue introducido originalmente por medios numéricos para evitar las rápidas oscilaciones en el espectro encontradas en la literatura para otros estados de las perturbaciones. Dichas oscilaciones podrían resultar en una amplificación de la potencia cuando se promedian sobre ciertos rangos de números de onda de Fourier. En esta tesis proporcionamos algunas ideas analíticas sobre por qué estas oscilaciones pueden estar causadas por la elección del estado de vacío y, de esta forma, pueden difuminar los efectos genuinos de la geometría cuántica en las predicciones observacionales si no se

evitan. También damos algunas condiciones, formuladas de forma analítica, que son necesarias en un estado de vacío para que sea del tipo NO, y demostramos que en el límite asintótico ultravioleta esta clase de vacíos satisface la propuesta de diagonalización asintótica. Finalmente, comparamos estas condiciones necesarias de comportamiento NO con una construcción de vacío propuesta recientemente por Ashtekar y Gupt. Esta construcción debería seleccionar el estado que es máximamente clásico al final de la inflación cosmológica, partiendo de una bola de estados que es elegida por la llamada Hipótesis de Homogeneidad e Isotropía Cuánticas (HHIC). Sin embargo, encontramos un paso en la construcción propuesta que no queda bien fijado y permite que el vacío de Ashtekar-Gupt exista fuera de la bola seleccionada por la HHIC. De hecho, demostramos numéricamente que, en un escenario inflacionario de corta duración cinéticamente dominado, considerado habitualmente en CCL, el vacío de Ashtekar-Gupt se encuentra fuera de la bola HHIC. No obstante, mostramos que las condiciones necesarias de tipo NO y la HHIC son mutuamente no excluyentes en este escenario.

I. Introducción

La pregunta sobre el origen del Universo ha permanecido elusiva e inescrutable a lo largo de la historia humana. Hasta tiempos recientes, esta pregunta tenía hipótesis y respuestas que no podían ser desmentidas a través de las observaciones. La aparición de la cosmología física ha cambiado este panorama de forma drástica y nos ha permitido estudiar ese tema de manera científica [1, 2]. La cosmología física descansa sobre los cimientos de la Teoría de la Relatividad General de Einstein y ha servido como uno de sus mayores triunfos [3,4]. Es posible describir el Universo en sus escalas más grandes teniendo en cuenta la homogeneidad e isotropía (aproximadas) que se observan, particularizando las ecuaciones de Einstein a esta situación. Sin embargo, este procedimiento predice la existencia de un suceso, al que llamamos *Big Bang*, en el que aparecen algunas singularidades en cantidades físicas. De hecho, el estudio de la física no es ajeno a las singularidades, que pueden entenderse como la forma en que la naturaleza pone en evidencia que una teoría es incompleta de alguna forma. Por lo tanto, podemos tomar la motivación de otros ejemplos previos en la ciencia (por ejemplo, el modelo del átomo de Bohr) y buscar la resolución de la singularidad del *Big Bang* a través de una descripción cuántica de la Relatividad General.

Hay una serie de requisitos que una explicación cuántica satisfactoria del *Big Bang* debe satisfacer. En primer lugar, se debe resolver la singularidad. La geometrodinámica, por ejemplo, a pesar de su éxito parcial en proporcionar una descripción cuántica de la geometría, no consigue evitar el *Big Bang* en su aplicación a la cosmología [5–7]. En segundo lugar, la contrapartida cuántica del *Big Bang* debe recuperar la cosmología relativista cuando la densidad de la materia en el Universo sea lo suficientemente pequeña. Esto se debe a que, para estos regímenes, la teoría de Einstein ha sido comprobada con un grado considerable de precisión [8, 9]. En tercer lugar, la teoría debe ser matemáticamente consistente y conducir a predicciones que finalmente pudieran ser contrastadas. Finalmente, la consideración del caso cosmológico, altamente simétrico, podría servir para arrojar luz en la búsqueda de una teoría de gravedad cuántica completa.

Un candidato de tal teoría de gravedad cuántica es la Gravedad Cuántica de Lazos (GCL). La GCL es una cuantización canónica, independiente del fondo (*background*) y no perturbativa de la Relatividad General [10, 11]. Entre los resultados más importantes de la GCL está la demostración de que los operadores geométricos que miden longitud, área y volumen tienen espectros discretos [12–15]. Esto significa que la GCL predice que la propia geometría es discreta. Sin embargo, una formulación completa de la teoría que sea satisfactoria sigue siendo difícil de alcanzar.

Para comprobar si las técnicas de la GCL pueden predecir el Universo que observamos, podemos introducir simetrías en la teoría general antes de su cuantización, truncando así los grados de libertad considerados. En estos escenarios simplificados, algunas de las dificultades de la teoría completa desaparecen, por ejemplo aquellas que afectan más severamente la representación cuántica de la ligadura hamiltoniana y la determinación de su núcleo (*kernel*). El formalismo cuántico resultante se conoce generalmente como Cosmología Cuántica de Lazos (CCL) [16–20]. Uno de los resultados más importantes de la CCL es que proporciona un mecanismo robusto para evitar la singularidad del *Big Bang*, que es reemplazada por un *Big Bounce* en estados cuánticos con un comportamiento adecuado [21–23]. De hecho, que la geometría espaciotemporal sea discreta es lo que en última instancia explica por qué las cantidades físicas, tales como la densidad del Universo, permanecen acotadas en toda la evolución cosmológica.

Para extraer predicciones de teorías cosmológicas como la CCL, es especialmente importante estudiar las fluctuaciones cuánticas primordiales en el Universo temprano. Se cree ampliamente que estas fluctuaciones fueron las semillas de las inhomogeneidades observadas del Universo, y que han pasado por un periodo de inflación después de haberse originado en épocas de alta curvatura [1, 24]. En condiciones tan extremas, es razonable esperar que los efectos de la gravedad cuántica puedan haberlas afectado. Además, las huellas dejadas por estos efectos pueden haber sobrevivido al periodo inflacionario si el Universo observado era del tamaño de Planck cuando los fenómenos de gravedad cuántica eran relevantes. El estudio de las fluctuaciones primordiales puede servir entonces como banco de prueba de nuestra teoría cuántica, ya que esta debería ser capaz de explicar las anisotropías e inhomogeneidades presentes y a la vez dar cabida a algunas discrepancias con respecto a los resultados de la Relatividad General. Ha habido muchos intentos de lidiar con campos no homogéneos en la cosmología cuántica (ver, por ejemplo, [25–34]). Sin embargo, en esta tesis nos vamos a centrar principalmente en la llamada propuesta de cuantización híbrida, diseñada originariamente para CCL [35–41]. En el enfoque híbrido, el espacio de representación cinemático del sistema es un producto tensorial del espacio de Hilbert del fondo simétrico (normalmente elegido como el estándar de CCL) y un espacio de Fock para los campos cuánticos (bosónicos o fermiónicos [42, 43]) inhomogéneos [35, 44–46].

Hay una importante ambigüedad inherente a la selección de ese espacio de Fock, y con ella a la elección de un estado de vacío. La existencia de esta ambigüedad puede parecer extraña desde el punto de vista de la teoría cuántica de campos en el espaciotiempo de Minkowski, donde las simetrías del fondo seleccionan el estado de Poincaré como el vacío preferido [47,48]. Desafortunadamente, cuando se trabaja en espaciotiempos curvos (incluso en los cosmológicos, considerablemente simétricos), los argumentos de simetría no son generalmente suficientes para señalar un vacío único [49–51]. Es precisamente en la introducción de criterios físicos que guíen esta elección de estado de vacío en lo que se centra esta tesis, centrando la atención en el caso de fluctuaciones primordiales en CCL híbrida.

Más específicamente, la primera parte de esta tesis está principalmente dedicada a la determinación de un estado de vacío físicamente viable para las perturbaciones fermiónicas en CCL híbrida. Este estudio se realiza después de truncar la acción del sistema a orden cuadrático en las perturbaciones. Si bien la mayor parte de la literatura sobre cosmología cuántica se centra en las perturbaciones cosmológicas escalares y tensoriales, las partículas de espín semientero no se han discutido con el mismo nivel de detalle [52]. Estas partículas fermiónicas pueden describir contenidos materiales realistas, y su estudio gana relevancia si se consideran órdenes superiores en la teoría de perturbaciones, ya que entonces se acoplan con las perturbaciones escalares y tensoriales. La elección del estado de vacío para un campo de

Dirac en el enfoque de cuantización híbrida generalmente se realiza mediante la definición de ciertas variables específicas de aniquilación y creación para cada uno de los modos en la descomposición de Fourier del campo [53]. En CCL híbrida, esta definición se introduce de forma bastante sencilla tras realizar unas transformaciones canónicas adecuadas que nos permiten mezclar los grados de libertad homogéneos y inhomogéneos y que conducen a un hamiltoniano fermiónico con buenas propiedades físicas. En la literatura previa sobre los campos de Dirac en cosmología de Friedmann-Lemaître-Robertson-Walker (FLRW) plana, se demostró que existe una familia única de vacíos que son invariantes bajo las transformaciones de simetría del fondo cosmológico y que tienen una evolución de Heisenberg unitariamente implementable. Sin embargo, todavía hay mucha libertad disponible en la definición del vacío [54]. Aquí eliminamos esta libertad imponiendo requisitos físicos adicionales.

La segunda parte de la tesis proporciona información analítica para definir el vacío de las perturbaciones escalares y tensoriales más allá del paradigma inflacionario (p.ej. en CCL), de forma tal que sus espectros de potencias no sean funciones con una oscilación rápida en el número de onda (de Fourier). Para comenzar esta discusión, hacemos notar primero que todos los modos de Fourier de las perturbaciones invariantes de *gauge* (por ejemplo, el llamado campo de Mukhanov-Sasaki) satisfacen ecuaciones de tipo oscilador armónico con una masa dependiente del fondo cuando se trunca la acción del sistema a orden perturbativo cuadrático [1,55–59]. De esta manera, una elección de condiciones iniciales para dichas ecuaciones determina una solución para las perturbaciones, y con ella una elección de vacío que, a su vez, fija el espacio de Fock para estas perturbaciones. Cuando las perturbaciones se introdujeron por primera vez en CCL, los estados de vacío propuestos para ellas eran los llamados estados adiabáticos [32, 60]. Los estados adiabáticos se construyen a partir de cierto estado adiabático de orden cero a través de un proceso iterativo y, a un orden lo suficientemente alto, conducen a un tensor de energía-momento renormalizable [61–63]. En última instancia, a un orden adiabático infinito, uno alcanzaría lo que se conoce como un estado de tipo Hadamard [62,64–67]. Pronto quedó claro que los espectros de potencias de los estados adiabáticos de órdenes finitos eran altamente oscilatorios en CCL. No obstante, estas oscilaciones no tienen por qué ser una consecuencia intrínseca de la CCL y pueden estar enmascarando artificialmente efectos genuinos de la geometría cuántica. Para resolver estos problemas, Martín de Blas y Olmedo presentaron una propuesta para seleccionar un estado de vacío con propiedades no oscilantes (NO) [68]. Sin embargo, esta propuesta fue originalmente concebida para estudios numéricos. Antes de nuestro trabajo, no había disponible ninguna descripción analítica de vacíos NO que pudiera permitir un estudio más detallado de estos estados.

1. Introduction

the origin of the Universe has remained elusive and inescrutable along the human history. Until recent times, this question only had hypotheses and answers that could not be falsified through observations. The advent of physical cosmology has drastically changed this panorama and allowed us to study this issue in a scientific way [1,2]. Physical cosmology rests upon the foundation of Einstein's Theory of General Relativity and has served as one of its greatest triumphs [3,4]. One can describe the Universe at its largest scales by taking into account its observed (approximated) homogeneity and isotropy, particularizing Einstein's equations to this situation. However, this procedure predicts the existence of an event, which we call the Big Bang, in which some singularities appear in physical quantities. In fact, the study of Physics is no stranger to singularities, which can be understood as a way of Nature telling us that a theory is somehow incomplete. Thus, one may take motivation from other previous examples in Science (e.g. Bohr model of the atom) and seek the resolution of the Big Bang singularity in a quantum mechanical description of General Relativity.

There are a number of requirements that a successful quantum explanation of the Big Bang should satisfy. First of all, the singularity should be resolved. Geometrodynamics, for example, in spite of its partial success to provide a quantum description of the geometry, fails to avoid the Big Bang in its application to cosmology [5–7]. Second, the quantum counterpart to the Big Bang must be such that relativistic cosmology is recovered when the matter density in the Universe is sufficiently small. This is because, for these regimes, Einstein theory has been tested to a considerable degree of accuracy [8,9]. Third, the theory should be mathematically consistent and lead to predictions that can be eventually falsified. Finally, the consideration of the highly symmetric cosmological case would ideally enlighten the search for a full quantum theory of gravity.

A candidate of such a theory of quantum gravity is Loop Quantum Gravity (LQG). LQG is a non-perturbative and background-independent canonical quantization of General Relativity [10,11]. Among the most important results in LQG is the proof that the geometric operators that measure length, area, and volume have discrete spectra [12–15]. This means that LQG predicts geometry itself to be discrete. However, a complete and fully satisfactory formulation of the theory remains elusive.

In order to check if LQG techniques can predict the Universe that we observe, we can introduce symmetries in the general theory before its quantization, truncating in this way the considered degrees of freedom. In these simplified scenarios, some of the difficulties of the full theory disappear, e.g. those more severely affecting the quantum representation of the Hamiltonian constraint and the determination of its kernel. The resulting quantum formalism is generally known as Loop Quantum Cosmology (LQC) [16–20]. One of the most important results of LQC is that it provides a robust mechanism to avoid the Big Bang singularity, which is replaced by a big bounce in quantum states of suitable behavior [21–23]. In fact, it is the discreteness of the spacetime geometry that ultimately explains why physical quantities, such as e.g. the density of the Universe, remain bounded in the whole cosmological evolution.

To extract predictions from cosmological theories such as LQC, it is especially important to study primordial quantum fluctuations in the Early Universe. It is widely believed that these fluctuations were the seeds of the observed inhomogeneities of the Universe, and that they have undergone a period of inflation after being originated in epochs of high curvature [1, 24]. In such extreme conditions, it is reasonable to expect that quantum gravity effects may have affected them. Moreover, the imprint left by these effects can survive the inflationary period if the observed Universe was of Planck size when quantum gravity phenomena were relevant. The study of primordial fluctuations can then serve as a test of our quantum theory, as it should be able to explain the present anisotropies and inhomogeneities while ideally predicting some discrepancies with respect to the results of General Relativity. There have been many attempts to deal with inhomogenous fields in quantum cosmology (see e.g. [25–34]). However, in this thesis we are mostly going to focus on the so-called hybrid quantization proposal, originally designed for LQC [35–41]. In the hybrid approach, the kinematical representation space of the system is a tensor product of the Hilbert space of the symmetric background (usually chosen as the standard one of LQC) and a Fock space for the quantum (bosonic or fermionic [42, 43]) inhomogeneous fields [35, 44–46].

A serious ambiguity is inherent to the selection of that Fock space, and within it the choice of a vacuum state. The existence of this ambiguity may seem odd from the viewpoint of quantum field theory in Minkowski spacetime, where the symmetries of the background pick out the Poincaré state as the preferred vacuum [47, 48]. Unfortunately, when one works in curved spacetimes (even in the considerably symmetric cosmological ones), symmetry arguments are generically not enough to single out a unique vacuum state [49–51]. The aim of this thesis is precisely to introduce physical criteria to select the vacuum state, focusing on the important case of primordial fluctuations in hybrid LQC.

More specifically, the first part of this thesis is mostly focused on the determination of a preferred physical vacuum state for fermionic perturbations in hybrid LQC. This study is developed after truncating the action of the system at quadratic order in the perturbations. While most of the quantum cosmology literature centers on scalar and tensor cosmological perturbations, half-spin particles have not been discussed at the same level of detail [52]. These fermionic particles can describe realistic matter contents, and their study gains relevance when one considers higher orders in perturbation theory, since they then couple with the scalar and tensor perturbations. The choice of vacuum state for a Dirac field is usually done through the definition of some concrete annihilation and creation variables for each of the modes of the Fourier decomposition of the field [53]. In hybrid LQC, this definition is introduced in a rather straightforward way after performing some suitable canonical transformations which allow us to mix the homogeneous and inhomogenous degrees of freedom and which lead to a fermionic Hamiltonian with good physical properties. In the previous literature regarding Dirac fields in flat Friedmann–Lemaître–Robertson–Walker (FLRW) cosmology, it was proven that there exists a unique family of vacua that are invariant under the symmetry transformations of the cosmological background and have a unitarily implementable Heisenberg evolution. However, much freedom is still available in the definition of the vacuum [54]. We eliminate this freedom by imposing additional physical requirements.

The second part of the thesis provides analytic insights to define vacua for the scalar and tensor perturbations beyond the inflationary paradigm (e.g. in LQC), such that their power spectra are not rapidly oscillating functions of the (Fourier) wavenumber. To start this discussion, we first notice that all Fourier modes of the gauge invariant perturbations (e.g. the so-called Mukhanov-Sasaki field) follow harmonic oscillator equations with a background-dependent mass when one truncates the action of the system at quadratic perturbative order [1, 55–59]. In this manner, a choice of initial conditions for these equations determines a solution for the perturbations, and with it a choice of vacuum which, in turn, fixes the Fock space for these perturbations. When perturbations were first introduced in LQC, the vacuum states proposed for them were the so-called adiabatic states [32, 60]. Adiabatic states are constructed from certain zeroth order state through an iterative process and, at high enough order, they lead to a renormalizable energy-momentum tensor [61–63]. Ultimately, at infinite adiabatic order, one would reach what is known as a Hadamard state [62, 64–67]. It soon became clear that the power spectra of adiabatic states of finite order were highly oscillatory in LQC. Nonetheless, these oscillations need not be an intrinsic consequence of LQC itself, and they may be artificially blurring the genuine effects of the quantum geometry. To solve these problems, a proposal to select a vacuum state with non-oscillating (NO) properties was introduced by Martín de Blas and Olmedo [68]. However, this proposal was originally conceived for numerical studies. Analytical descriptions of NO vacua, which allow for a more detailed study of this type of states, were not available before our work.

2. Objectives and results of the thesis

When fermions were first introduced in hybrid LQC, it was noticed that, for suitably motivated physical states, one ended up with a Schrödinger-type equation for the fermionic degrees of freedom [53]. This equation includes a quantity that accounts for the difference between the evolution of the perturbed geometry and the unperturbed one, and that can be consequently interpreted as a fermionic backreaction. This quantity is possibly divergent, as it has been was-well known from the pioneering work of D'Eath and Halliwell [52], who considered fermions in quantum geometrodynamics. In the first analyses carried out in LQC, it was suggested that the these divergences could be cured through a "substraction of infinities" regularization scheme [53]. Nevertheless, one usually expects that a true quantum theory of gravity would be able to avoid these divergences without the need of employing such schemes. The objective of the first article in this thesis is to investigate if one can eliminate the aforementioned divergence by adopting a more suitable choice of Fock quantization of the fermionic field and its vacuum state. Indeed, we prove that the backreaction term can be made finite by performing a convenient canonical transformation to new annihilation and creation variables. The asymptotic ultraviolet behavior of these variables is restricted in this way. In fact, this restriction also lowers the asymptotic order of the interaction part of the fermionic Hamiltonian, which creates and annihilates pairs of particles and antiparticles. Further restrictions on this asymptotic behavior then guarantee that the resulting fermionic Hamiltonian is represented by a well-defined quantum operator in the Fock subspace spanned by the set of n particle/antiparticle states. [69][1]

As a continuation of this goal, the second objective of the thesis is to find a unique asymptotic expansion for the definition of the annihilation and creation variables that removes all the nondiagonal (or interactive) terms of the fermionic Hamiltonian in the ultraviolet regime. This leads to an optimal quantum evolution for the fermionic operators, at least in the asymptotic limit, because they only change in a phase. Such an asymptotic diagonalization is attained by means of a totally deterministic recursive relation which fixes the definition of the annihilation and creation variables in the considered limit. This procedure defines the most suitable vacuum, dynamically stationary in the asymptotic regime, because the annihilation operators would have a completely diagonal evolution in this regime according to our previous comments. In addition, we find that the backreaction for this state is not only finite, but of an arbitrarily small asymptotic order. Finally, the associated fermionic Hamiltonian is clearly a well-defined operator in the Fock subspace spanned by the set of n particle/antiparticle states.

Our next objective is to compare the vacuum state selected by these physical requirements with other vacua proposed in the literature, the most common of which are the adiabatic states [70–72]. Adiabatic states are obtained by an iterative process, the ultimate (infinite) step of which would ideally produce a Hadammard state. A construction of this kind of states, leading to well-defined Fock spaces, exists for fermionic fields [70]. However, it was formulated in a different representation of the Clifford algebra than

[1] This article was published previous to my enrollment in the PhD programme and, as such, it is referenced and not attached. However it is included as part of the thesis so that the overall line of reasoning is complete.

the one used so far in our previous works. We adapt this construction in our representation and show that all adiabatic states allow for a unitarily implementable Heisenberg evolution. Besides, for higher than/equal to the first adiabatic order, they lead to a generally convergent backreaction.

The final objective pursued in our study of fermions is to apply in full detail the asymptotic diagonalization scheme for the particular cosmological solution of a de Sitter Universe [73], and discuss the result. For this model, a general diagonalization of the fermionic Hamiltonian leads to coefficients in the desired canonical transformation that depend on some integration constants. However, the recursive relation that defines the asymptotic diagonalization can now be solved exactly and, in fact, it can be used to fix the aforementioned integration constants completely (except for an irrelevant phase). This means that the asymptotic diagonalization procedure serves to fix the vacuum uniquely. We study the corresponding positive-frequency decomposition of the fermionic field and conclude that it coincides with the one corresponding to the fermionic Bunch-Davies vacuum [1, 74–78].

Placing next the attention on the consideration of NO vacua for scalar and tensor primordial perturbations, our first objective is to derive some analytic conditions that characterize the definition of these states. To achieve this goal, we reparametrize the equation that describes the evolution of the Mukhanov-Sasaki field in a way inspired by the procedure of asymptotic diagonalization of the Hamiltonian, commented above for fermions and developed for scalar and tensor perturbations in Ref. [79]. Then, we show that the squared norm of any solution actually follows the well known Ermakov-Pinney equation [80,81]. This equation allows to isolate the possibly oscillatory part of this norm, and to identify some necessary conditions on the initial conditions in order to define NO vacua. Moreover, we argue that NO vacua are in fact the most natural states to choose in LQC, because the mode oscillations present in the primordial power spectrum for other vacua can erase the information on the physical effects of the quantum geometry. Finally, we show that all these vacua must asymptotically behave as the one selected by the aforementioned procedure of Hamiltonian diagonalization.

As a natural continuation of the above study, the final objective is to investigate other vacua proposed in the LQC literature in the light of the derived conditions on NO vacua. In particular, we revisit a construction put forward by Asthekar and Gupt [82,83]. Their proposal is meant to select the maximally classical state at the end of inflation (where quantum effects should be negligible) within a ball of states that is singled out by the Quantum Homogeneity and Isotropy Hyptohesis (QHIH). The QHIH is a quantum generalization of Penrose's hypothesis that the initial state of the Universe should have vanishing Weyl curvature [84, 85]. We find that the necessary conditions on NO vacua are not incompatible with the restriction to this QHIH ball, for a kinetically dominated early universe with short-lived inflation in hybrid LQC. Since the Ashtekar-Gupt vacuum is known to lead to a oscillatory power spectrum, its existence may put into question the possible classicality of any NO vacuum. However, we find a loose step in the Ashtekar-Gupt construction, which explains that the ball from which they select the vacuum differs in general from the QHIH ball. In fact, we numerically show that the Ashtekar-Gupt vacuum is out of this ball for the considered scenario in hybrid LQC.

2.1. Notation and structure of the thesis

In this thesis we use natural units such that $\hbar = c = G = 1$, where $\hbar$ is Planck reduced constant, c is the speed of light in a vacuum and G is Newton gravitational constant. We use the first letters of the Greek alphabet for spatial-temporal indices, $\mu, \nu ... = 0, 1, 2, 3$, the first letters of the Latin alphabet for spatial indices, $a, b, c, ... = 1, 2, 3$, and the middle letters of the Latin alphabet for indices of the internal gauge group, $i, j, k, ...$. They go from one to three for triads, which have internal group $SU(2)$, and from one to four for tetrads, with internal group $SO(3, 1)$. Finally, hats over phase space functions denote their operator counterpart in the corresponding quantum representation.

The structure of the thesis is as follows:

- Section 3 introduces preliminary concepts, convenient to understand the results of the thesis.
  - Subsection 3.1 summarizes the reformulation of General Relativity as a canonical theory of connections. This classical reformulation is the starting point for LQG.
  - Subsection 3.2 is an introduction to LQC. Specifically, we review the construction of the quantum Hilbert space that describes the background geometry in the hybrid approach. This is done in the context of an inflationary flat FLRW cosmology.
  - Subsection 3.3 explains the introduction of inhomogeneous perturbations to the homogeneous sector of cosmological systems, so that they form a canonical set that describes the perturbative gauge-invariant degrees of freedom. In this thesis, we truncate the action at quadratic perturbative order.
  - In subsection 3.4, a Dirac field is minimally coupled to the cosmological spacetime and treated as a perturbation.
  - Subsection 3.5 summarizes the key features of a hybrid quantization for the previously described system. Namely, one chooses a Hilbert space for the homogeneous sector adopting LQC techniques and suitable Fock spaces for the inhomogenous sectors.
  - In the context of the hybrid approach, one needs physical criteria to choose the Fock spaces for the inhomogeneous sector. Subsection 3.6 summarizes the known result that there is a unique (unitarily equivalent) family of vacua for fermionic fields that leads to a unitarily implementable quantum (Heisenberg) evolution.
  - Subsection 3.7 reviews the framework in which an NO vacuum was originally formulated. Namely, in hybrid LQC the evolution of the Fourier modes of the gauge-invariant scalar and tensor perturbations can be seen as that of a harmonic oscillator with a background-dependent mass. In this context, the choice of vacuum state is equivalent to the choice of a set of positive-frequency solutions to this equation, or alternatively of their initial conditions because their evolution is a well-posed Cauchy problem. One can then choose initial conditions

that minimize time-dependent (generally also mode-dependent) oscillations in the norm of their solutions that can blur the quantum gravity effects in the primordial power spectrum.

- Section 4 is a summary of the techniques and results used in the articles in order to obtain the goals that we have detailed.

  - Subsection 4.1 describes our investigations to define suitable vacuum states for fermionic perturbations around a flat FLRW cosmology. First, in the context of hybrid LQC we require that they avoid divergences in the backreaction terms without renormalization schemes based on a "subtraction of infinities" [69][2] . Second, we impose that they lead to an optimal quantum fermionic dynamics in the asymptotic limit of large Fourier wavenumbers. The next step is to compare the vacuum selected by these criteria with adiabatic states, which are commonly used in the literature. Finally, we apply these techniques to the tractable case of a de Sitter Universe, showing that our criteria indeed select a unique vacuum which, in fact, corresponds to the Bunch-Davies one.

  - Subsection 4.2 presents our analytic insights for the determination of NO vacua. On the one hand, we derive some necessary conditions on these vacua, and explain why the oscillatory nature of other vacua should not be directly assigned to quantum geometry effects. On the other hand, these necessary conditions are compared with the restrictions that underlie the Ashtekar-Gupt construction of a vacuum state.

It should be noted that while Section 3 on preliminary concepts is conceived to facilitate a somewhat straight line of reasoning, there are many concepts that are not necessary if one is interested only in one of the two main topics investigated in this thesis. A reader that is only interested in fermions may want to skip Subsection 3.7, while one who is only interested in NO vacua for scalar and tensor perturbations can skip Subsections 3.4 and 3.6.

[2]See footnote 1.

3. Preliminary concepts

3.1. General Relativity in terms of Asthekar-Barbero Variables

The work contained in this thesis is related to applications of Loop Quantum Gravity, whose starting point is a canonical reformulation of General Relativity [10, 86]. So, we first quickly review the Hamiltonian formulation of General Relativity [3, 87, 88]. Let us consider a globally hyperbolic spacetime. This spacetime admits a global function of time, and hence a 3+1 decomposition in terms of spatial hypersurfaces. The spacetime metric can be expressed using the lapse function N, the shift vector N_a, and the induced 3-metric on the spatial hypersurfaces h_{ab}. The lapse function and the shift vector do not describe true physical degrees of freedom, but they are rather Lagrange multipliers that encode information about the particular foliation adopted. The dynamical behavior of the system can then be captured in Hamiltonian equations for the metric h_{ab} and its canonically conjugated momentum, which is determined by the extrinsic curvature $K_{ab} = 1/2\pounds_n h_{ab}$, where $\pounds_n$ is the Lie derivative along the normal n to the spatial hypersurface. However, to correctly describe General Relativity, one needs to take into account in addition its symmetries, given by time reparametrizations and spatial diffeomorphisms. This is done by imposing, respectively, the Hamiltonian and diffeomorphisms constraints on the system.

Motivated in part by other theories that have been successfully quantized in a non-perturbative way (e.g Yang-Mill theories [89]), we search for a reformulation of the Hamiltonian description of General Relativity in terms of gauge connections [90,91]. We start by defining inertial reference frames (or triads) e_i^a, and their inverse, the co-triads e_a^i, which are related to the spatial metric by

$$h_{ab} = \delta_{ij} e_a^i e_b^j, \tag{3.1}$$

where $i, j = 1, 2, 3$ and δ_{ij} is the Kronecker delta. One can see that (3.1) introduces physically spurious degrees of freedom, since one can locally redefine the triads by an $SO(3)$ rotation and obtain the same 3-metric. To take this into account, one includes an additional set of gauge constraints on the theory, called Gauss constraints, that generate the commented internal rotations. Actually, we can take as gauge group the universal cover of $SO(3)$, i.e. $SU(2)$, which is a compact group. We denote its Lie algebra as $su(2)$. This procedure is necessary when one introduces fermions, which couple directly to the internal group and distinguish between the two leaves in the universal cover.

In practice, one does not take as (part of the) canonical variables the triads themselves, but rather adopts the densitized triads $E_i^a = \sqrt{h} e_i^a$, where h is the determinant of the 3-metric. One may choose as canonically conjugated variables the components of the Ashtekar-Barbero connection $A_a^i = \Gamma_a^i + \gamma K_a^i$, where $K_a^i = K_{ab} e_j^b \delta^{ij}$ and Γ_a^i is an $su(2)$ connection, called the spin connection, which defined in such a way that the triads are annihilated by the covariant derivative (that acts on both spatial and internal gauge indices). The parameter γ is a non-zero real number known as the Immirzi parameter [92–94] (and its value is usually fixed by arguments related to black hole entropy).

In terms of these canonical variables, one constructs the basic variables of the system which, in order to extract directly the gauge-invariant information, are instead given by the holonomy-flux algebra, formed by holonomies along (piecewise analytic) edges e,

$$h_e(A) = \mathcal{P}\exp\int_e A_a^i \tau_i dx^a,$$

and smeared fluxes through surfaces,

$$E(S,f) = \int_S f^i \varepsilon_{abc} E_i^a dx^b dx^c,$$

where $\mathcal{P}$ denotes path ordering, ε_{abc} is the totally antisymmetric symbol, τ_i are $-i/2$ times the Pauli matrices and f^i are $su(2)$-valued smearing functions [11]. The elementary Poisson brackets are obtained from

$$\{E_i^a(\vec{x}), E_j^b(\vec{x}')\} = \{A_a^i(\vec{x}), A_b^j(\vec{x}')\} = 0,$$
$$\{E_i^a(\vec{x}), A_b^j(\vec{x}')\} = -8\pi\gamma\delta_b^a\delta_i^j\delta^3(\vec{x}-\vec{x}'), \tag{3.2}$$

where $\delta^3(\vec{x}-\vec{x}')$ is the Dirac delta on the spatial hypersurfaces. Apart from the Gauss constraints that have a trivial action on the holonomies and fluxes,

$$\mathcal{G}_i = \partial_a E_i^a + \delta^{kl}\epsilon_{ijk} A_a^j E_l^a = 0, \tag{3.3}$$

the system is subject to the spatial diffeomorphisms and Hamiltonian constraints H_a and H, that modulo the Gauss contraints can be expressed in the form

$$8\pi\gamma H_a = F_{ab}^i E_i^b = 0, \tag{3.4}$$
$$16\pi H = \frac{E_i^a E_j^b}{\sqrt{|\det E|}}\left[\delta_{kl}\epsilon^{ijk} F_{ab}^l - 2(1+\gamma^2) K_{[a}^i K_{b]}^j\right] = 0. \tag{3.5}$$

Here, F_{ab}^i is the curvature of the connection A_a^i, i.e. $F_{ab}^i = 2\partial_{[a}A_{b]}^i + \delta^{il}\epsilon_{ljk}A_a^j A_b^k$, we have used squared brackets as a notation for the standard antisymmetrization of indices and $\det E$ is the determinant of the densitized triad (whose absolute value equals h).

3.2. LQC for Friedmann–Lemaître–Robertson–Walker spacetimes

Let us consider the case of a FLRW spacetime with flat spatial hypersurfaces [95–98]. For convenience, we take these hypersurfaces to be compact, isotropic to a three-torus with compactification period denoted by ℓ_0. In addition, we use coordinates adapted to the spatial homogeneity. In such a cosmological spacetime, our configuration variables E_i^a and A_a^i possess each only one independent component, and we can express them as [17, 18, 20]:

$$A_a^i = c\, \ell_0^{-1}\, {}^0e_a^i, \quad E_i^a = p\, \ell_0^{-2}\sqrt{{}^0h}\, {}^0e_i^a. \tag{3.6}$$

Here, ${}^0e_i^a$ is a fiducial flat diagonal triad with no physical content, and ${}^0h$ is its determinant. We have that p is related to the usual scale factor by $a = \ell_0^{-1}\sqrt{|p|}$, whereas $|c| = \gamma\ell_0|\dot{a}/N|$ in the classical theory, where $\dot{a}$ is the time derivative of a. The fundamental Poisson bracket, obtained from (3.2), is

$$\{c, p\} = \frac{8\pi\gamma}{3}. \tag{3.7}$$

In this thesis we are mainly concerned with inflationary universes [99]. To introduce inflation into this system, we minimally couple a homogeneous scalar field ϕ with a potential, typically a quadratic term $m^2\phi^2/2$ with real mass m. Together with its canonical momentum π_ϕ, the field provides a new pair of canonical variables:

$$\{\phi, \pi_\phi\} = 1. \tag{3.8}$$

The spacetime symmetries and our conventions lead to spatial diffeomorphisms contstraints (and Gauss constraints) that are trivially satisfied. Only the Hamiltonian constraint needs to be taken into account. This constraint can be rewritten as

$$H_{|0} = -\frac{3}{8\pi\gamma^2}c^2|p|^{1/2} + \frac{\pi_\phi^2}{2|p|^{3/2}} + \frac{1}{2}m^2\phi^2|p|^{3/2}. \tag{3.9}$$

To define the quantum kinematics of the system, we must determine a set of elementary variables and provide an operator representation of them. Following LQG techniques, we introduce the holonomy-flux algebra given by holonomies h_e, defined by the connection A_a^i along edges e, and fluxes of E_i^a accross two-dimensional surfaces S. Given the assumed homogeneity and isotropy, it actually suffices to consider straight edges in the fiducial directions and square surfaces with edges parallel to those directions. It is important to notice that it is at the step of quantizing this algebra where LQC departs from the Wheeler-DeWitt formalism in cosmology, because the latter employs a continuous representation of the elementary variables which are directly (i.e. linearly) related to c and p [6, 7], while LQC uses a discrete representation of the holonomies of c. In our canonical formalism, we use Dirac's proposal for the quantization of constrained systems. Thus, physical states ultimately belong to a *dynamical* Hilbert space constructed from the intersection of the kernels of the quantum operators that represent the constraints on the *kinematical* Hilbert space that we use as starting point [100].

As we have commented, in our cosmological system we only have to consider holonomies along straight edges oriented in the fiducial directions, with length $\mu\ell_0$, where μ is an arbitrary real number.

The holonomy along an edge in the i-th direction is

$$h_i^{\mu}(c) = e^{\mu c \tau_i} = \cos\left(\frac{\mu c}{2}\right) \mathbb{I}_2 + 2\sin\left(\frac{\mu c}{2}\right) \tau_i, \tag{3.10}$$

where $\mathbb{I}_2$ is the identity matrix in two dimensions. Since the matrix elements of these holonomies are linear combinations of complex exponentials, we can take as our elementary configuration variables the exponentials $\mathcal{N}_\mu(c) = e^{i\mu c/2}$, which for $\mu \in \mathbb{R}$ form the algebra of quasi-periodic functions of c [101]. On the other hand, the fluxes are simply linear functions of p, with coefficients that depend only on the smearing functions and the surface. In total, the phase space of LQC for our considered geometries can then coordinatized by the variables $\mathcal{N}_\mu(c)$ and p. Their Poisson bracket is

$$\{\mathcal{N}_\mu(c), p\} = i\frac{4\pi\gamma}{3}\mu\mathcal{N}_\mu(c). \tag{3.11}$$

The Hilbert space naturally chosen in LQC for these variables is $\mathcal{H}_{\text{kin}}^{\text{grav}} = L^2(\mathbb{R}_{\text{Bohr}}, d\mu_{\text{Bohr}})$, where $\mathbb{R}_{\text{Bohr}}$ is the Bohr compactification of the real line and $d\mu_{\text{Bohr}}$ is its Haar measure [101, 102]. This representation mimics that found in full LQG, which is non-continuous in the connection, so that there is no operator corresponding (unambiguously) to c [11,17,20]. This Hilbert space for LQC is isomorphic to the space of square-summable functions in $\mathbb{R}$ with respect to the discrete measure, which is usually called the polymeric Hilbert space. This space can be regarded, in turn, as the completion of the linear span generated by the functions $\mathcal{N}_\mu$ (which may be identified as *kets* $|\mu\rangle$), span that sometimes is denoted as Cil_S, and which is dense in $\mathbb{R}_{\text{Bohr}}$ with the internal product

$$\langle\mu|\mu'\rangle = \delta_{\mu\mu'}. \tag{3.12}$$

The delta appearing in this product is the Kronecker one, a fact that makes manifest the discreteness of the corresponding measure. The action of $\hat{\mathcal{N}}_\mu$ on these ket states is a translation on their label:

$$\hat{\mathcal{N}}_\mu|\mu'\rangle = |\mu + \mu'\rangle. \tag{3.13}$$

Now, using (3.11) and Dirac's rule for the correspondence between basic Poisson bracekts and commutators, $\{\cdot,\cdot\} \leftrightarrow -i\,[\,\widehat{\cdot}\,,\widehat{\cdot}\,]$, we define the action of $\hat{p}$ as

$$\hat{p}|\mu\rangle = \frac{4\pi\gamma\mu}{3}|\mu\rangle. \tag{3.14}$$

Since the measure is discrete in this representation, so is the spectrum of $\hat{p}$.

One may wonder whether this polymeric representation is equivalent to that of geometrodynamics, given the Stone-von Neumann uniqueness theorem [103,104]. However, a key hypothesis in this theorem is that of continuity, which the LQC representation fails to satisfy. This means that the LQC quantization may be (and indeed is) inequivalent to the conventional quanitzation used in the Wheeler-DeWitt formalism [6,7]. To complete our quantum description, we choose $L^2(\mathbb{R}, d\phi)$ as the Hilbert space $\mathcal{H}_{\text{kin}}^{\text{matt}}$ for the homogeneous scalar field, where $d\phi$ is just the Lebesgue measure on $\mathbb{R}$. This is the space of squared integrable functions with $\widehat{\phi}$ acting by multiplication and $\hat{\pi}_\phi = -i\partial_\phi$. The total kinematic Hilbert space is the tensor product of those for LQC and the scalar field.

To describe the quantum dynamics, we first notice that the part of $H_{|0}$ that depends on the spacetime geometry is just the particularization of the (spatial integration of the) general expression of the Hamiltonian constraint (3.5) to this homogeneous system,

$$16\pi\gamma^2\ell_0^{-3}H_{|0} = -\frac{E_i^a E_j^b \delta_{kl}\epsilon^{ijk}F_{ab}^l}{\sqrt{|\det E|}}, \tag{3.15}$$

where we have used that the second term in (3.5) coincides for flat cosmologies with the first one except for a numerical factor. As in the full LQG theory, we cannot express the Hamiltonian constraint as an operator in a straightforward manner because it contains powers of the connection. To overpass these complications, we can start with the holonomy along a square $\square_{jk}$ in the jk-plane,

$$h^\mu_{\square jk} = h^\mu_j h^\mu_k (h^\mu_j)^{-1}(h^\mu_k)^{-1}. \tag{3.16}$$

Using it, the curvature can be written as follows:

$$F^i_{ab} = -2 \lim_{A\square\to 0} \text{tr}\left(\frac{h^\mu_{\square jk} - \delta_{jk}}{A_\square}\tau_l \delta^{il}\right) \, {}^0e^j_a \, {}^0e^k_b, \tag{3.17}$$

where tr denotes the trace and $A_\square = \ell_0^2\mu^2$ is the fiducial area of the square. Whereas this expression is well defined in the classical theory, the limit would diverge if we consider its operator version in LQC. It is the discreteness of the spacetime geometry, as described in the full LQG theory, what permits us to define a meaningful counterpart of this limit. For this, we use the fact that the quantum area operator has a smallest non-zero eigenvalue Δ_g in LQG [105], and then replace the limit with an evaluation in the auxiliary square whose physical area is equal to Δ_g, so that

$$F^i_{ab} = -2\text{tr}\left(\frac{h^{\tilde{\mu}}_{\square jk} - \delta_{jk}}{\ell_0^2\tilde{\mu}^2}\tau_l \delta^{il}\right) \, {}^0e^j_a \, {}^0e^k_b, \tag{3.18}$$

where $\tilde{\mu} = \sqrt{\Delta_g/|p|}$.

We still have to define the specific operators $\hat{\mathcal{N}}_{\pm\tilde{\mu}}$ that are necessary for the representation of (3.18). Since c cannot be expressed as a well-defined operator and $\tilde{\mu}$ is a function p, then $\hat{\mathcal{N}}_{\pm\tilde{\mu}}$ cannot be unambiguously expressed in terms of our elementary operators $\hat{\mathcal{N}}_\mu$ and $\hat{p}$. To introduce a definition, one appeals to geometric considerations. We can introduce a suitable parameter v so that $\hat{\mathcal{N}}_{\pm\tilde{\mu}}$ would produce constant translations in it. Taking into account the canonical algebra, v is the affine parameter associated with a vector field proportional to $\partial_v = \tilde{\mu}(p)\partial_p$. In this manner, we conclude that

$$v(p) = \frac{\text{sgn}(p)|p|^{3/2}}{2\pi\gamma\sqrt{\Delta_g}}. \tag{3.19}$$

Its canonically conjugate variable is indeed $b = \tilde{\mu}c$, with $\{b, v\} = 2$. In these variables, the Hamiltonian becomes

$$H_{|0} = \frac{1}{4\pi\gamma\sqrt{\Delta_g}|v|}\left(\pi_\phi^2 - 3\pi v^2 b^2 + 4\pi^2\gamma^2\Delta_g v^2 m^2 \phi^2\right). \tag{3.20}$$

The magnitude of v has a geometric meaning, because it is proportional to the physical volume of the spatial sections[3] $V = 2\pi\gamma\sqrt{\Delta_g}|v|$. Since the variable v is well adapted to the implementation of $\hat{\mathcal{N}}_{\pm\tilde{\mu}}$, we reindex the label of the states $|\mu\rangle$ so that this holonomy operator becomes indeed a unit translation, $\hat{\mathcal{N}}_{\pm\tilde{\mu}}|v\rangle = |v \pm 1\rangle$, and $\hat{v}$ acts by multiplication, $\hat{v}|v\rangle = v|v\rangle$.

Finally, we need a strategy to define the inverse of the scale factor (or rather, of the volume), present in the Hamiltonian constraint. Since zero is in the discrete spectrum of $\hat{v}$ (given the discrete measure of LQC), we cannot use the spectral theorem to define the inverse of the volume (i.e., we cannot simply divide by v). Once again, we adopt LQG techniques and make use of the classical identity [10, 106]

$$\left(\frac{1}{V}\right)^{1/3} = \frac{1}{|p|^{1/2}} = \frac{\text{sgn}(p)}{2\pi\gamma\tilde{\mu}}\text{tr}\left(\sum_i \tau_i h_i^{\tilde{\mu}}\{(h_i^{\tilde{\mu}})^{-1}, |p|^{1/2}\}\right). \tag{3.21}$$

Using this, $\widehat{1/V}$ can be defined as the cube of $\widehat{1/\sqrt{|p|}}$, this operator being

$$\widehat{\frac{1}{\sqrt{|p|}}} = \frac{3}{4\pi\gamma\sqrt{\Delta_g}}\widehat{\text{sgn}(p)}\widehat{\sqrt{|p|}}\left(\hat{\mathcal{N}}_{-\tilde{\mu}}\widehat{\sqrt{|p|}}\,\hat{\mathcal{N}}_{\tilde{\mu}} - \hat{\mathcal{N}}_{\tilde{\mu}}\widehat{\sqrt{|p|}}\,\hat{\mathcal{N}}_{-\tilde{\mu}}\right). \tag{3.22}$$

The final step for quantization is a procedure to replace the positive powers of $\hat{p}$ and $\widehat{1/p}$ (or, equivalently $\hat{V}$ and $\widehat{1/V}$), and select the factor ordering of all operators. For this, we will use the prescription given in Ref. [23], which avoids problems with the state $|v = 0\rangle$ and treats carefully the quantum counterpart of the sign sgn(p). In particular, it involves a symmetric algebraic ordering of the powers of the volume operator. This decouples the null volume state, so that it can be eliminated in practice from the geometric part of the kinematical Hilbert space. Furthermore, one can prove that the action of the resulting Hamiltonian constraint operator does not mix the subspaces $\mathcal{H}_\varepsilon^\pm$ spanned by states $|v\rangle$ with v supported on the semilattices $\mathcal{L}_\varepsilon^\pm = \{\pm(\varepsilon + 4n)|n \in \mathbb{N}\}$ with $\varepsilon \in (0, 4]$ [21–23]. These subspaces $\mathcal{H}_\varepsilon^\pm$ are frequently called superselection spaces. We notice that the variable v related to the volume has an strictly positive minimum ε, or an strictly negative maximum $-\varepsilon$, on each superselection sector. Finally, taking into account the symmetry of the system under parity, we can restrict the discussion of physical states in LQC, for example, to $\mathcal{H}_\varepsilon^+$, with strictly positive values for v, namely $v \in \mathcal{L}_\varepsilon^+$.

We may further restrict the discussion to certain physical states with a pronounced semiclassical

[3] The physical volume is related to the scale factor, that we will employ in many classical formulas, by $V = \ell_0^3 a^3$.

behavior for large volumes and that stay highly peaked during the entire quantum evolution [107]. The evolution of these states is governed by the Hamiltonian constraint. It has been shown that their peak follows a trajectory that is dictated by Einstein's equations when the matter density is small enough (less than one percent of Planck density). However, when this density grows, the Universe stops following the dynamics of General Relativity. If it was contracting, the density grows until it reaches a critical value (around 41 percent of Planck density) and the scale factor a minimum, and then starts expanding. The instant the Universe ceases to collapse is called the Big Bounce. This resolves the Big Bang singularity, because all relevant physical quantities remain bounded in the commented process [21–23, 108].

3.3. Scalar and tensor perturbations

While the FLRW cosmology we considered so far is an acceptable first order approximation, we can clearly observe that the Universe is actually inhomogeneous. It is thought that these small inhomogeneities were seeded by quantum fluctuations of small inhomogeneities in the Early Universe. We may introduce such perturbations both in the geometry ($g_{\mu\nu} = {}^0g_{\mu\nu} + \Delta g_{\mu\nu}$) and in the inflaton field ($\Phi = \phi + \Delta\Phi$), in a manner described e.g. in Refs. [39, 41, 53]. To exploit the spatial symmetry of the background system, we can expand our fields in eigenmodes of the Laplace-Beltrami operator on the homogeneous spatial slices. These modes provide a basis to decompose the perturbations. In particular, in absence of matter vector fields, the physically relevant, gauge-invariant part of the perturbations can be expressed in our cosmological system in terms of scalar and tensor harmonics. The Hamiltonian H of the complete system truncated at quadratic order in the action adopts the form

$$H = N_0 \left(H_{|0} + \sum_{\vec{k}} \tilde{H}^{\vec{k}}_{(s)} + \sum_{\vec{k},\epsilon} \tilde{H}^{\vec{k},\epsilon}_{(t)} \right) + \sum_{\vec{k}} N_{\vec{k}} H_{|1,\vec{k}} + \sum_{\vec{k}} \tilde{N}_{\vec{k}} H_{-1,\vec{k}}, \tag{3.23}$$

where N_0 is the zero mode[4] of the lapse function, $\vec{k}$ is the wavevector label of the Fourier modes (taken different from zero in order not to include zero modes), and $\epsilon = +, \times$ represents the two admissible polarizations of the tensor modes. The terms $\tilde{H}^{\vec{k}}_{(s,t)}$ are quadrative in the perturbations and contain only scalar or tensor contributions, depending on the label (s) or (t), respectively. Furthermore, $N_{\vec{k}}$ and $\tilde{N}_{\vec{k}}$ describe the (scalar) perturbations of the lapse and shift . Actually, their canonical momenta are not present in the total Hamiltonian, indicating that they do not represent true degrees of freedom. They must be handled as Lagrange multipliers, associated to the terms $H_{|1,\vec{k}}$ and $H_{-1,\vec{k}}$, which are linear in the perturbations. We call them the linear (Hamiltonian and diffeomorphisms) perturbative constraints. They reflect the freedom to perform perturbative time reparametrizations and perturbative spatial diffeomorphisms, respectively.

One must take into account that geometries that are related by any of these perturbative transformations correspond in fact to the same physical perturbed spacetime. So, we want to consider only that

[4] In this expansion, the zero mode of the lapse function and the contribution $H_{|0}$ to the Hamiltonian constraint are formally the same as those of the unperturbed system.

part of the phase space of the perturbations that contains gauge-invariant information [1], which is not affected by the aforementioned transformations. A perturbative variable is gauge-invariant if and only if its Poisson bracket with the linear perturbative constraints is null, taking the background variables as fixed [109]. This is automatically the case for the tensor perturbations, since the linear perturbative constraints do not depend on them. But it is not the situation found generically for the scalar perturbations. Nonetheless, we can perform a suitable background-dependent canonical transformation of the variables that describe the scalar perturbations and arrive to a new canonical set that contains a complete set of gauge invariants. For instance, the new gauge-invariant variables can be chosen as the so-called Mukhanov-Sasaki variables (together with their canonical, gauge-invariant momenta). In this way, we can construct a phase space for the perturbations that is coordinatized by the MS variables, the tensor perturbations and the linear perturbative constraints, together with their respective momenta. In order to do this, an obstruction is found in the fact that the linear perturbative constraints do not commute. This problem is solved by replacing $\tilde{H}^{\vec{k}}_{|1}$ with an *Abelianized* version of it that is still linear in the scalar perturbations. This replacement can be compensated in the total Hamiltonian with a change in the Lagrange multiplier that corresponds to the zero mode of the lapse function, change that consists in the addition of a term that is quadratic in perturbations [39].

Since the employed canonical transformation is background-dependent, the new perturbative variables no longer commute with the homogenous variables when the background is not regarded as fixed anymore. So, to obtain a set that is canonical in both the homogeneous and inhomogeneous sectors, we must modify the zero modes of the geometry and of the scalar field. The simplest way to obtain new variables for the homogeneous sector forming a canonical set for the whole system, at the order of our perturbative truncation in the action, is to rewrite the Legendre part of this action (that contains the information about the symplectic structure) in a canonical way, i.e., as a sum of products of the time derivative of configuration variables multiplied by their momenta, modulo surface contributions at the initial and final times. This is done in detail in Ref. [39] using that the relation between the old and new perturbative variables is linear and does not mix modes[5]. After a series of integrations by parts, and truncating the result at quadratic order in the perturbations, the general form of the Hamiltonian constraint is formally the same as in (3.23), but the perturbative terms appearing in it have now a different dependence on the new canonical variables and the geometric interpretation of the Lagrange multipliers is changed slightly.

3.4. Fermionic perturbations

We now introduce fermionic content in our cosmological system. This serves as a test of our formalism and extends our treatment to realistic matter fields. Let us summarize how to couple a Dirac field Ψ with mass M to the system [53]. We treat this Dirac field as a perturbation, including its possible zero

[5] Unless specified otherwise, in the following we will not make an explicit distinction in our notation between old and new zero modes.

modes. The field dynamics is determined by the fermionic part of the Einstein-Dirac action,

$$S_D = -i \int d^4x \, \sqrt{-\,{}^0g} \left[\frac{1}{2} (\Psi^\dagger \gamma^0 \, {}^0e_i^\nu \gamma^i \nabla_\nu^s \Psi - H.c.) - M \Psi^\dagger \gamma^0 \Psi \right], \tag{3.24}$$

where ${}^0e_\nu^i$ is the frame field, or tetrad, of the homogeneous metric (defined in a similar way as the triads but with respect to the 4-metric instead), and ${}^0g = \det\, {}^0g_{\mu\nu}$ is the determinant of this metric. In addition, we have in this case $i = 0, 1, 2, 3$ as an internal gauge index, γ^i are the constant Dirac matrices in the Weyl representation of the Clifford algebra, and the dagger denotes the Hermitian conjugate, whereas $H.c.$ corresponds to the Hermitian conjugate of the previous term displayed. Finally, we define $\nabla_\mu^s = \partial_\mu + \frac{1}{4} e_\nu^i (e^{\nu j})_{;\mu} \gamma_i \gamma_j$, where the semicolon denotes the covariant derivative corresponding to the homogeneous metric. Note that (3.24) is quadratic in the fermionic contributions. This means that we can couple the Dirac field directly to the homogeneous metric either before or after correcting the homogeneous variables to maintain the canonical structure in the total system. Any difference from this change of variables will be a contribution of a higher perturbative order than those kept by our truncation. A useful consequence of this fact is that the fermionic degrees of freedom are actually gauge-invariant perturbations at this order of truncation.

We adopt the so-called temporal gauge so that $e_0^j = 0$, for convenience in the treatment of the Hamiltonian [52]. This choice of gauge plays an irrelevant role for the non-fermionic part of the system. Its effect on the spin structure of the homogeneous manifold is a restriction that can be reinterpreted as an assigment of a spin structure on each of the spatial sections. In this manner we can describe the Dirac field with two bi-component spinors on T^3, φ^A and $\bar{\chi}_{A'}$, of defined chirality and parametrized by the time t. In our notation, $A, B, ... = 1, 2$ are *left-handed* components, and $A', B', ... = 1', 2'$ are *right-handed.* In addition, we denote complex conjugation by an overhead bar. Explicitly, we have then

$$\Psi = \begin{pmatrix} \varphi^A \\ \bar{\chi}_{A'} \end{pmatrix}.$$

The components of these spinors are treated as Grassmann variables, to incorporate the anticommuting behavior of fermions. Spinorial indices are raised and lowered with the antisymmetric matrices ε, defined so that $\varepsilon^{12} = \varepsilon^{1'2'} = \varepsilon_{12} = \varepsilon_{1'2'} = 1$, and $\varepsilon^{AB} = -\varepsilon^{BA}$, $\varepsilon^{A'B'} = -\varepsilon^{B'A'}$, etc. After eliminating the second-class constraints that relate the Dirac field with its momentum (owing to the fact that the action is of first order in the derivative of the field), we obtain, at fixed time, the anticommutative Dirac brackets

$$\{a^{3/2}\Psi^\dagger(\vec{x}), a^{3/2}\Psi(\vec{x}')\}_D = -i\delta^3(\vec{x} - \vec{x}')\mathbb{I}_4, \tag{3.25}$$

where $\mathbb{I}_4$ is the 4-dimensional identity matrix.

Each of the chiral components of the Dirac field can be expanded in an eigenspinor basis of the Dirac operator on T^3. The spectrum of this operator is discrete and characterized by eigenvalues $\pm\omega_k =$

$\pm 2\pi|\vec{k}+\vec{\tau}|/\ell_0$, with $\vec{k}\in\mathbb{Z}^3$, and $2\vec{\tau}=\sum_I \tau_I \vec{v}^I$ characterizes the spin structure, where $I=1,2,3$, $\vec{v}^I$ can be any of the constant vectors that form the orthonormal basis of $\mathbb{Z}^3$, and $\tau_I\in\{0,1\}$, giving a total of eight possible spin structures on T^3 [110]. In an effort to avoid technicalities, we will not discuss in this summary the potential zero-modes in the expansion of the Dirac field, only present for the trivial spin structure on T^3 (the reader can find their contribution in Ref. [53]). On the other hand, since ω_k grows like $|\vec{k}|$ when the latter tends to infinity, we notice that the density of states with eigenvalues in an interval $(\omega_k, \omega_k+\Delta\omega_k]$ grows asymptotically as $\omega_k^2\Delta\omega_k$. Extracting a global factor $a^{3/2}$ from our expansions for convencience and taking into account (3.25), we obtain

$$\varphi_A = \frac{1}{{\ell_0}^{3/2}a^{3/2}}\sum_{\vec{k}}\left(m_{\vec{k}} w^{+}_{\vec{k},A} + \bar{r}_{\vec{k}} w^{-}_{\vec{k},A}\right) \tag{3.26}$$

$$\bar{\chi}'_A = \frac{1}{{\ell_0}^{3/2}a^{3/2}}\sum_{\vec{k}}\left(\bar{s}_{\vec{k}} \bar{w}^{+}_{\vec{k},A'} + t_{\vec{k}} \bar{w}^{-}_{\vec{k},A'}\right) \tag{3.27}$$

The time-dependent coefficients $m_{\vec{k}}, s_{\vec{k}}, r_{\vec{k}}$ and $t_{\vec{k}}$, are Grassmann variables. In fact, the pairs formed by each of these variables and their complex conjugate are canonical. For the specific form of the Dirac eigenspinors $w^{\pm}_{\vec{k},A}$ and $\bar{w}^{\pm}_{\vec{k},A'}$ (with eigenvalue $\pm\omega_k$ according to the sign $\pm$) we refer the reader to Ref. [53]. The zero mode of the total Hamiltonian constraint on the complete cosmological system is then

$$H_{|0} + \sum_{\vec{k}} \tilde{H}^{\vec{k}}_{(s)} + \sum_{\vec{k},\epsilon} \tilde{H}^{\vec{k},\epsilon}_{(t)} + \sum_{\vec{k}} H_{\vec{k}}, \tag{3.28}$$

where (for all non-zero modes)

$$\begin{aligned} H_{\vec{k}} = {} & M(s_{-\vec{k}-2\vec{\tau}} m_{\vec{k}} + \bar{m}_{\vec{k}} \bar{s}_{-\vec{k}-2\vec{\tau}} + r_{-\vec{k}-2\vec{\tau}} t_{\vec{k}} + \bar{t}_{\vec{k}} \bar{r}_{-\vec{k}-2\vec{\tau}}) \\ & - \frac{\omega_k}{a}(\bar{m}_{\vec{k}} m_{\vec{k}} + \bar{t}_{\vec{k}} t_{\vec{k}} - r_{\vec{k}} \bar{r}_{\vec{k}} - s_{\vec{k}} \bar{s}_{\vec{k}}). \end{aligned} \tag{3.29}$$

We call $H_D = \sum_{\vec{k}} H_{\vec{k}}$ to shorten the notation. With the change of variables introduced in the previous subsection, the system is symplectic at the considered truncation order. Finally, the only constraints remaining on it are the zero mode of the Hamiltonian constraint and the linear perturbative constraints.

3.5. Hybrid quantization in Loop Quantum Cosmology

In the hybrid approach, one adopts a conveniently chosen quantum representation for each of the sectors of the cosmological system, each of them with its own Hilbert or Fock space. The constraints of the system are given by operators that are well defined in the tensor product of these representation spaces. These constraints are imposed following the Dirac approach, which means that we expect physical states to be annihilated by them [100]. This is non-trivial, since the zero mode of the Hamiltonian constraint mixes the homogeneous sector, for which we choose an LQC quantization, with the inhomogeneous sectors that are quantized with Fock techniques.

Starting from the homogeneous geometry, we define $\mathcal{H}_{\text{kin}}^{\text{grav}}$ as its representation space in LQC, along the lines explained in Section 3.2. For the zero mode of the scalar field, we call its kinematical space $\mathcal{H}_{\text{kin}}^{\text{matt}}$, given again by the Hilbert space $L^2(\mathbb{R}, d\phi)$ of squared integrable functions over the real numbers, with $\hat{\phi}$ acting by multiplication and $\hat{\pi}_\phi = -i\partial_\phi$. For the perturbations, we adopt symmetric Fock spaces for the scalar and tensor perturbations, that we call $\mathcal{F}_s$ and $\mathcal{F}_t$ respectively, and an antisymmetric Fock space for the fermionic perturbations, called $\mathcal{F}_D$. Bases of these Fock spaces are given by the n-particle(/antiparticle) states $|\mathcal{N}_s\rangle$, $|\mathcal{N}_t\rangle$ and $|\mathcal{N}_D\rangle$, where $\mathcal{N}$ denotes occupation numbers in each of the considered Fock representations.

Let us consider the linear perturbative constraints. In fact, it makes sense to treat these linear constraints as the generalized momenta of their canonical pairs. In this manner, one can use a representation where these perturbations act as generalized derivatives. As such, their imposition simply implies that physical states only depend on gauge-invariant perturbative degrees of freedom and on the homogeneous sector. The only constraint that remains to be imposed on the system is the zero mode of the Hamiltonian constraint. Using the representation space $\mathcal{H} = \mathcal{H}_{\text{kin}}^{\text{matt}} \otimes \mathcal{H}_{\text{kin}}^{\text{grav}} \otimes \mathcal{F}_S \otimes \mathcal{F}_t \otimes \mathcal{F}_D$, the construction of the operator for this constraint is then carried out according to the prescriptions explained in Refs. [23, 39, 41, 53].

Finally, one would have to determine the kernel of the (adjoint) of the zero mode of Hamiltonian constraint. A convenient strategy is based on the fact that, for physically interesting states, we rarely expect quantum transitions of the background to be mediated by the perturbations (as well as on the fact that the modes of different types of perturbations are mutually decoupled at this order of truncation). This motivates ansatz of separation of variables, in which only the homogeneous scalar field ϕ is contained in all the factors and, in certain regimes, it may act as an internal time [23, 39, 41, 53]. Explicitly, we search for states with wave functions Ξ such that:

$$\Xi(V, \phi, \mathcal{N}_s, \mathcal{N}_T, \mathcal{N}_D) = \Gamma(V, \phi)\psi_s(\mathcal{N}_s, \phi)\psi_T(\mathcal{N}_T, \phi)\psi_D(\mathcal{N}_D, \phi). \tag{3.30}$$

Additionally, we restrict our considerations to normalized states Γ in $\mathcal{H}_{\text{kin}}^{\text{grav}}$ with unitary evolution in ϕ. With this ansatz, the imposition of the Hamiltonian constraint[6] leads to a collection of Scrödinger-like equations with respect to ϕ for the perturbations, in which all the terms related to the unperturbed geometry are given by expectation values of the operators that describe it. In particular, we obtain the fermionic Schrödinger equation

$$i\partial_\phi \psi_D(\mathcal{N}_D, \phi) = \frac{\langle \widehat{VH_D} \rangle_\Gamma - C_D^{(\Gamma)}(\phi)}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} \psi_D(\mathcal{N}_D, \phi). \tag{3.31}$$

Here, $\hat{\tilde{\mathcal{H}}}_0$ is the self-adjoint and positive operator that generates the unitary evolution in ϕ of the quantum

[6]Some other well motivated approximations are needed but we refer the reader to the Refs. [23, 39, 41, 53] for the detailed calculations.

state Γ of the homogeneous geometry. The term $C_D^{(\Gamma)}$, on the other hand, appears in the equation

$$C_D^{(\Gamma)} + C_s^{(\Gamma)} + C_t^{(\Gamma)} + \frac{\langle \hat{\mathcal{H}}_0^{(2)} + i[\partial_{\tilde{\phi}}, \hat{\tilde{\mathcal{H}}}_0] - (\hat{\tilde{\mathcal{H}}}_0)^2 \rangle_\Gamma}{2\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} = 0, \tag{3.32}$$

where $C_t^{(\Gamma)}$ and $C_s^{(\Gamma)}$ are similar terms arising from the scalar and tensor perturbations, and $\hat{\mathcal{H}}_0^{(2)}$ is the operator whose square root would generate the evolution on the unperturbed quantum geometry. Consequently, $C_D^{(\Gamma)}$ measures in average (i.e. after taking expectation values) how much the partial FLRW state Γ can differ from being an exact solution of the unperturbed system as a result of the fermionic perturbations. In this sense, it can be understood as a quantum backreaction term of the fermionic sector on the homogeneous background.

3.6. Unitarily implementable evolution for fermionic perturbations

The last step in the quantization would be to find the physical states of the system and endow them with a Hilbert structure. To do so, we must first specify the kinematical Fock space for the fermionic part of these states. A usual way to characterize this Fock space is by defining a set of annihilation and creation variables that are straightforwardly promoted to operators. These variables can be introduced by means of canonical transformations which, in general, mix the homogeneous and inhomogeneous sectors of the system:

$$\begin{aligned} a_{\vec{k}}^{\lambda} &= f_1^{\vec{k},\lambda}(a,\phi) x_{\vec{k}} + f_2^{\vec{k},\lambda}(a,\phi) \bar{y}_{-\vec{k}-2\vec{\tau}}, \\ \bar{b}_{\vec{k}}^{\lambda} &= g_1^{\vec{k},\lambda}(a,\phi) x_{\vec{k}} + g_2^{\vec{k},\lambda}(a,\phi) \bar{y}_{-\vec{k}-2\vec{\tau}}, \end{aligned} \tag{3.33}$$

together with their complex conjugate expressions, where $(x_{\vec{k}}, y_{\vec{k}})$ is any of the ordered pairs $(m_{\vec{k}}, s_{\vec{k}})$ or $(t_{\vec{k}}, r_{\vec{k}})$, that have well-defined and opposite helicity $\lambda = \pm 1$. It is understood that the coefficients $h_l^{\vec{k},\lambda}$, with $h = f, g$ and $l = 1, 2$, may depend also on the momenta of the homogeneous variables. In order to satisfy the standard anticommutation canonical relations, it is necessary that [53]

$$g_1^{\vec{k},\lambda} = e^{iJ_{\vec{k}}^{\lambda}} \bar{f}_2^{\vec{k},\lambda}, \qquad g_2^{\vec{k},\lambda} = -e^{iJ_{\vec{k}}^{\lambda}} \bar{f}_1^{\vec{k},\lambda}, \tag{3.34}$$

$$f_2^{\vec{k},\lambda} = e^{iF_2^{\vec{k},\lambda}} \sqrt{1 - \left| f_1^{\vec{k},\lambda} \right|^2}, \tag{3.35}$$

where $J_{\vec{k}}^{\lambda}, F_2^{\vec{k},\lambda} \in \mathbb{R}$ are two (possibly) background-dependent phases.

We see that Eqs. (3.33) allow for an infinite number of choices of vacua. This ambiguity may be alleviated by considering only vacua that are invariant under the spatial symmetries of the background and/or the symmetries of the dynamical equations. In particular, we restrict our considerations to coefficients that only depend on the eigenvalue ω_k, as opposed to a dependence on $\vec{k}$. On the other hand, since the spacetime is non-stationary, requiring that the vacuum be invariant under the evolution is not a suitable strategy, at least in principle. Instead, we can ask for vacua that lead to a Heisenberg dynamics for the annihilation and creation variables that can be implemented as unitary transformations in the Fock space (when the Dirac field is treated as a test field propagating on a fixed FLRW cosmology). It was proven in Ref. [54] that this condition univocally fixes the asymptotic behavior of the annihilation and creation variables in the limit of infinitely large ω_k, so that they must satisfy [54]

$$f_1^{k,\lambda} \sim \frac{Ma}{2\omega_k} e^{iF_2^{k,\lambda}} + \theta^{k,\lambda}, \quad \text{with} \quad \sum_{\vec{k}\in\mathbb{Z}^3} \left|\theta^{k,\lambda}\right|^2 < \infty, \tag{3.36}$$

where the $\sim$ symbol denotes the same asymptotic order in the limit $\omega_k \to \infty$. Note that, even after imposing this restriction coming from unitarity, there is still much freedom left (even in the asymptotic limit) in our choice of annihilation and creation variables. Nevertheless, it has been proven that all Fock representations corresponding to these possible choices of vacua are at least unitarily equivalent, so that they allow for the same physics [54].

3.7. Effective LQC and non-oscillating vacua

As explained in section 3.2, one can evolve certain families of semiclassical states with the LQC Hamiltonian constraint until one reaches in the past an epoch in which the matter density of the Universe was large, of the Plack order. These states avoid the Big Bang singularity while remaining highly peaked. Moreover, the trajectory of the peak follows an effective dynamics generated by an effective Hamiltonian constraint [107]. This effective constraint $H_{|0}^{eff}$ can be obtained by replacing the classical variable b in the expression (3.20) of $H_{|0}$ by $\sin b$, namely

$$H_{|0}^{eff} = \frac{1}{4\pi\gamma\sqrt{\Delta_g}|v|}\left(\pi_\phi^2 - 3\pi v^2 \sin^2 b + 4\pi^2\gamma^2\Delta_g v^2 m^2 \phi^2\right). \tag{3.37}$$

This replacement comes from the fact that the connection variable b is not well defined as a local operator in LQC, and is then represented in terms of holonomies which contain imaginary exponentials of b. If we now consider cosmological perturbations with a background state Γ that follows this effective LQC dynamics with negligible backreaction, the expectation values on the homogeneous geometry that appear in the dynamical equations of the perturbations can be approximated by their evaluation on the effective trajectory of the peak of Γ. From this perspective, to specify the effect of Γ on these equations we only need to provide initial conditions on the four canonical variables of the homogeneous sector, since these will fix the effective LQC solution that describes the peak of the state. These homogeneous variables are, however, not independent, because they must satisfy the effective Hamiltonian constraint $H_{|0}^{eff}$. This can be employed to find the initial value of e.g. the inflaton momentum in terms of the initial conditions for the other three homogeneous variables. On the other hand, a convenient choice is to set the initial time at the bounce. There, the time derivative of the scale factor (and consequently of the volume) vanishes, a fact that serves to specify part of the initial data on the geometry. Additionaly, since we have the freedom to set a reference scale of distances, we can simply set the initial scale factor equal to one at this initial time. This means that a rescaling will be necessary if we are ever to compare our results with (observational) cosmological data, for which the scale factor is commonly set to one at the present time. In conclusion, we see that we only have to give the initial value of the inflaton at the bounce to fix the effective trajectory of the homogeneous sector. If we are considering a mass term as the inflaton potential, we can also add the value of this mass as a piece of data that must be determined. Usually, the initial value of the inflaton and its mass are chosen so that one obtains power spectra for the perturbations that can reproduce the observed CMB spectrum, while still allowing for the pressence of quantum effects in it. In this thesis, we study the scenario that is phenomenologically more interesting, namely, a kinetically dominated regime followed by a short-lived inflation. This situation is found for initial values of the inflaton at the bounce, ϕ_B, slightly smaller than one, and for a mass of the order of 10^{-6}, both of them in Planck units. For concreteness, we are going to run all of our numerical simulations for the values $m = 1.2 \times 10^{-6}$ and $\phi_B = 0.97$, as done in Refs. [111,112]. In addition, we take the Immirzi parameter equal to 0.2375, a standard choice based on the Bekenstein-Hawking formula [113–115].

In hybrid LQC, one obtains effective equations of the Mukhanov-Sasaki and tensor perturbations that describe the dynamics of harmonic oscillators with a time-dependent mass that is a function of the homogeneous cosmology [39]. Calling $v_{\vec{k}}$ any of the perturbative mode variables (and $\vec{k}$ its labels for simplicity), we get

$$v''_{\vec{k}} + (k^2 + s)v_{\vec{k}} = 0, \tag{3.38}$$

where the prime denotes the derivative with respect to the conformal time and, within the considered effective regime, the time dependent mass s for the scalar (s) and tensor (t) perturbations is given by

$$s^{(s)} = s^{(t)} + U_{ms}, \tag{3.39}$$

$$s^{(t)} = \left(2\pi\gamma\sqrt{\Delta_g}v\right)^{2/3}\left(\frac{\sin^2 b}{\gamma^2\Delta_g} - 4\pi m^2\phi^2\right), \tag{3.40}$$

$$U_{ms} = \left(2\pi\gamma\sqrt{\Delta_g}v\right)^{2/3}\left(m^2 + \frac{4\pi_\phi \sin(2b) m^2\phi}{v\sin^2 b} + 24\pi m^2\phi^2 - \frac{32\pi^2\gamma^2\Delta_g m^4\phi^4}{\sin^2 b}\right). \tag{3.41}$$

For calculations of the power spectrum of the perturbations, in practice, one takes the eigenvalue k of the Fourier modes as a continuous quantity. This continuum limit can be defined rigorously in the system, as proven in Ref. [116].

The same type of mode equations is also found in other approaches to quantum cosmology, including LQC, such as the so-called dressed metric approach introduced by Ashtekar, Agullo and Nelson [30, 32, 33, 117]. The key difference between this approach and hybrid LQC is the expression of the time-dependent mass that appears in these equations. Nonetheless, this difference between the masses is only non-negligible in epochs with large matter density [118], because both approaches reproduce the results of General Relativity at low densities.

On the other hand, let us consider a set $\{\mu_k\}$ of complex solutions to (3.38), for all $k \in \mathbb{R}$, that becomes a basis together with their complex conjugates. It is well known [49] that any such set univocally defines a quantum Fock representation of the considered field if it is normalized as

$$\mu_k \bar{\mu}_k' - \mu_k' \bar{\mu}_k = i. \tag{3.42}$$

It is important to note that, because of this normalization, and the reality and linearity of (3.38), any two choices of basis elements in which the modes are not mixed, $\tilde{\mu}_k$ and μ_k, must be related to each other by a linear Bogoliubov transformation of the form

$$\tilde{\mu}_k = \alpha_k (\tilde{\mu}_k, \mu_k) \mu_k + \beta_k (\tilde{\mu}_k, \mu_k) \bar{\mu}_k. \tag{3.43}$$

The normalization condition (3.42) holds provided that the constant Bogoliubov coefficients satisfy

$$|\alpha_k (\tilde{\mu}_k, \mu_k)|^2 - |\beta_k (\tilde{\mu}_k, \mu_k)|^2 = 1. \tag{3.44}$$

We may refer to the vacuum state selected by a specific set $\{\mu_k\}$ as $|0_\mu\rangle$. The power spectrum corresponding to this vacuum can be obtained from the quantity

$$\mathcal{P}_{\mathcal{V}}(k,\eta) = \frac{k^3}{2\pi^2} |\mu_k(\eta)|^2, \tag{3.45}$$

evaluated at the value for the conformal time η corresponding to the end of inflation, η_{end}.

Some widely studied vacua in LQC have been the adiabatic states which, much like in the case of the fermionic perturbations, are built by and iterative procedure that should eventually determine a Hadammard state. From a certain adiabatic order on, these vacua lead to a renormalizable energy-momentum tensor. However, they have been seen to provide oscillatoy power spectra, a behavior that, after its averaging, usually amplifies the power and may blur the genuine quantum gravity effects that ocurred in the pre-inflationary epoch. To find a possible solution to this problem, a criterion for the choice of a vacuum has been proposed [68] in which one requires numerically a non-oscillating behavior by minimizing the quantity

$$\int_{\eta_i}^{\eta_f} d\eta \left| \partial_\eta \left(|\mu_k|^2 \right) \right|, \tag{3.46}$$

where the integration limits η_i and η_f are usually chosen to be the bounce and the time for which ϕ' vanishes for the first time. This minimization takes into account the fact that the oscillations in the wavenumbers are often related to the time oscillations that the norm of the solutions μ_k may have experienced in the period before inflation.

4. Article summary

4.1. Fermionic perturbations

4.1.1. Backreaction of fermionic perturbations in the Hamiltonian of Hybrid LQC

When one considers quantum matter fields coupled to curved spacetimes, treated as classical entities, divergences frequently appear [64,119–125]. In fact, it is not straightforward to get rid of these divergences by simple renormalization techniques and it is commonly believed that these pathologies are due to the classical treatment adopted for the geometry. We have already motivated the search for a quantum theory of gravity as a way to remove or at least alleviate the singularities that exist in General Relativity. From this perspective, we find in the divergences of quantum field theory in curved spacetimes a good arena to put into test the possible consequences of a quantum theory of gravity, specially if this line of attack can remove the divergences without using any "substraction of infinities" scheme. A possibly divergent quantity is present in (3.31), describing a quantum backreaction from the fermionic perturbations on the geometry. To study it further, we start with any set of annihilation and creation variables that satisfies (3.36), written in the convenient form (inspired by Refs. [52, 53])

$$f_1^{k,\lambda} \sim \sqrt{\frac{\xi_k - \omega_k}{2\xi_k} + \frac{Ma}{2\omega_k}\left[e^{iF_2^{k,\lambda}} - 1\right] + \theta_k^\lambda} \quad \text{with} \quad \sum_{\vec{k}} \left|\theta_k^\lambda\right|^2 < \infty, \tag{4.1}$$

where we have defined[7]

$$\xi_k = \sqrt{\omega_k^2 + M^2 a^2}, \tag{4.2}$$

and we keep generic phases for the moment. We consider that $F_2^{k,\lambda}$ and θ_k^λ do not depend on the inflaton or its momentum and restrict ourselves to transformations such that

$$\partial_a^n h_l^{k,\lambda} = \mathcal{O}(h_l^{k,\lambda}), \qquad \partial_{\pi_a}^n h_l^{k,\lambda} = \mathcal{O}(h_l^{k,\lambda}), \tag{4.3}$$

for $h = f, g$ and $l = 1, 2$, integers n at least up to three, and where the considered derivatives act order by order in the asymptotic expansions for large ω_k (at least for the relevant orders in our discussion). Here, a contribution is $\mathcal{O}(.)$ when it is of the asymptotic order of the corresponding argument (or smaller). Our restriction excludes, in particular, the possibility of absorbing in the phases of $h_1^{k,\lambda}$ and $h_2^{k,\lambda}$ any of the dominant oscillations in conformal time that the Dirac field displays in the limit of large ω_k, when it is treated as a test field obeying the Dirac equation in a classical FLRW cosmology.

Since the coefficient (4.1) is allowed to depend on homogeneous variables, the annihilation and creation variables cannot form a full canonical set together with the homogeneous cosmological ones. Then, by a procedure similar to that explained in Subsection 3.3, we must change our set of homogeneous variables.

[7] In the original publication we actually let the coefficients depend on the Fourier label $\vec{k}$, while in subsequent articles we restricted the study to a dependence on the eigenvalue ω_k, owing to symmetry considerations. In this summary, we adopt this last viewpoint to avoid lengthier calculations that would obscure the results.

At our order of truncation, and denoting with the new variables with a tilde, the change is

$$\tilde{a} - a = \Delta a \quad = \quad \frac{i}{2}\sum_{\vec{k},\lambda}[(\partial_{\pi_a} x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_{\pi_a}\bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_{\pi_a} y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_{\pi_a}\bar{y}_{\vec{k}})y_{\vec{k}}], \tag{4.4}$$

$$\pi_{\tilde{a}} - \pi_a = \Delta\pi_a \quad = \quad -\frac{i}{2}\sum_{\vec{k},\lambda}[(\partial_a x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_a\bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_a y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_a\bar{y}_{\vec{k}})y_{\vec{k}}]. \tag{4.5}$$

We will ignore the tilde in the new variables after these redefinitions, in order to simplify the notation. This change of variables naturally gives rise then to a modification of the terms corresponding to perturbative contributions in the zero mode of the Hamiltonian constraint. At our truncation order, the final result is the new fermionic Hamiltonian

$$\sum_{\vec{k},\lambda}\Bigg[\left(\frac{1}{2a}\xi_k + h_D^{k,\lambda}\right)\left(\bar{a}_{\vec{k}}^{\lambda}a_{\vec{k}}^{\lambda} - a_{\vec{k}}^{\lambda}\bar{a}_{\vec{k}}^{\lambda} + \bar{b}_{\vec{k}}^{\lambda}b_{\vec{k}}^{\lambda} - b_{\vec{k}}^{\lambda}\bar{b}_{\vec{k}}^{\lambda}\right) + h_J^{k,\lambda}\left(\bar{b}_{\vec{k}}^{\lambda}b_{\vec{k}}^{\lambda} - b_{\vec{k}}^{\lambda}\bar{b}_{\vec{k}}^{\lambda}\right)$$
$$+ e^{i(J_k^{\lambda} - F_2^{k,\lambda})}a^{-1}\left(2\omega_k\bar{\theta}_k^{\lambda} + \bar{h}_I^{k,\lambda}\right)a_{\vec{k}}^{\lambda}b_{\vec{k}}^{\lambda} - e^{-i(J_k^{\lambda} - F_2^{k,\lambda})}a^{-1}\left(2\omega_k\theta_k^{\lambda} + h_I^{k,\lambda}\right)\bar{a}_{\vec{k}}^{\lambda}\bar{b}_{\vec{k}}^{\lambda}\Bigg], \tag{4.6}$$

where $h_D^{k,\lambda}$ and $h_J^{k,\lambda}$ are real functions that depend on the coefficients appearing in (3.33). In the asymptotic regime of large ω_k, $h_I^{k,\lambda}$ is given by

$$h_I^{k,\lambda} = i\frac{2\pi M}{3\ell_0^3\omega_k}\pi_a e^{iF_2^k} + \mathcal{O}[\mathrm{Max}(\theta_k^{\lambda}, \omega_k^{-2})], \tag{4.7}$$

where Max(., .) denotes the maximum of its two arguments. Notice that θ_k^{λ} must be (at least) asymptotically negligible compared to $\omega_k^{-3/2}$ in order to satisfy (4.1)[8]. Then $h_I^{k,\lambda}$, in the interactive part of the Hamiltonian, has asymptotic order $\mathcal{O}[\mathrm{Max}(\omega_k\theta_k^{\lambda}, \omega_k^{-1})]$, a fact that implies that its square is not absolutely convergent. This means that, as long as θ_k^{λ} does not depend on the cosmological variables, the operator version of the Hamiltonian constraint is not well-defined in the dense subset spanned by n-particle/antiparticle states of the Fock space.

Let us then proceed to quantize the system in the manner described in the previous sections. We introduce a state dependent conformal time η_Γ given by

$$d\eta_\Gamma = \frac{\ell_0\langle\hat{V}^{2/3}\rangle_\Gamma}{\langle\hat{\tilde{\mathcal{H}}}_0\rangle_\Gamma}d\phi, \tag{4.8}$$

which is well-defined thanks to the the positivity of $\hat{\tilde{\mathcal{H}}}_0$ and the lower positive bound on the volume in each superselection sector of LQC. Then, for asymptotically infinitely large ω_k, (3.31) defines the

[8]Recall that we are summing over all wavenumbers $\vec{k}$ and that, for asymptotically large ω_k, the density of states grows proportional to ω_k^2. Therefore, sequences of asymptotic order $\mathcal{O}(\omega_k^{-3/2})$ or bigger are not generally square summable.

following Heisenberg equations on our annihilation and creation variables, evaluated at $\eta_\Gamma = \eta$:

$$\begin{aligned} d_{\eta_\Gamma} \hat{a}_{\vec{k}}^{\lambda}(\eta,\eta_0) &= -iF_k^{(\Gamma)} \hat{a}_{\vec{k}}^{\lambda}(\eta,\eta_0) + G_k^{(\Gamma)} \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta,\eta_0), \\ d_{\eta_\Gamma} \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta,\eta_0) &= i\left(F_k^{(\Gamma)} + \tilde{J}_k^{(\Gamma)}\right) \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta,\eta_0) - \bar{G}_k^{(\Gamma)} \hat{a}_{\vec{k}}^{\lambda}(\eta,\eta_0), \end{aligned} \tag{4.9}$$

where

$$G_k^{(\Gamma)} = \frac{2i\omega_k \langle \widehat{e^{i(F_2^{k,\lambda} - J_k^\lambda)} V^{2/3}} \theta_k^\lambda \rangle_\Gamma + i\langle \widehat{e^{i(F_2^{k,\lambda} - J_k^\lambda)} V^{2/3}} h_I^{k,\lambda} \rangle_\Gamma}{\langle \hat{V}^{2/3} \rangle_\Gamma}. \tag{4.10}$$

The expressions of $F_k^{(\Gamma)}$ and $\tilde{J}_k^{(\Gamma)}$ will not be needed here.

Equations (4.9) can be integrated to obtain the Bogoliubov transformation corresponding to the dynamical evolution:

$$\begin{aligned} \hat{a}_{\vec{k}}^{\lambda}(\eta,\eta_0) &= \alpha_k(\eta,\eta_0) \hat{a}_{\vec{k}}^{\lambda}(\eta_0) + \beta_k(\eta,\eta_0) \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta_0), \\ \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta,\eta_0) &= -e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \, \tilde{J}_k^{(\Gamma)}} \bar{\beta}_k(\eta,\eta_0) \hat{a}_{\vec{k}}^{\lambda}(\eta_0) + e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \, \tilde{J}_k^{(\Gamma)}} \bar{\alpha}_k(\eta,\eta_0) \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta_0). \end{aligned} \tag{4.11}$$

This Bogoliubov transformation can be used to find solutions to the Schrödinger equation (3.31) as long as it is implementable as a unitary operator on the Fock space $\mathcal{F}_D$. This is indeed the case for all coefficients of the form (4.1)[9]. In particular, we can define rigorously the evolution of the vacuum state.

The fact that the evolved vacuum must be a solution to the (3.31) implies that, in the asymptotic limit of inifinitely large wavenumbers, the fermionic backreaction term behaves as [53]

$$C_D^{(\Gamma)}(\phi) \sim l_0 \langle \hat{V}^{2/3} \rangle_\Gamma \sum_{\vec{k},\lambda} \left[\frac{|G_k^{(\Gamma)}|^2}{2\omega_k} - d_{\eta_\Gamma} c_{\vec{k}}^{\lambda} \right]. \tag{4.12}$$

where $c_{\vec{k}}^{\lambda} \in \mathbb{R}$ is an undetermined phase. Clearly, one can easily make this backreaction finite by a "subtraction of infinities", adjusting the phase $c_{\vec{k}}^{\lambda}$ so that the contribution of each mode vanishes. This is possible even for a divergent sum in the first term of $C_D^{(\Gamma)}$. We will not consider this possibility here, but rather investigate whether the hybrid approach can avoid these problems by a suitable choice of vacuum for the fermions, as we motivated previously and in the spirit of Dirac's ideas about what one should expect when gravity is quantized. Actually, this goal can be accomplished by noting that the quantity $G_k^{(\Gamma)} \omega_k^{-1/2}$ can be made square summable by further restricting the asymptotic freedom in (4.1) so that

$$\theta_k^\lambda = -i \frac{\pi M}{3\ell_0^3 \omega_k^2} \pi_a e^{iF_2^k} + \vartheta_k^\lambda, \qquad \text{with} \qquad \sum_{\vec{k}} \omega_k |\vartheta_k^\lambda|^2 < \infty. \tag{4.13}$$

Hence, $\vartheta_{\vec{k}}^{\lambda}$ is subdominant with respect to ω_k^{-2}. In fact, one can prove that this restriction on the choice of annihilation and creation variables makes the interactive part of the fermionic Hamiltonian decay

[9] This is so because the beta coefficients are square summable [54, 126].

asymptotically as $\omega_k \vartheta_k^\lambda$, which can be chosen as a square summable sequence by further restricting the dominant order of ϑ_k. The new choice of vacuum would then succeed in both achieving a finite backreaction term and ensuring that the fermionic part of the Hamiltonian constraint is well defined as an operator in the dense subset spanned by n-particle/antiparticle states. [10]

4.1.2. Asymptotic diagonalization of the fermionic Hamiltonian in Hybrid LQC

In the previous subsection, we showed that imposing good mathematical and physical conditions on the quantum theory actually restricts the freedom in the choice of vacuum state. We achieved this by restricting the choice of annihilation and creation variables in the limit of asymptotically large wavenumbers. One can go a step further and ask whether, among the still available choices of vacua, there is one preferred by the quantum dynamics. Our previous procedure actually lowered the asymptotic order of the interactive part of the fermionic contribution to the Hamiltonian. It is thus natural to look now for a procedure that removes this term completely, at least asymptotically. For a general definition of annihilation and creation variables, the fermionic contribution $\breve{H}_D$ to the zero-mode of the Hamiltonian constraint has the form

$$\breve{H}_D = \sum_{\vec{k},\lambda} \Bigg[h_D^{k,\lambda} \left(\bar{a}_{\vec{k}}^\lambda a_{\vec{k}}^\lambda - a_{\vec{k}}^\lambda \bar{a}_{\vec{k}}^\lambda + \bar{b}_{\vec{k}}^\lambda b_{\vec{k}}^\lambda - b_{\vec{k}}^\lambda \bar{b}_{\vec{k}}^\lambda \right) + h_J^{k,\lambda} \left(\bar{b}_{\vec{k}}^\lambda b_{\vec{k}}^\lambda - b_{\vec{k}}^\lambda \bar{b}_{\vec{k}}^\lambda \right) + \bar{h}_I^{k,\lambda} \left(a_{\vec{k}}^\lambda b_{\vec{k}}^\lambda \right) - h_I^{k,\lambda} \left(\bar{a}_{\vec{k}}^\lambda \bar{b}_{\vec{k}}^\lambda \right) \Bigg]. \quad (4.14)$$

In the calculation of $\breve{H}_D$, one has to take into account the redefinition of the homogeneous cosmological variables that is needed to keep the system canonical. The non-diagonal part of the Hamiltonian, which is the part that we are interested in, is given by

$$h_I^{k,\lambda} = e^{-iJ_k^\lambda} \left[i f_1^{k,\lambda} \{ f_2^{k,\lambda}, H_{|0} \} - i f_2^{k,\lambda} \{ f_1^{k,\lambda}, H_{|0} \} + \frac{2\omega_k}{a} f_1^{k,\lambda} f_2^{k,\lambda} + M \left(f_1^{k,\lambda} \right)^2 - M \left(f_2^{k,\lambda} \right)^2 \right], \quad (4.15)$$

where $\{\cdot,\cdot\}$ are the Poisson brackets of our (truncated) system.

In order to explore this system in the asymptotic limit of large wavenumbers, we write $f_1^{k,\lambda}$ as the following asymptotic series expansion in inverse powers of ω_k:

$$f_1^{k,\lambda} = e^{iF_2^{k,\lambda}} \sum_{n=1}^{\infty} \frac{(-i)^{n+1} \gamma_n}{\omega_k^n}, \quad (4.16)$$

with $\gamma_n \in \mathbb{R}$. The normalization condition in (3.35) implies then that the asymptotic form of $f_2^{k,\lambda}$ must be

$$f_2^{k,\lambda} = e^{iF_2^{k,\lambda}} \sum_{n=0}^{\infty} \frac{(-i)^n \tilde{\gamma}_n}{\omega_k^n}, \quad (4.17)$$

[10] See footnote 1.

with $\tilde{\gamma}_n \in \mathbb{R}$ again, and where the coefficients $\tilde{\gamma}_n$ are defined as $\tilde{\gamma}_0 = 1$, $\tilde{\gamma}_{2n-1} = 0$, and

$$\tilde{\gamma}_{2n} = (-1)^{n+1} \left[\frac{1}{2}\Gamma_{2n} + \sum_{m=2}^{\infty} \frac{(2m-3)!!}{(2^m)m!} \sum_{i_{m-1}=1}^{n} \dots \sum_{i_1=1}^{i_2} \Gamma_{2n-2i_{m-1}} \dots \Gamma_{2i_1} \right], \quad \forall n \geq 1 \tag{4.18}$$

with

$$\Gamma_0 = 0, \quad \Gamma_{2n} = \sum_{i=1}^{2n} (-1)^{n+i} \gamma_i \gamma_{2n-i}, \quad \forall n \geq 1. \tag{4.19}$$

Note that $\tilde{\gamma}_n$ is completely determined via (4.18) by γ_m with $m \leq n$.

The interactive part of the Hamiltonian vanishes when

$$i f_1^{k,\lambda} \{f_2^{k,\lambda}, H_{|0}\} - i f_2^{k,\lambda} \{f_1^{k,\lambda}, H_{|0}\} + \frac{2\omega_k}{a} f_1^{k,\lambda} f_2^{k,\lambda} + M \left(f_1^{k,\lambda}\right)^2 - M \left(f_2^{k,\lambda}\right)^2 = 0. \tag{4.20}$$

If we plug our asymptotic expansions into this expression, we get the recursive relation

$$\gamma_{n+1} = -\frac{Ma}{2}\tilde{\gamma}_n + \frac{a}{2} \sum_{l=1}^{n} \Big[\tilde{\gamma}_{n-l} \{H_{|0}, \gamma_l\} - \gamma_l \{H_{|0}, \tilde{\gamma}_{n-l}\} - \frac{2}{a} \tilde{\gamma}_l \gamma_{n+1-l} - M(\gamma_l \gamma_{n-l} + \tilde{\gamma}_l \tilde{\gamma}_{n-l}) \Big], \tag{4.21}$$

for all $n \geq 0$. Since $\tilde{\gamma}_0 = 1$ from the normalization condition, we can get the first term of the series (4.16) from this equation, namely $\gamma_1 = -\frac{1}{2}Ma$. We can then univocally obtain the rest of unknown coefficients with our formulas, because the terms in the right hand side of (4.21) only involve contributions of $\tilde{\gamma}_m$ with $m \leq n$. A simple calculation shows that $\gamma_2 = -\frac{\pi M}{3\ell_0^3 \omega_k^2} \pi_a$. In this manner, we recover the results of unitarily implementable evolution and finite backreaction[11].

With this choice of annihilation and creation variables, we get (in the asymptotic sector) the Heisenberg equations

$$d_{\eta_\Gamma} \hat{a}_{\vec{k}}^{\lambda}(\eta, \eta_0) = -i F_k^{(\Gamma)} \hat{a}_{\vec{k}}^{\lambda}(\eta, \eta_0), \quad d_{\eta_\Gamma} \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta, \eta_0) = i \left(F_k^{(\Gamma)} + \tilde{J}_{\vec{k}}^{(\Gamma)} \right) \hat{b}_{\vec{k}}^{\dagger\lambda}(\eta, \eta_0), \tag{4.22}$$

where we have called

$$F_k^{(\Gamma)} = \frac{2\langle \widehat{V^{2/3} a h_D^{k,\lambda}} \rangle_\Gamma}{\langle \widehat{V}^{2/3} \rangle_\Gamma}, \quad \tilde{J}_k^{(\Gamma)} = \frac{2\langle \widehat{V^{2/3} a h_J^{k,\lambda}} \rangle_\Gamma}{\langle \widehat{V}^{2/3} \rangle_\Gamma}. \tag{4.23}$$

These Heisenberg equations can be easily integrated as the following Bogoliubov transformation:

$$\hat{a}_{\vec{k}}^{\lambda}(\eta, \eta_0) = e^{-iF_{\eta,k}^{(\Gamma)}} \hat{a}_{\vec{k}}^{\lambda}(\eta_0) \quad \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta, \eta_0) = e^{i\left(F_{\eta,k}^{(\Gamma)} + \tilde{J}_{\eta,k}^{(\Gamma)}\right)} \hat{b}_{\vec{k}}^{\lambda\dagger}(\eta_0), \tag{4.24}$$

where we have defined

$$F_{\eta,k}^{(\Gamma)} = \int_{\eta_0}^{\eta} d\eta_\Gamma \, F_k^{(\Gamma)}, \quad \tilde{J}_{\eta,k}^{(\Gamma)} = \int_{\eta_0}^{\eta} d\eta_\Gamma \, \tilde{J}_k^{(\Gamma)}. \tag{4.25}$$

[11] For the sake of simplicity, the recursive equation has not been written exactly as it appears in the article.

Some features of this quantization in the asymptotic region are:

- This Bogoliubov transformation is clearly unitary [126], since the antilinear part of the transformation vanishes asymptotically.
- The vacuum is stationary under the evolution dictated by the evolution operator.
- The backreaction is not only finite, but can be made to have an arbitrarily low asymptotic order.
- The fermionic Hamiltonian is properly defined in the dense subset of $\mathcal{F}_D$ spanned by the n-particle/antiparticle states.

4.1.3. Fock quantization of the Dirac field in hybrid quantum cosmology: Relation with adiabatic states

In the previous subsections we discussed how one can impose good physical properties to restrict the choice of vacuum of fermionic perturbations in the context of hybrid LQC. It is a good idea, then, to see how these criteria relate to other vacua in the literature. In quantum field theory in cosmological spacetimes, on the other hand, a well-studied family of vacua are the adiabatic states. The consideration of such states is very common in the case of scalar and tensor fields, but there are less works on this topic in the case of Dirac fields. One construction of fermionic adiabatic states in cosmology is provided in Ref. [70][12]. However, it was carried out in the Dirac representation of the Clifford algebra, instead of the Weyl representation that we are employing. So, we first contruct these states in the Weyl representation following the same line of reasoning of Ref. [70].

At a given initial time η_0, any set of annihilation and creation variables selects a decomposition of the Dirac field of the form

$$\Psi(\eta, \vec{x}) = \sum_{\vec{k}\in\mathbb{Z}^3} \sum_{\lambda=\pm1} \left[u_{\vec{k},\lambda}(\eta,\vec{x}) A_{\vec{k},\lambda} + v_{\vec{k},\lambda}(\eta,\vec{x}) \bar{B}_{\vec{k},\lambda} \right], \tag{4.26}$$

where λ is the helicity, we have introduced the (annihilation and creation-like) constant coefficients

$$A_{\vec{k},\lambda} = a^{\lambda}_{\vec{k}}(\eta_0), \qquad \bar{B}_{\vec{k},\lambda} = \bar{b}^{\lambda}_{-\vec{k}}(\eta_0), \tag{4.27}$$

and, for trivial spin structure on T^3 and setting for simplicity $J^{\lambda}_{k} = 0$,

$$u_{\vec{k},\lambda}(\eta,\vec{x}) = \frac{e^{i2\pi\lambda\vec{k}\vec{x}/\ell_0}}{\sqrt{\ell_0^3 a^3}} \begin{pmatrix} h^{I}_{k,\lambda}(\eta)\xi_\lambda(\vec{k}) \\ \lambda h^{II}_{k,\lambda}(\eta)\xi_\lambda(\vec{k}) \end{pmatrix}, \qquad v_{\vec{k},\lambda}(\eta,\vec{x}) = \lambda\gamma^2 \bar{u}_{\vec{k},\lambda}(\eta,\vec{x}), \tag{4.28}$$

where γ^2 is the second Dirac matrix. The bispinor $\xi_\lambda(\vec{k})$ is normalized so that $\xi^{\dagger}_{\lambda}\xi_\lambda = 1$. In addition, the functions $(h^{I}_{k,\lambda}, h^{II}_{k,\lambda})$ provide a basis of mode solutions of the Dirac equation, normalized such that

[12] A different construction of adiabatic states for fermions in FLRW cosmology has been proposed in Ref. [71]. Nonetheless, we proved that one cannot build a Fock representation based on the states determined by this construction.

$|h^{I}_{k,\lambda}|^2 + |h^{II}_{k,\lambda}|^2 = 1$. They are related to the coefficients of our annihilation and creation variables by

$$\boldsymbol{h}(\eta) = \begin{pmatrix} h^{I}_{k,\lambda} \\ h^{II}_{k,\lambda} \end{pmatrix} = \left[I - \frac{1-\lambda}{2}(I - i\sigma_2) \right] \begin{pmatrix} \bar{f}^{k,\lambda}_1(\eta)\alpha_{k,\lambda}(\eta,\eta_0) - f^{k,\lambda}_2(\eta)\bar{\beta}_{k,\lambda}(\eta,\eta_0) \\ \bar{f}^{k,\lambda}_2(\eta)\alpha_{k,\lambda}(\eta,\eta_0) + f^{k,\lambda}_1(\eta)\bar{\beta}_{k,\lambda}(\eta,\eta_0) \end{pmatrix}. \tag{4.29}$$

In order for the Dirac field to be a solution of the Dirac equation, the variables $(h^{I}_{k,\lambda}, h^{II}_{k,\lambda})$ need to satisfy the Schrödinger-like equation [54]

$$i\partial_\eta \boldsymbol{h} = \boldsymbol{H}(\eta)\boldsymbol{h}, \qquad \boldsymbol{H} = \lambda \begin{pmatrix} -\omega_k & Ma \\ Ma & \omega_k \end{pmatrix}. \tag{4.30}$$

The adiabatic construction begins by diagonalizing the time-dependent Schrödinger Hamiltonian $\boldsymbol{H}(\eta)$, performing an explicitly time-dependent change of variables by means of a unitary matrix. These new variables satisfy a similar equation, but with a lower dominant asymptotic order in the non-diagonal part. This process is applied repeatedly. At the n-th step, the solution can be approximated as

$$\boldsymbol{h}_{|n}(\eta) = \left(\prod_{i=0}^{n} \boldsymbol{U}_i(\eta) \right) \tilde{\boldsymbol{U}}_n(\eta,\eta_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \tilde{\boldsymbol{U}}_n = \mathrm{diag}\left(\exp\left(-i \int_{\eta_0}^{\eta} \Omega_n \right), \exp\left(i \int_{\eta_0}^{\eta} \Omega_n \right) \right). \tag{4.31}$$

The matrices U_i are defined as the unitary matrices necessary to diagonalize the Hamiltonian at the i-th adiabatic step, and Ω_n are the diagonal elements of the Hamiltonian at the nth step. The approximation $\boldsymbol{h}_{|n}(\eta)$ is different from the solution only by terms of asymptotic order $\mathcal{O}(\omega_k^{-n})$. It is worth noting that the frequency Ω_n is manifestly positive in the asymptotic regime of infinitely large ω_k. This adiabatic approximation was motivated in Ref. [70] in order to select positive frequencies. It can be checked that, as expected, this construction is indeed equivalent to that carried out in the Dirac representation.

Let us now analyze the properties of the resulting adiabatic quantization and its associated annihilation and creation operators. With respect to the asymptotic expansion in the limit $\omega_k \to \infty$, the adiabatic construction is such that $f^{k,\lambda}_{1|n}$ mantains, for each adiabatic order $n \geq 1$, the same dominant terms that appear in $f^{k,\lambda}_{1|n-1}$ up to order $\mathcal{O}(\omega_k^{-n-1})$. Computing just the two first adiabatic orders in classical cosmology, one gets

$$f^{k,\lambda}_{1|0}(\eta) = \frac{Ma(\eta)}{2\omega_k} + \mathcal{O}(\omega_k^{-2}), \tag{4.32}$$

$$f^{k,\lambda}_{1|1}(\eta) = \frac{Ma(\eta)}{2\omega_k} + \frac{iMa'(\eta)}{4\omega_k^2} + \mathcal{O}(\omega_k^{-3}) = \frac{Ma(\eta)}{2\omega_k} - i\frac{\pi M \pi_a(\eta)}{3l_0^3\omega_k^2} + \mathcal{O}(\omega_k^{-3}). \tag{4.33}$$

The choice of initial time η_0 does not affect the construction of the adiabatic states, except for a phase that is irrelevant in the choice of Fock space. Comparing these asymptotic terms and those that are characteristic of the family of Fock quantizations admissible in hybrid quantum cosmology according to our physical criteria, we can prove that all adiabatic vacua belong indeed to this family. Furthermore, for adiabatic orders other than zero, those adiabatic vacua can be associated with annihilation and creation operators that lead to a well defined quantum fermionic Hamiltonian and backreaction term in the only non-trivial constraint of the system.

4.1.4. Unique fermionic vacuum in de Sitter spacetime from hybrid quantum cosmology

At this point, we have physical criteria to select a preferred vacuum in the case of fermionic cosmological perturbations for a generic FLRW cosmology. Insight about the properties of this vacuum can be gained by studying a particularly interesting cosmological solution and applying to it our procedures, namely, a de Sitter spacetime. This is a perfect arena to check whether the asymptotic diagonalization procedure is consistent and whether it can indeed fix a unique vacuum. A de Sitter spacetime can actually provide a good approximation to the inflationary epoch of the Universe.

The differential equation (4.20) can be written as an equation on the function $\varphi_{k,\lambda} = f_1^{k,\lambda}/f_2^{k,\lambda}$ for any $f_2^{k,\lambda} \neq 0$:

$$a\{\varphi_{k,\lambda}, H_{|0}\} + 2i\omega_k\varphi_{k,\lambda} + iaM\varphi_{k,\lambda}^2 - iaM = 0. \tag{4.34}$$

In fact, if one introduces the asymptotic expansion

$$\varphi_{k,\lambda} \sim \frac{1}{2\omega_k}\sum_{n=0}^{\infty}\left(-\frac{i}{2\omega_k}\right)^n Z_n, \tag{4.35}$$

the recursive relations previously shown in Subsection 4.1.2 become

$$Z_0 = Ma, \quad Z_{n+1} = a\{H_{|0}, Z_n\} + Ma\sum_{m=0}^{n-1} Z_m Z_{n-(m+1)}, \qquad \forall n \geq 0. \tag{4.36}$$

We may particularize this asymptotic expansion to the expanding chart of de Sitter spacetime, described by a constant potential for the inflaton ϕ and a scale factor that behaves as

$$a = -(\eta H_\Lambda)^{-1}, \qquad -\infty < \eta < 0, \tag{4.37}$$

where H_Λ is the Hubble constant and η the conformal time. In this de Sitter background, the general condition (4.34) that cancels the interaction terms in the fermionic Hamiltonian becomes the following Riccati equation:

$$\varphi'_{k,\lambda} + 2i\omega_k\varphi_{k,\lambda} - iM(\eta H_\Lambda)^{-1}\varphi_{k,\lambda}^2 + iM(\eta H_\Lambda)^{-1} = 0, \tag{4.38}$$

where the prime denotes the derivative with respect to η. To solve this equation, we use the change of variable

$$\varphi_{k,\lambda} = i\eta M^{-1}H_\Lambda[\ln(e^{iMt}w_{k,\lambda})]', \tag{4.39}$$

where t is the cosmic time, and then define the mode-dependent complex time $T_k = -2i\omega_k\eta$. In this manner, we find that the general solution is given by the following linear combination of convergent hypergeometric functions:

$$w_{k,\lambda} = A\,{}_1F_1\left(-iMH_\Lambda^{-1}; 1-2iMH_\Lambda^{-1}; T_k\right) + B\,T_k^{2iMH_\Lambda^{-1}}\,{}_1F_1\left(iMH_\Lambda^{-1}; 1+2iMH_\Lambda^{-1}; T_k\right), \tag{4.40}$$

where A and B are arbitrary complex integration constants.

Let us now prove that the asymptotic diagonalization process picks out a unique vacuum by determining the constants A and B, at least up to a global multiplicative factor that is irrelevant for our definition of creation and annihilation variables. We begin by expanding $w_{k,\lambda}$ as an asymptotic series

$$w_{k,\lambda} \sim T_k^{iMH_\Lambda^{-1}} \sum_{n=0}^{\infty} (-T_k)^{-n} w_n, \qquad \text{with} \qquad w_1 = \left(MH_\Lambda^{-1}\right)^2 w_0. \tag{4.41}$$

The imaginary power of T_k that appears in the above expression is needed to eliminate the term of order 1 in $\varphi_{k,\lambda}$, so that the function $T_k\varphi_{k,\lambda}$ behaves like iMH_Λ^{-1} at dominant order in the asymptotic limit. Introducing this expansion for $w_{k,\lambda}$ in the confluent hypergeometric equation that it must fulfill, we obtain a recursion relation for the constant coefficients w_n,

$$w_{n+1} = \frac{\left(n+iMH_\Lambda^{-1}\right)\left(n-iMH_\Lambda^{-1}\right)}{n+1} w_n. \tag{4.42}$$

The solution is

$$w_n = \frac{w_0}{n!}\left(iMH_\Lambda^{-1}\right)_n \left(-iMH_\Lambda^{-1}\right)_n \tag{4.43}$$

where w_0 is an arbitrary constant and we have employed the notation

$$(b)_n = \begin{cases} 1 & \text{if } n = 0, \\ b(b+1)...(b+n-1) & \text{if } n > 0, \end{cases} \tag{4.44}$$

for any number b. Using some identities satisfied by special functions [127, 128], our formulas allow us to fix the integration constants:

$$A = w_0 \frac{\Gamma\left(2iMH_\Lambda^{-1}\right)}{\Gamma\left(iMH_\Lambda^{-1}\right)}, \qquad B = w_0 \frac{\Gamma\left(-2iMH_\Lambda^{-1}\right)}{\Gamma\left(-iMH_\Lambda^{-1}\right)}. \tag{4.45}$$

where Γ is the usual gamma function.

The solution (4.40) with integration constants (4.45) can be shown to lead in (4.28) to the positive frequency solution

$$u_{\vec{k},\lambda}(\eta,\vec{x}) = \frac{e^{i2\pi\lambda\vec{k}\vec{x}/l_0}}{\sqrt{\ell_0^3 a^3}}\left[I - \frac{1-\lambda}{2}(I+i\gamma^0)\right]\sqrt{\frac{\pi\omega_k\eta}{8}}e^{i\Theta+\pi M H_\Lambda^{-1}/2}\begin{pmatrix}[H^{(2)}_{\mu-1}(\omega_k\eta)+iH^{(2)}_{\mu}(\omega_k\eta)]\xi_\lambda(\vec{k})\\ [H^{(2)}_{\mu-1}(\omega_k\eta)-iH^{(2)}_{\mu}(\omega_k\eta)]\xi_\lambda(\vec{k})\end{pmatrix}, \tag{4.46}$$

where $\mu = iMH_\Lambda^{-1} + 1/2$ and Θ is a constant global phase, irrelevant for the definition of the vacuum. On the other hand, the solutions that describe antiparticles are given by the charge conjugate of these ones, namely via the second equation in (4.28).

We end this subsection by noting that the constant phase Θ includes all the dependence of the basis of solutions on the choice of initial time η_0, and hence the definition of the annihilation and creation constant coefficients that results from our procedure, and thus the associated vacuum, are independent of that choice. Let us finally point out that the leading time dependence of our basis of solutions follows the behavior $u_{\vec{k},\lambda} \sim a^{-3/2}\exp(-i\omega_k\eta)$, $v_{\vec{k},\lambda} \sim a^{-3/2}\exp(i\omega_k\eta)$, something that is often demanded on physical grounds as a necessary feature of the corresponding Fock representation of fields in conformally flat spacetimes [65, 67]. In particular, the Bunch-Davies Hadamard vacuum for scalar fields in de Sitter spacetime has this dominant plane wave behavior [1, 75–78]. In fact, we can show that the asymptotic diagonalization procedure singles out the usual Bunch-Davies vacuum in de Sitter.

4.2. Properties of NO vacua

4.2.1. NO power spectra in LQC

As we discussed in the Introduction, there are many different ways to fix a vacuum for the scalar and tensor perturbations of a homogenous inflationary cosmology with a relevant pre-inflationary period. One of the most studied proposals is the choice of adiabatic states, that leads to vacua with certain desirable physical properties, such as a renormalizable energy-momentum tensor, but that in typical scenarios arising in LQC have some phenomenologically undesirable attributes, like a highly oscillatory power spectrum. Another recent proposal is the NO vacuum. This proposal directly adresses the problem of the superimposed oscillations in the power spectrum, which often produce power amplification in the average and may blur or hide the quantum gravity effects [68]. This choice of vacuum was originally characterized by means of a numerical procedure, a fact that makes difficult the comparison with other vacua and even the discussion of its physical properties. Our goal now is to overcome these complications and gain analytic insights into the qualitative behavior of the NO vacuum states. Let us start with the following generic expression of a positive-frequency mode solution μ_k:

$$\mu_k = \frac{1}{\sqrt{-2\mathrm{Im}(h_k)}}e^{i\int d\eta\,\mathrm{Im}(h_k)}, \tag{4.47}$$

where $\text{Im}(h_k)$ must be strictly negative and, for (3.38) to be satisfied, h_k must be a complex solution to the Ricatti equation

$$h_k' = k^2 + s + h_k^2. \tag{4.48}$$

This last equation is in fact equivalent to the set of coupled equations

$$\text{Re}(h_k)' = k^2 + s + \text{Re}(h_k)^2 - \text{Im}(h_k)^2, \tag{4.49}$$

$$\text{Im}(h_k)' = 2\text{Re}(h_k)\text{Im}(h_k). \tag{4.50}$$

Let us call $p_k = |\mu_k|^2$ the part of the solution on which the power spectra truly depends. From (4.50), we have

$$p_k' = \frac{\text{Re}(h_k)}{\text{Im}(h_k)}. \tag{4.51}$$

One can see that, in the case of a (background-dependent) mass s (like e.g. in hybrid LQC) and given (4.49) and (4.50), p_k can only have one minimum (if any), and therefore cannot oscillate, at time intervals and wavenumbers where $k^2 + s \leq 0$.

We can write this quantity as $p_k = \rho_k^2/2$, where ρ_k is a real non-zero function that, in virtue of (4.48), must satisfy the equation

$$\rho_k'' + (k^2 + s)\rho_k = \frac{1}{\rho_k^3}. \tag{4.52}$$

This is the so-called Ermakov-Pinney equation [80, 81] which has been widely employed in the context of FLRW cosmology and its perturbations (see e.g. [129–132]). Thus, the advantage of our procedure is that we can obtain all possible solutions to (3.38) in terms of one particular real solution ψ_k of the Ermakov-Pinney equation. In fact, the resulting formula manifestly displays the possible oscillatory behavior of p_k. This is because the general real solution of any Ermakov-Pinney equation of the form (4.52) can be expressed as [81]

$$\rho_k^2 = \psi_k^2 \left[A\cos^2(\phi_k) + B\sin^2(\phi_k) + C\sin(2\phi_k)\right], \quad C^2 = AB - 1, \tag{4.53}$$

where A, B, and C are constants that must be real and such that ρ_k^2 be positive, and

$$\phi_k' = \psi_k^{-2}. \tag{4.54}$$

The function p_k is then given by

$$p_k = \frac{1}{4}\psi_k^2 \left[A + B + (A - B)\cos(2\phi_k) + 2C\sin(2\phi_k)\right]. \tag{4.55}$$

It is clear from (4.54) that ϕ_k grows monotonically in time, so that the sine and cosine functions appearing in this formula oscillate in time, generally in a k-dependent way[13]. It then follows that we can characterize the NO spectra by restricting our considerations to real solutions of the Ermakov-Pinney equation such that $|\psi_k'\psi_k|$ is small when $k^2 + s > 0$ and the constants A and B take values in a small neighbourhood of 1. The condition that $|\psi_k'\psi_k|$ be small ensures that the relative variation of the global factor ψ_k^2 is slower than the frequency of the sinusoidal part of the solution.

In terms of h_k this last condition requires in particular that, at any initial time where $s \geq 0$,

$$|\text{Re}(h_k)(\eta_0)| = \epsilon_k |\text{Im}(h_k)(\eta_0)|, \tag{4.56}$$

where ϵ_k is a positive real number smaller than one (or much smaller than one, if preferred). To satisfy this condition in a small neighbourhood of η_0, it is necessary that the derivative of $\text{Re}(h_k)\text{Im}(h_k)^{-1}$ is also small initially. Using Eqs. (4.49) and (4.50), we obtain the requirement

$$\left| \frac{k^2 + s(\eta_0)}{\text{Im}(h_k)(\eta_0)} - (1 + \epsilon_k^2)\text{Im}(h_k)(\eta_0) \right| < 1. \tag{4.57}$$

In general, ϵ_k^2 provides a subdominant contribution to the second summand. Thus, at times η_0 for which the time dependent mass is such that $k^2 + s(\eta_0) \geq 1$, (4.57) requires that

$$\text{Im}(h_k)(\eta_0) = -\sqrt{k^2 + s(\eta_0)} + \delta_k, \qquad \frac{|\delta_k|}{\sqrt{k^2 + s(\eta_0)}} < 1. \tag{4.58}$$

This situation always happens e.g. in hybrid LQC near the bounce for phenomenologically interesting situations, where s is roughly of Planck order.

The power spectra of the perturbations at the end of the kinetically dominated period should ideally include information about features originated at the epoch after the bounce where effective LQC corrections are important. A highly oscillatory behavior (even more when averaged over wavenumber bins) can easily blur most of this information. Furthermore, these (averaged) oscillations can result in an enhancement of power that is not due to any quantum cosmology effect nor it is intrinsic to the classical behavior of spacetime shortly after the loop quantum bounce. Rather, it may correspond to details of the specific set of normalized solutions chosen for the perturbations. So, it makes sense that power spectra with few to no oscillations provide the most natural candidates to capture genuine LQC corrections on the evolution of the perturbations, without introducing artificial modifications in the part of the pre-inflationary era that is essentially Einsteinian.

[13] We recall that this may only happen for intervals of time and wavenumbers k such that $k^2 + s > 0$.

To investigate the ultraviolet properties of NO power spectra, we can use the proposal of an asymptotic diagonalization of the Hamiltonian of the perturbations. We thus focus on the asymptotic regime of unboundedly large wavenumbers k, and adopt an expansion of the form [79]

$$kh_k^{-1} \sim i\left[1 - \frac{1}{2k^2}\sum_{n=0}^{\infty}\left(\frac{-i}{2k}\right)^n h_n\right]. \tag{4.59}$$

The coefficients h_n are real, only depend on time, and, taking into account the Riccati equation that the complex function h_k must satisfy, turn out to be given by the following iterative relation, that is deterministic together with the data $h_0 = s$:

$$h_{n+1} = -h_n' + 4s\left[h_{n-1} + \sum_{m=0}^{n-3} h_m h_{n-(m+3)}\right] - \sum_{m=0}^{n-1} h_l h_{n-(m+1)}. \tag{4.60}$$

We define $h_{-n} = 0$ for all $n > 0$. This leads to a unique asymptotic expansion of, at least, one solution h_k to (4.48), with imaginary part that is strictly negative [79]. Therefore, it provides in turn a precise asymptotic expansion of, at least, one normalized solution to (3.38), via (4.47). We call (any) such solution $\tilde{\mu}_k$. Its associated square norm $\tilde{p}_k = |\tilde{\mu}_k|^2$ is of the form

$$\tilde{p}_k = \frac{1}{2k}\left(1 - \Gamma_k\right), \tag{4.61}$$

where Γ_k has the following asymptotic behavior:

$$\Gamma_k \sim \frac{1}{2k^2}\left[1 - \frac{1}{2k^2}\sum_{n=0}^{\infty}\left(\frac{i}{2k}\right)^{2n} h_{2n}\right]^{-1}\sum_{n=0}^{\infty}\left(\frac{i}{2k}\right)^{2n}\left[h_{2n} - \frac{1}{2k^2}\sum_{m=0}^{2n}(-1)^m h_m h_{2n-m}\right]. \tag{4.62}$$

Each summand of the series depends on the wavenumber k only through an even inverse power. Since we know that $\tilde{p}_k = \tilde{\psi}_k^2/2$ where $\tilde{\psi}_k$ is a real solution to the Ermakov-Pinney equation (4.52), our ultraviolet diagonalization fixes as well (up to sign) a specific asymptotic expansion of, at least, one solution $\tilde{\psi}_k$ to that equation, for unboundedly large k. We can identify it (or one of them, if there are more than one) as the particular solution appearing in the general formula (4.55) for any other power spectrum. Then, for any function p_k that is given by the square norm of a normalized solution to (3.38), we have

$$p_k = \frac{1}{4k}\left(1 - \Gamma_k\right)\left[A + B + (A - B)\cos(2k\eta + 2\theta_k) + 2C\sin(2k\eta + 2\theta_k)\right]. \tag{4.63}$$

The function Γ_k admits the asymptotic expansion (4.62) and θ_k is a phase that has a dominant contribution in the ultraviolet of order k^{-1}. In this asymptotic regime, since Γ_k is of order k^{-2}, p_k has the dominant term

$$\frac{1}{4k}\left[A + B + (A - B)\cos(2k\eta + 2\theta_k) + 2C\sin(2k\eta + 2\theta_k)\right]. \tag{4.64}$$

This is a highly oscillatory function for large k unless we strictly impose that the constants A and B are equal to one, in which case p_k reduces to $\tilde{p}_k$ (recall that $C^2 = AB - 1$). In fact, this choice of constants is the only one that eliminates, order by order in the expansion of p_k in inverse powers of k, all the scale dependent oscillations in the studied asymptotic regime. We then conclude that all NO vacua must possess the asymptotic behavior of $\tilde{\mu}_k$ for sufficiently large k.

4.2.2. NO vacuum states and the quantum homogeneity and isotropy hypothesis in LQC

Given the analytic conditions we now have to study the NO vacua, it is natural to compare them to other vacua proposed in the LQC literature. One such vacuum has been put forward by Ashtekar and Gupt [82, 83]. Its construction is motivated by Penrose's hypothesis that the initial conditions on the Universe should guarantee that its Weyl curvature vanish [84, 85]. The hypothesis is extended by Ashtekar and Gupt to the quantum realm. This quantum counterpart is called the quantum homogeneity and isotropy hypothesis (QHIH). However, in a quantum gravity approach, the quantum operators corresponding to that Weyl curvature of a perturbed homogeneous cosmology cannot vanish all at once. This happens because its components are canonically conjugated variables and so their commutator cannot be zero in the quantum theory. As such, Penrose's hypothesis must be modified to ask for a Weyl curvature (and an associated quantum uncertainty) that is as small as possible. The Weyl curvature is constructed using the tensor perturbations. The above requirements are satisfied on it at an instant η_0 if the quantum state of these perturbations is the zeroth order adiabatic state $|0_{\mu^{\eta_0}}\rangle$ defined by positive-frequency solutions $\mu_k^{\eta_0}$ with initial conditions

$$\mu_k^{\eta_0}(\eta_0) = \frac{1}{\sqrt{2k}}, \quad \mu_k^{\eta_0\prime}(\eta_0) = -i\sqrt{\frac{k}{2}}. \tag{4.65}$$

Since the cosmological background is not stationary, the evolution of the considered adiabatic states is not trivial. As a consequence, there may be many more quantum states that are in the same footing as $|0_{\mu^{\eta_0}}\rangle$ as far as the QHIH is concerned. Therefore, the family of states allowed in the analysis carried out by Ashtekar and Gupt is larger than simply $|0_{\mu^{\eta_0}}\rangle$. This family is given by

$$B = \left\{ |0_{\tilde{\mu}}\rangle \;\middle|\; |\beta_k(\tilde{\mu}_k, \mu_k^{\eta})|^2 \leq \sup_{\eta_0,\eta_1 \in I} |\beta_k(\mu_k^{\eta_0}, \mu_k^{\eta_1})|^2 \quad \forall k \in \mathbb{R}^+, \forall \eta \in I \right\}, \tag{4.66}$$

where I is a compact interval outside which quantum gravity effects are expected to be negligible, and $\beta_k(.,.)$ is the beta coefficient of the Bogoliubov transformation between the states defined by its two arguments. For concreteness, we take the interval I as the period in which the matter density of the Universe is smaller than 10^{-4} in Planck units.

To extract predictions from this proposal, a single vacuum state must be chosen within this Weyl uncertainty ball. The choice made by Ashtekar and Gupt is the maximally classical state at the end of inflation, which minimizes the quantity $|\mu_k(\eta_{end})|^2$ within this ball. This minimization problem is complicated, even numerically. So, Ashtekar and Gupt proceeded to look instead at states in the union over I of *instantaneous* Weyl uncertainty balls B_{η_0} defined as follows:

$$B_{\eta_0} = \left\{ |0_{\tilde{\mu}}\rangle \,\middle|\, |\beta_k(\tilde{\mu}_k, \mu_k^{\eta_0})|^2 \leq \sup_{\eta \in I} |\beta_k(\mu_k^{\eta}, \mu_k^{\eta_0})|^2 \quad \forall k \in \mathbb{R}^+ \right\}. \tag{4.67}$$

The maximally classical states in B_{η_0} for all $\eta_0 \in I$ form a 1-parameter family of states $|0_{\nu^{\eta_0}}\rangle$ defined by the Bogoliubov transformation [82, 83]

$$\nu_k^{\eta_0}(\eta) = \sqrt{1 + (r_k^{\eta_0})^2}\, \mu_k^{\eta_0}(\eta) + r_k^{\eta_0} e^{-i\theta_k^{\eta_0}} \bar{\mu}_k^{\eta_0}(\eta), \tag{4.68}$$

where

$$r_k^{\eta_0} = \sup_{\eta \in I} |\beta_k(\mu_k^{\eta}, \mu_k^{\eta_0})|, \qquad \theta_k^{\eta_0} = \pi - 2 \arg\left[\mu_k^{\eta_0}(\eta_{end})\right], \tag{4.69}$$

and arg denotes the argument of the complex quantity. The unique state corresponding to the global minimum is the Ashtekar-Gupt vacuum. Let us comment that, owing to the similarities between the dynamics of the tensor and scalar perturbations, the QHIH has also been proposed to select a preferred quantum state for the Mukhanov-Sasaki field.

A problem arises with the definition of the Ashtekar-Gupt vacuum, because one was originally looking for it in the total Weyl uncertainty ball of states B, rather than in the union of instantaneous balls $\bigcup_{\eta_0 \in I} B_{\eta_0}$, and we have shown that these two sets do not coincide. We prove this by means of a counterexample. Assuming smooth beta coefficients, and given a compact interval I, there must exist times η_-^k and η_+^k in I such that

$$\left|\beta_k\left(\mu_k^{\eta_-^k}, \mu_k^{\eta_+^k}\right)\right|^2 = \sup_{\eta_0, \eta_1 \in I} |\beta_k\left(\mu_k^{\eta_0}, \mu_k^{\eta_1}\right)|^2. \tag{4.70}$$

Fixing any positive $\tilde{k}$, let us now consider the state $|0_{\mu^S}\rangle$ defined by the Bogoliubov transformation

$$\mu_k^S(\eta) = \bar{\alpha}_k\left(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}}\right) \mu_k^{\eta_+^{\tilde{k}}}(\eta) + \beta_k\left(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}}\right) \bar{\mu}_k^{\eta_+^{\tilde{k}}}(\eta). \tag{4.71}$$

It is clear that $|0_{\mu^S}\rangle$ is in the instantaneous ball $B_{\eta_+^{\tilde{k}}}$, and therefore it is an element of $\bigcup_{\eta_0 \in I} B_{\eta_0}$. However, one can check that

$$\left|\beta_{\tilde{k}}\left(\mu_{\tilde{k}}^S, \mu_{\tilde{k}}^{\eta_-^{\tilde{k}}}\right)\right|^2 \geq 4 \sup_{\eta_0, \eta_1 \in I} \left|\beta_{\tilde{k}}\left(\mu_{\tilde{k}}^{\eta_0}, \mu_{\tilde{k}}^{\eta_1}\right)\right|^2, \tag{4.72}$$

This inequality implies that $|0_{\mu^S}\rangle$ does not belong to B, and hence we conclude that $B \neq \bigcup_{\eta_0 \in I} B_{\eta_0}$.

Given this difference, we restrict our attention to the ball B motivated by the QHIH and investigate whether there may exist NO vacua in it. By considering the Bogoliubov transformation between a possible NO-vacuum and a zeroth order adiabatic state $|0_{\mu^\eta}\rangle$, we obtain

$$
\begin{aligned}
|\mu_k^{NO}(\eta)| &= \frac{1}{\sqrt{2k}}|\alpha_k(\mu_k^{NO},\mu_k^\eta)+\beta_k(\mu_k^{NO},\mu_k^\eta)|, \\
|\mu_k^{NO\prime}(\eta)| &= \sqrt{\frac{k}{2}}\,|\alpha_k(\mu_k^{NO},\mu_k^\eta)-\beta_k(\mu_k^{NO},\mu_k^\eta)|.
\end{aligned} \tag{4.73}
$$

Let us call h_k any function that defines an NO-vacuum via (4.47). The above identities then imply that a state satisfying the first necessary NO-vacuum condition (4.56) can belong to the total Weyl uncertainty ball B only if, for all times η (at least) at the end of I,

$$
[1+\epsilon_k^2(\eta)]|\mathrm{Im}(h_k)(\eta)| \in \left[kz_k - k\sqrt{z_k^2-[1+\epsilon_k^2(\eta)]}, kz_k + k\sqrt{z_k^2-[1+\epsilon_k^2(\eta)]}\right], \tag{4.74}
$$

where $z_k = 1+2\sup_{\eta_0,\eta_1\in I}|\beta_k(\mu_k^{\eta_0},\mu_k^{\eta_1})|^2$. On the other hand, the second necessary condition (4.57) for an NO-vacuum at those times is satisfied if and only if

$$
[1+\epsilon_k^2(\eta)]|\mathrm{Im}(h_k)(\eta)| \in \left(\frac{1}{2}\sqrt{1+4[k^2+s(\eta)][1+\epsilon_k^2(\eta)]}-\frac{1}{2}, \frac{1}{2}\sqrt{1+4[k^2+s(\eta)][1+\epsilon_k^2(\eta)]}+\frac{1}{2}\right). \tag{4.75}
$$

Since ϵ_k is expected to be much smaller than the unity for an NO vacuum, at leading order we can ignore the contribution of this parameter in our expressions. With this approximation, the two necessary conditions for the NO vacuum can be compatible with the QHIH (formulated in terms of the ball B) only if, (at least) for all instants of time η near the end of I,

$$
\left[kz_k - k\sqrt{z_k^2-1}, kz_k + k\sqrt{z_k^2-1}\right] \bigcap \left(\frac{1}{2}\sqrt{1+4[k^2+s(\eta)]}-\frac{1}{2}, \frac{1}{2}\sqrt{1+4[k^2+s(\eta)]}+\frac{1}{2}\right) \neq \emptyset. \tag{4.76}
$$

Finally, we can discuss the consequences of our results in the case of background cosmologies derived from effective LQC. As it was explained in Section 3.7, we consider situations in which the Universe experiences a short-lived inflation with a kinematicaly dominated pre-inflationary period. One can numerically integrate the cosmological background solution and, with it, determine the time-dependent mass of the perturbations and the corresponding bound z_k. Remarkably, for hybrid LQC, Fig. 1 shows that none of the states $|0_{\nu^{\eta_0}}\rangle$ belongs to the physically motivated ball B. This implies that the Ashtekar-Gupt vacuum is outside of the QHIH ball. In addition, Fig. 2 shows that the intersection (4.76) is actually non-empty for all relevant values of k. This means that the NO conditions and the QHIH are non-exclusive in the case of hybrid LQC.

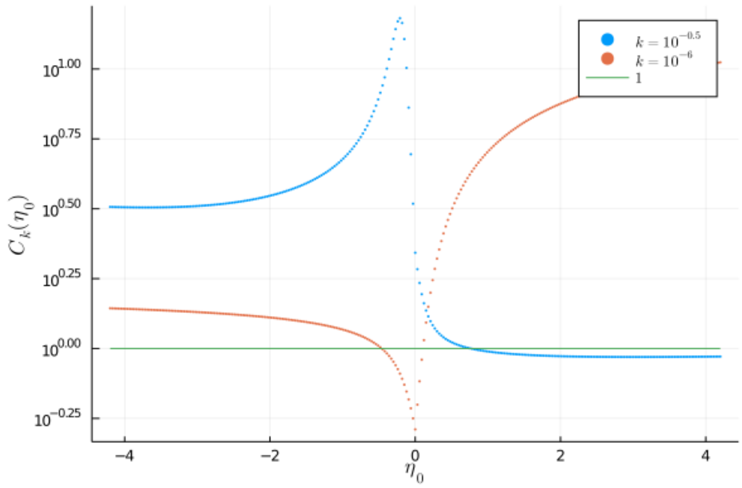

Figure 1: The quantity $C_k(\eta_0) = (z_k)^{-1} \max_{\eta \in I} \left(1 + 2|\beta(\nu_k^{\eta_0}, \mu_k^{\eta})|^2\right)$ compared with 1 for $k = 10^{-6}$ and $k = 10^{-0.5}$, with $I = [-4.2, 4.2]$ in conformal time ($\eta = 0$ corresponds to the bounce). There exists no value of η_0 such that the two curves remain below or equal to 1, a fact that implies that no state $|0_{\nu^{\eta_0}}\rangle$ belongs to B.

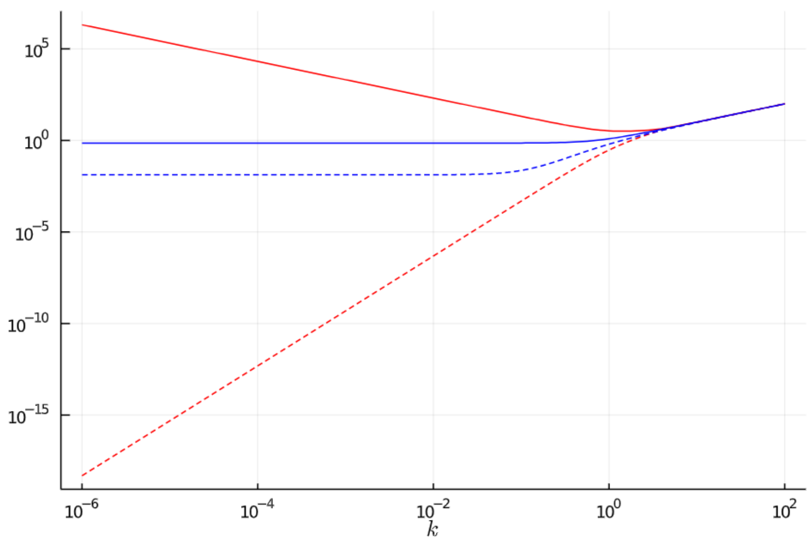

Figure 2: The bounds imposed by the Weyl uncertainty ball, $k\left(z_k - \sqrt{z_k^2 - 1}\right)$ and $k\left(z_k + \sqrt{z_k^2 - 1}\right)$, in red dashed and solid lines respectively, compared with the bounds imposed by the NO-condition, $\frac{1}{2}\sqrt{1 + 4[k^2 + s(\eta)]} - \frac{1}{2}$ and $\frac{1}{2}\sqrt{1 + 4[k^2 + s(\eta)]} + \frac{1}{2}$, in blue dashed and solid lines respectively, for different modes k. These are evaluated for the mass $s(\eta)$ obtained in the hybrid approach to LQC, where $I = [-4.2, 4.2]$ and $\eta = 4.2$, time near which the mass varies slowly. The intersection given by these bounds is not empty for any k.

5. Conclusions

We have investigated and successfully restricted the freedom inherent to the choice of a vacuum state for cosmological perturbations, paying a special attention to cosmological models found in hybrid Loop Quantum Cosmology (LQC) or, more generally, in hybrid approaches to quantum cosmology in which the perturbations are described using Fock representations. The determination of a vacuum state for the cosmological perturbations is essential to be able to extract robust physical predictions from any formalism in cosmology in which one expects relevant phenomena in epochs without a quasi-de Sitter dynamics. Our proposals for the choice of vacuum states are based on requiring certain physically desirable conditions. We have considered in detail two interesting scenarios with perturbations around Friedmann-Lemaître-Robertson-Walker (FLRW) spacetimes, either classical or motivated by LQC: fermionic perturbations, on the one hand, and scalar and tensor perturbations with a non-oscillating (NO) primordial power spectrum, on the other hand.

5.1. Specific results

- For fermionic fields treated as perturbations about inflationary cosmologies, we have managed to restrict the choice of a vacuum state so that the associated quantum backreaction that appears on the geometry in the Hamiltonian constraint be finite.
- This choice can be refined so that the Hamiltonian constraint can be represented by a well-defined operator on the dense subset of the fermionic Fock space spanned by n-particle/antiparticle states.
- We have put forward a choice of vacuum with all the above properties that in addition diagonalizes asymptotically the fermionic contribution to the Hamiltonian constraint, so that, in the limit of large Fourier wavenumbers, the Hamiltonian terms that create and annihilate pairs of particles have an arbitrarily low asymptotic order.
- We have analyzed the hybrid quantization of a FLRW cosmology with a perturbative Dirac field when the fermionic Fock space is determined by this asymptotic diagonalization, obtaining all the desired good physical properties: a diagonal evolution of the fermionic part, a backreaction of arbitrarily low asymptotic order, and a fermionic contribution to the Hamiltonian constraint that is rigorously well-defined as a quantum operator.
- We have described the construction of adiabatic fermionic states in FLRW cosmology, using the Weyl representation of the Clifford algebra.
- We have compared these adiabatic states with the vacuum selected by the physical criteria explained above. All adiabatic states evolve unitarily, and from the first adiabatic order on, their backreaction contribution to the Hamiltonian constraint is finite and allows for a well-defined fermionic Hamiltonian on the basis of n-particle/antiparticle states.

- We have demonstrated that the asymptotic diagonalization procedure fixes a unique vacuum in the case of a classical de Sitter cosmology.
- This unique vacuum has a plane wave behavior in the asymptotic limit of large wavenumbers and we can identify it with the usual Bunch-davies state, which is generally considered a preferred vacuum for de Sitter.
- For scalar and tensor perturbations about inflationary cosmologies, we have related their choice of vacuum with the solutions of the Ermakov-Pinney equation, and used the properties of those solutions to single out states with NO power spectra (if they exist). Oscillations in the spectra arising from other choices of vacuum state can blur the effects that genuinely come from quantum gravity phenomena.
- Taking into account that the choice of a vacuum state is equivalent to a choice of initial conditions for the perturbations, we have derived a necessary condition on these initial data to avoid highly oscillatory spectra.
- We have studied the stability of this necessary condition, and derived from that a second condition that is always applicable in situations in which the time-dependent mass of the gauge-invariant perturbations is of Planck order or higher, as it happens in interesting scenarios of hybrid LQC.
- We have revisited the Ashtekar-Gupt construction, proposed to determine a specific vacuum state in the framework of LQC, and noticed that, in general, this construction is not consistent with the so-called quantum homogeneity and isotropy hypothesis (QHIH) originally introduced to motivate physically this choice.
- We have found some analytic conditions that are necessary so that NO vacua belong to the family of states satisfying the QHIH.
- We have proved that these conditions are met for effective backgrounds with a short-lived inflation in hybrid LQC. therefore, the QHIH and the restriction to NO vacua are mutually non-exclusive in principle.
- Finally, we have shown that the vacuum selected with the Ashtekar-Gupt construction in these effective backgrounds of hybrid LQC is a state that does not belong to the family picked out by the QHIH.

In summary, we have investigated the search for a vacuum state in relevant scenarios in cosmology by focusing on physical criteria. On the one hand, we have carried out a rigorous study of fermionic fields in quantum cosmology that clarifies a field that has not been explored in depth and sometimes even in discordant ways. On the other hand, we have carried out a study of NO vacua that sheds light on which initial conditions are physically suitable for the equations that govern the evolution of primordial cosmological perturbations. These two studies allow advances in LQC and its hybrid approach that facilitate the extraction of falsifiable predictions.

V. Conclusiones

Hemos estudiado y restringido con éxito la libertad inherente a la elección de un estado de vacío para las perturbaciones cosmológicas, prestando especial atención a modelos cosmológicos descritos mediante Cosmología Cuántica de Lazos (CCL) híbrida o, más generalmente, mediante enfoques híbridos de cosmología cuántica en los que las perturbaciones se describen utilizando representaciones de Fock. La determinación de un estado de vacío para las perturbaciones cosmológicas es esencial para poder extraer predicciones físicas robustas a partir de cualquier formalismo en cosmología en el que se espera que existan fenómenos relevantes en épocas sin una dinámica cuasi-de Sitter. Nuestras propuestas para la elección de estados de vacío se basan en requerir ciertas condiciones físicamente deseables. Hemos considerado en detalle dos escenarios interesantes con perturbaciones sobre espaciotiempos de Friedmann-Lemaître-Robertson-Walker (FLRW), ya sean clásicos o motivados por CCL: perturbaciones fermiónicas, por un lado, y perturbaciones escalares y tensoriales con un espectro de potencias primordial no oscilante (NO), por otro lado.

V.1. Resultados concretos

- Para campos fermiónicos tratados como perturbaciones sobre cosmologías inflacionarias, hemos logrado restringir la elección del estado de vacío para que la *backreaction* cuántica asociada que aparece sobre la geometría en la ligadura hamiltoniana sea finita.

- Esta elección puede refinarse de tal forma que la ligadura hamiltoniana puede representarse mediante un operador bien definido en el subconjunto denso del espacio de Fock generado por estados de n-partículas/antipartículas.

- Hemos propuesto una elección de vacío con todas las propiedades anteriores que además diagonaliza asintóticamente la contribución fermiónica a la ligadura hamiltoniana, de modo que, en el límite de números de onda de Fourier grandes, los términos hamiltonianos que crean y aniquilan pares de partículas tienen un orden asintótico arbitrariamente bajo.

- Hemos analizado la cuantización híbrida de una cosmología FLRW con un campo de Dirac perturbativo cuando el espacio de Fock fermiónico está determinado por esta diagonalización asintótica, obteniendo todas las buenas propiedades físicas deseadas: una evolución diagonal de la parte fermiónica, una *backreaction* de la parte fermiónica de orden asintótico arbitrariamente bajo y una contribución fermiónica a la ligadura hamiltoniana que está rigurosamente bien definida como operador cuántico.

- Hemos descrito la construcción de estados fermiónicos adiabáticos en cosmologías de FLRW, usando la representación de Weyl del álgebra de Clifford.

- Hemos comparado estos estados adiabáticos con el vacío seleccionado por los criterios físicos explicados anteriormente. Todos los estados adiabáticos evolucionan unitariamente y, a partir del primer orden adiabático, su contribución de *backreaction* a la ligadura hamiltoniana es finita y permiten un hamiltoniano fermiónico bien definido sobre la base de estados de n-partículas/antipartículas.

- Hemos demostrado que el procedimiento de diagonalización asintótica fija un vacío único en el caso de una cosmología clásica de de Sitter.

- Este vacío único tiene un comportamiento de onda plana en el límite asintótico de números de onda grandes y podemos identificarlo con el estado habitual de Bunch-Davies, que generalmente se considera un vacío preferente para de Sitter.

- Para perturbaciones escalares y tensoriales sobre cosmologías inflacionarias, hemos relacionado la elección de vacío con las soluciones de la ecuación de Ermakov-Pinney, y hemos usado las propiedades de esas soluciones para seleccionar estados con espectros NO (si existen). Las oscilaciones en los espectros que surgen de otras elecciones de estado de vacío pueden enmascarar los efectos que realmente provienen de fenómenos de gravedad cuántica.

- Teniendo en cuenta que la elección de un estado de vacío es equivalente a la elección de condiciones iniciales para las perturbaciones, hemos deducido una condición necesaria sobre estos datos iniciales para evitar espectros altamente oscilatorios.

- Hemos estudiado la estabilidad dinámica de esta condición necesaria, y de ahí hemos deducido una segunda condición que siempre es aplicable en situaciones en las que la masa dependiente del tiempo de las perturbaciones invariantes de *gauge* es de orden uno en unidades de Planck, como sucede en escenarios interesantes de CCL híbrida.

- Hemos revisado la construcción de Ashtekar-Gupt, propuesta para determinar un estado de vacío específico en el marco de la CCL, y así hemos hecho notar que, en general, esta construcción no es consistente con la llamada hipótesis de homogeneidad e isotropía cuántica (HHIC), introducida originariamente para motivar físicamente esta elección.

- Hemos encontrado ciertas condiciones que son necesarias para que el vacío NO pueda pertenecer a la familia de estados que satisfacen la HHIC.

- Hemos demostrado que estas condiciones se cumplen para fondos (*backgrounds*) efectivos con inflación de corta vida en CCL híbrida. Por lo tanto, la HHIC y la restricción a vacíos NO, en principio, no se excluyen mutuamente.

- Finalmente, hemos demostrado que el vacío seleccionado con la construcción de Ashtekar-Gupt en estos fondos efectivos para CCL híbrida es un estado que no pertenece a la familia seleccionada por la HHIC.

En resumen, hemos investigado la búsqueda de un estado de vacío para escenarios relevantes en cosmología centrándonos en criterios físicos. Por una parte, hemos llevado a cabo un estudio riguroso de campos fermiónicos en cosmología cuántica que esclarece un campo poco explorado y de maneras a veces discordantes. Por otro lado, hemos realizado un estudio de vacíos NO que arroja luz sobre qué condiciones iniciales son físicamente adecuadas para las ecuaciones que gobiernan la evolución de perturbaciones cosmológicas primordiales. Estos dos estudios permiten el avance de la CCL y su enfoque híbrido hacia la obtención de predicciones falsificables.

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VI. List of publications produced during the Thesis

1. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado, Asymptotic diagonalization of the fermionic Hamiltonian in hybrid loop quantum cosmology, Phys. Rev. D **99**, 063535 (2019).

2. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado, Fock quantization of the Dirac field in hybrid quantum cosmology: Relation with adiabatic states, Phys. Rev. D **100**, 125003 (2019).

3. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado, Unique fermionic vacuum in de Sitter spacetime from hybrid quantum cosmology, Phys. Rev. D **101**, 123530 (2020).

4. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado, Non-oscillating power spectra in Loop Quantum Cosmology, Class. Quantum Grav. **38** 035001 (2021).

5. J. Cortez, B. Elizaga Navascués, G. A. Mena Marugán, S. Prado, J. M. Velhinho, Uniqueness Criteria for the Fock Quantization of Dirac Fields and Applications in Hybrid Loop Quantum Cosmology, Universe 2020, **6**(12), 241, (2020).

6. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado, Non-oscillating vacuum states and the quantum homogeneity and isotropy hypothesis in Loop Quantum Cosmology, Phys. Rev. D **104**, 083541 (2021).

VI.1. Publication produced between the Master Thesis defense and the beginning of the PhD Thesis

7. B. Elizaga Navascués, G.A. Mena Marugán, and S. Prado Loy, Backreaction of fermionic perturbations in the Hamiltonian of hybrid loop quantum cosmology, Phys. Rev. D **98**, 063535 (2018).[14]

[14] Added as an appendix at the end.

Asymptotic diagonalization of the fermionic Hamiltonian in hybrid loop quantum cosmology

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We use the freedom available in hybrid loop quantum cosmology to split the degrees of freedom between the geometry and the matter fields so as to build a quantum field theory for the matter content with good quantum properties. We investigate this issue in an inflationary, flat cosmology with inhomogeneous perturbations, and focus the discussion on a Dirac field, minimally coupled to the cosmological background and treated as a perturbation. After truncating the action at the lowest nontrivial order in perturbations, one must define canonical variables for the matter content, for which one generally employs canonical transformations that mix the homogeneous background and the perturbations. Each of these possible definitions comes associated with a different matter contribution to the Hamiltonian of the complete system, that may, in general, contain terms that are quadratic in creationlike variables, and in annihilationlike variables, with the subsequent production and destruction of pairs of fermionic particles and antiparticles. We determine a choice of the fermionic canonical variables for which the interaction part of the Hamiltonian can be made as negligible as desired in the asymptotic regime of large particle/antiparticle wave numbers. Finally, we study the quantum dynamics for this choice, imposing the total Hamiltonian constraint on the quantum states and assuming that their gravitational part is not affected significantly by the presence of fermions. In this way, we obtain a Schrödinger equation for the fermionic degrees of freedom in terms of quantum expectation values of the geometry that leads to asymptotically diagonal Heisenberg relations and Bogoliubov evolution transformations, with no divergences in the associated normal-ordered Hamiltonian.

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I. INTRODUCTION

Choosing a Fock representation for the quantization of matter fields in curved spacetimes, and with it a vacuum state, is a nontrivial task even in the case of linear fields. In quantum mechanics, when one is considering systems with finite degrees of freedom, one can make use of results like the Stone-von Neumann theorem that guarantees that there exists only one representation of the Weyl relations, up to unitary equivalence, with the desired properties, namely a strongly continuous, irreducible, and unitary representation [1,2]. Nevertheless, when one has to deal with fields that are systems with infinite degrees of freedom, there is no such theorem at our disposal and, in the best of cases, one has to appeal to symmetries or other kinds of physical arguments in order to select a vacuum. In Minkowski spacetime, for instance, the most natural thing to ask for is Poincaré invariance, which in fact picks out a unique representation, up to unitary transformations [3,4]. For stationary spacetimes, the so-called energy criterion can be used to select a preferred complex structure (which essentially fixes the Fock representation) out of the infinite many that are possible [5,6]. In spite of all this, no general uniqueness result has been found for systems with fieldlike degrees of freedom in nonstationary spacetimes, such as cosmologies [7,8]. Actually, in nonstationary spacetimes, and after imposing invariance under the spatial isometries that the system possesses, one could expect that the ambiguity that affects the choice of representation could be solved, not by demanding invariance under time evolution, since the dynamics is not a symmetry anymore, but by requiring that, at least, the quantum evolution of the creation and annihilation operators can be implemented in a unitary way. For a variety of cosmological systems, it has been recently proven that this criterion of unitarity (together with the invariance under spatial symmetries) indeed

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determines a preferred family of vacua, which are all unitarily related [9–19].

The system that we study in this work is a flat Friedmann-Lemaître-Robertson-Walker (FLRW) cosmology with a Dirac field that will be regarded as a perturbation, including its zero mode if it is not identically vanishing. Since we are not concerned here about infrared divergences, in order to simplify the discussion and keep all definitions rigorous we restrict our considerations to compact FLRW spatial sections. More specifically, we analyze the case of sections with the topology of a three-torus. In this system, it has been proven that there is a unique family of Fock representations of the Dirac field, all related among them by unitary transformations, for which the vacuum is invariant under the isometries of the spatial sections and the Heisenberg dynamics of the creation and annihilation operators is unitarily implementable (once one adopts a standard convention for particles and antiparticles), provided that one treats the FLRW spacetime as a classical or *effective* background [20].

Furthermore, the system was further studied within the hybrid approach for the quantization of gravitational models, in which the (matter) fields are quantized with suitable Fock representations and the homogeneous geometry is quantized with techniques inspired by nonperturbative quantum gravity, typically with methods of the canonical formalism known as loop quantum gravity (LQG) [21]. This hybrid approach has been successfully used in cosmological scenarios with perturbations [22–24]. In our particular system, we treat the degrees of freedom of the homogeneous cosmology exactly and truncate the action at quadratic order in the perturbations, that is the lowest order with a nonvanishing contribution. With this truncation, the zero mode of the Hamiltonian constraint is formally equal to the constraint of the homogeneous cosmology plus a contribution that is quadratic in the perturbations. Nevertheless, it is worth pointing out that there is an inherent freedom in the way in which one decides to separate the degrees of freedom of the homogeneous cosmology from the inhomogeneous perturbations, since they can always be remixed using transformations that preserve the canonical symplectic structure at the level of the perturbative truncation of the system. Actually, instead of considering this freedom a nuisance, the idea that was put forward in Ref. [25] was to exploit the freedom to define canonical variables for which the Hamiltonian of the perturbative Dirac variables had certain nice properties. In fact, when fermions were first studied within the hybrid approach in Ref. [26], the choice of fermionic variables was based only on the requirements of invariance of the resulting Fock vacuum under the spatial symmetries, a unitarily implementable Heisenberg evolution in the regime of quantum field theory in curved spacetimes, and a standard convention for particles and antiparticles. But it was already shown there that ultraviolet divergences appeared in the resulting Schrödinger equation for the fermionic degrees of freedom (after a convenient sort of Born-Oppenheimer approximation in the imposition of the full quantum constraint). These divergences could only be solved by either a regularization scheme with *substraction of infinities* or by introducing a further restriction on the choice of perturbative variables that define the vacuum [25]. In practice, this new restriction lowered the asymptotic order of the interaction part of the fermionic Hamiltonian at large wave numbers (identified as the eigenvalues of the Dirac operator on the spatial sections), diminishing the production of pairs of particles and antiparticles in this asymptotic regime.

In the present work, we go one step beyond in the same direction and, by further taking advantage of the freedom to split the degrees of freedom between the geometry and the perturbations, prove that one can absorb the interaction terms of the fermionic Hamiltonian so as to make them as negligible as desired in the asymptotic regime of large eigenvalues (in absolute value) of the modes of the Dirac field. Moreover, in this way we not only improve the quantum behavior of the fermionic contribution to the Hamiltonian of our gravitational model, but we also reduce the ambiguity in our choice of Fock representation and the vacuum for the Dirac field, leaving only some remaining asymptotic freedom in certain phases. In addition, we also notice that, since the resulting fermionic Hamiltonian contribution is diagonal, at least asymptotically, the dynamics that it generates is very simple for the vacuum of the representation, essentially a rotating phase. In this sense, one can think of this vacuum and our splitting of degrees of freedom in the hybrid quantization as those that are best adapted to the dynamics of the entire cosmological system.

The rest of the paper is organized as follows, in Sec. II, and following the procedure detailed in Ref. [26], we introduce the Dirac field as a perturbation around the flat FLRW cosmology, truncating the action at quadratic perturbative order. In Sec. III we consider a generic choice of creation and annihilationlike variables for the Dirac field, allowing definitions that depend on the homogeneous geometry. This dependence is captured in the coefficients of the linear transformations that relate our fermionic variables with the coefficients of the fermionic mode expansions. We also calculate the form of the fermionic contribution to the total Hamiltonian constraint for each of the possible choices of variables, paying special attention to the nondiagonal part of this contribution that provides the fermionic interaction terms. Then, in Sec. IV we adopt an *ansatz* for the creation and annihilationlike variables inspired in the analysis of Refs. [25,26], and we investigate the specific expression that these variables must take so that they asymptotically diagonalize the fermionic Hamiltonian. We also give the form of the remaining, diagonal part of the Hamiltonian. Finally, in Sec. V we briefly revisit the hybrid quantization of Ref. [26] to adapt it to our new variables.

In particular, we give the new Schrödinger equation, Heisenberg relations, Bogoliubov evolution transformation, and evolution operator for the new choice of vacuum. We conclude in Sec. VI, summarizing our results, and commenting on some lines for further research.

II. CLASSICAL MODEL

Let us start by briefly presenting the model that we study. The homogeneous sector consists of a flat FLRW spacetime with compact spatial sections that are isomorphic to the three-torus, T^3, and of a massive scalar field, ϕ, subject to a potential $V(\phi)$. This field plays the role of the inflaton. We use spacetime coordinates that exploit the symmetry of this cosmological background. The inhomogeneous sector is given by a Dirac field with mass M, which is treated as a perturbation. For all practical purposes, we include in this sector also the zero mode of the Dirac field if it does not vanish, regarding it as a perturbative degree of freedom. We then truncate the action at quadratic order in the perturbations [27,28], and use the canonical structure and the Hamiltonian of this truncated action to construct our description of the entire system.

In principle, we can also add perturbative inhomogeneities to the metric and the inflaton, as in Refs. [29,30], perturbations that we consider again as part of the inhomogeneous sector. These additional perturbations originate new quadratic contributions to the purely homogeneous part of the Hamiltonian constraint, and they furthermore introduce a whole family of linear perturbative constraints. The only perturbative quantities that are physically meaningful are those that commute with this family of constraints, and they are generally called gauge-invariant perturbations [31,32]. Invariant perturbations of this kind, for the case with flat spatial topology that we are discussing, are the tensor perturbations of the metric and the Mukhanov-Sasaki scalar [33–35], which mixes scalar perturbations of the metric and the inflaton. A phase space for the perturbations can then be constructed with these gauge invariants and with an Abelianized version of the perturbative linear constraints, together with suitable canonical momenta of all of them. Nonetheless, since the definitions of these variables make use of the homogeneous FLRW ones, they do not form a canonical set with the variables of the homogeneous sector, and these latter variables have to be modified with quadratic terms in the perturbations in order to render the whole set canonical again. On the other hand, since the Einstein-Dirac action is quadratic in the Dirac field, the fermionic perturbations, at our order of truncation, couple directly to the homogeneous tetrad and hence turn out to be gauge invariants (namely, they commute under Poisson brackets with the linear perturbative constraints arising from the perturbation of the tetrad).

It is convenient to rescale the Dirac field by a factor $e^{3\tilde{\alpha}/2}$ in order to get canonical Dirac brackets that are constant in the evolution, after imposing an internal time gauge on the homogeneous tetrad [36]. Here, $\tilde{\alpha}$ is the logarithm of the scale factor of the FLRW geometry up to an additive constant $\ln[4\pi/(3l_0)^3]/2$, where l_0 is the compactification length of the tori, and, in general, the tilde over a homogeneous variable indicates that it has been corrected with quadratic perturbative terms, as we have mentioned above. In the adopted internal time gauge, we can expand the two chiral components of the rescaled field in modes of the Dirac operator on the spatial sections. This expansion is especially suitable because the Dirac operator is invariant under the spatial isometries of the FLRW cosmology, a property that at the end of the day guarantees that the dynamical equations do not mix its eigenmodes. Since we are dealing with compact spatial sections, the spectrum of this operator is discrete. The eigenvalues for T^3 are $\pm\omega_k = \pm 2\pi|\vec{k}+\vec{\tau}|/l_0$, $\vec{k}\in\mathbb{Z}^3$, and where $\vec{\tau} = \sum \theta_I \vec{v}_I/2$ characterizes the spin structure on the spatial sections ($\theta_I = 0$ or 1 depending on the spin structure, and $\vec{v}_I$ is the standard $\mathbb{Z}^3$ basis). Then, the rescaled Dirac field can be described in terms of a set of time-dependent Grassmann variables $\{m_{\vec{k}}.\bar{r}_{\vec{k}}, \bar{s}_{\vec{k}}, t_{\vec{k}}\}$, where the bar denotes complex conjugation. The ordered pairs $(m_{\vec{k}}, \bar{r}_{\vec{k}})$ and $(s_{\vec{k}}, \bar{t}_{\vec{k}})$ are simply the coefficients of the Dirac eigenspinors of the left-handed and (the complex conjugate of the) right-handed components of the rescaled Dirac field, respectively, up to a multiplicative constant $[4\pi/(3l_0)]^{-3/4}$. The first variable of each of these pairs is associated with the eigenspinors that have positive eigenvalues, while the second variable corresponds to negative eigenvalues. Each of these mode coefficients is canonically conjugate to its complex conjugate, inasmuch as their Dirac bracket equals $-i$, whereas the rest of the Dirac brackets between our fermionic variables vanish [36].

III. FERMIONIC CONTRIBUTION TO THE HAMILTONIAN

Let us introduce the following family of annihilationlike variables of particles and creationlike variables of antiparticles for the Dirac field, respectively, defined by these linear combinations of the Grassman variables that determine the field,

$$a_{\vec{k}}^{(x,y)} = f_1^{\vec{k},(x,y)} x_{\vec{k}} + f_2^{\vec{k},(x,y)} \bar{y}_{-\vec{k}-2\vec{\tau}},$$
$$\bar{b}_{\vec{k}}^{(x,y)} = g_1^{\vec{k},(x,y)} x_{\vec{k}} + g_2^{\vec{k},(x,y)} \bar{y}_{-\vec{k}-2\vec{\tau}}. \tag{3.1}$$

Here, $(x_{\vec{k}}, \bar{y}_{\vec{k}})$ is any of the ordered pairs $(m_{\vec{k}}.\bar{s}_{\vec{k}})$ and $(t_{\vec{k}}, \bar{r}_{\vec{k}})$, and the superindex (x, y) means that the coefficients may be different for each of the pairs. Notice that, in the linear combinations that provide our creation and annihilationlike variables, we have imposed that they do not mix contributions from different modes of the spatial Dirac operator, labeled by the value of $\vec{k}$, so that our definitions respect the spatial symmetries of the fermionic dynamics (and hence the resulting complex structure is invariant under those symmetries) [20]. Since the variables given in Eq. (3.1) have to satisfy standard anticommutation relations, the coefficients of the linear combinations that define them must fulfil the relations [18]

$$f_2^{\vec{k},(x,y)} = e^{iF_2^{\vec{k},(x,y)}}\sqrt{1-\left|f_1^{\vec{k},(x,y)}\right|^2},$$
$$g_1^{\vec{k},(x,y)} = e^{iJ_{\vec{k}}^{(x,y)}}\bar{f}_2^{\vec{k},(x,y)},$$
$$g_2^{\vec{k},(x,y)} = -e^{iJ_{\vec{k}}^{(x,y)}}\bar{f}_1^{\vec{k},(x,y)}, \tag{3.2}$$

where $F_2^{\vec{k},(x,y)}$ and $J_{\vec{k}}^{(x,y)}$ are real phases.

In general, we allow linear combinations that depend on the variables of the homogeneous sector, namely $f_L^{\vec{k},(x,y)} \equiv f_L^{\vec{k},(x,y)}(\tilde{\alpha},\pi_{\tilde{\alpha}},\tilde{\phi},\pi_{\tilde{\phi}})$ and $g_L^{\vec{k},(x,y)} \equiv g_L^{\vec{k},(x,y)}(\tilde{\alpha},\pi_{\tilde{\alpha}},\tilde{\phi},\pi_{\tilde{\phi}})$, where $L=1,2$ and $\pi_{\tilde{z}}$ is the canonical momentum of the variable $\tilde{z}=\tilde{\alpha},\tilde{\phi}$. As a result, the new fermionic variables do not constitute a canonical set with $(\tilde{\alpha},\pi_{\tilde{\alpha}},\tilde{\phi},\pi_{\tilde{\phi}})$, a fact that calls for a suitable redefinition of the homogeneous variables, which must be corrected with quadratic perturbative terms along the lines that we have already explained in order to arrive at a new canonical set $(\alpha,\pi_\alpha,\phi,\pi_\phi)$. At our order of truncation, the desired corrections are [26]

$$z-\tilde{z} \equiv \Delta z = \frac{i}{2}\sum_{\vec{k},(x,y)}[(\partial_{\pi_{\tilde{z}}}x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_{\pi_{\tilde{z}}}\bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_{\pi_{\tilde{z}}}y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_{\pi_{\tilde{z}}}\bar{y}_{\vec{k}})y_{\vec{k}}], \tag{3.3}$$

$$\pi_z-\pi_{\tilde{z}} \equiv \Delta\pi_z = -\frac{i}{2}\sum_{\vec{k},(x,y)}[(\partial_{\tilde{z}}x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_{\tilde{z}}\bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_{\tilde{z}}y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_{\tilde{z}}\bar{y}_{\vec{k}})y_{\vec{k}}], \tag{3.4}$$

where $z=\alpha,\phi$ and the subindex (x,y) indicates that we are summing over both existing pairs. This change of variables gives rise then to alterations in the homogeneous part of the Hamiltonian constraint, producing new perturbative contributions from it. Truncating those contributions at the relevant perturbative order, one can see that the final result is a new fermionic contribution $\breve{H}_D$ to the zero mode of the Hamiltonian constraint, given by the expression [26]

$$\breve{H}_D = H_D - \partial_\alpha H_{|0}\Delta\alpha - \partial_{\pi_\alpha}H_{|0}\Delta\pi_\alpha - \partial_\phi H_{|0}\Delta\phi - \partial_{\pi_\phi}H_{|0}\Delta\pi_\phi, \tag{3.5}$$

where H_D is the old fermionic contribution and $H_{|0}$ is the Hamiltonian of the unperturbed model, with their dependence on the old homogeneous variables identified with the new ones.

Following calculations similar to those of Ref. [25],[1] we then obtain the fermionic contribution

$$\breve{H}_D = \sum_{\vec{k},(x,y)}\Big[h_D^{\vec{k},(x,y)}(\bar{a}_{\vec{k}}^{(x,y)}a_{\vec{k}}^{(x,y)} - a_{\vec{k}}^{(x,y)}\bar{a}_{\vec{k}}^{(x,y)} + \bar{b}_{\vec{k}}^{(x,y)}b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)}\bar{b}_{\vec{k}}^{(x,y)}) + h_J^{\vec{k},(x,y)}(\bar{b}_{\vec{k}}^{(x,y)}b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)}\bar{b}_{\vec{k}}^{(x,y)}) + \bar{h}_I^{\vec{k},(x,y)}(a_{\vec{k}}^{(x,y)}b_{\vec{k}}^{(x,y)}) - h_I^{\vec{k},(x,y)}(\bar{a}_{\vec{k}}^{(x,y)}\bar{b}_{\vec{k}}^{(x,y)})\Big], \tag{3.6}$$

where

$$h_D^{\vec{k},(x,y)} = \frac{\omega_k}{2e^\alpha}(|f_2^{\vec{k},(x,y)}|^2 - |f_1^{\vec{k},(x,y)}|^2) + \tilde{M}\Re(f_1^{\vec{k},(x,y)}\bar{f}_2^{\vec{k},(x,y)}) - \frac{i}{2}(\bar{f}_1^{\vec{k},(x,y)}\partial f_1^{\vec{k},(x,y)} + \bar{f}_2^{\vec{k},(x,y)}\partial f_2^{\vec{k},(x,y)}), \tag{3.7}$$

$$h_J^{\vec{k},(x,y)} = -\frac{1}{2}\partial J_{\vec{k}}^{(x,y)}, \tag{3.8}$$

$$h_I^{\vec{k},(x,y)} = e^{-iJ_{\vec{k}}^{(x,y)}}\Big[if_2^{\vec{k},(x,y)}\partial f_1^{\vec{k},(x,y)} - if_1^{\vec{k},(x,y)}\partial f_2^{\vec{k},(x,y)} + \frac{2\omega_k}{e^\alpha}f_1^{\vec{k},(x,y)}f_2^{\vec{k},(x,y)} + \tilde{M}(f_1^{\vec{k},(x,y)})^2 - \tilde{M}(f_2^{\vec{k},(x,y)})^2\Big]. \tag{3.9}$$

Here, we have introduced the rescaled mass $\tilde{M} = 2M\sqrt{\pi/(3l_0^3)}$, we have used $\Re$ to denote the real part of a complex number, and we have defined ∂ as the linear differential operator $\partial \equiv \{H_{|0},\cdot\}$, where $\{\cdot,\cdot\}$ are the Poisson brackets of our truncated system.

IV. DIAGONALIZATION OF THE FERMIONIC CONTRIBUTION

We know from Refs. [25,26] that, on the sector of large ω_k, one can lower the asymptotic order of $h_I^{\vec{k},(x,y)}$ with a suitable definition of creation and annihilationlike variables, restricting also in this way the freedom available in their choice. If one were to continue with this procedure, lowering more and more the asymptotic order, one would restrict more and more the choice of fermionic variables, with the hope that one would arrive at a unique choice, perhaps up to certain phases, in the limit of a complete asymptotic diagonalization of $\breve{H}_D$. Inspired by the analysis of Refs. [25,26], we adopt for $f_1^{\vec{k},(x,y)}$ the following asymptotic series expansion in inverse powers of ω_k:

[1]As in that reference, we now ignore the possible zero mode of the Dirac field, assuming that we can find a suitable representation for it. This is not important in our discussion, because we focus it on the ultraviolet sector of the field.

$$f_1^{\vec{k},(x,y)} = e^{iF_2^{\vec{k},(x,y)}} \sum_{n=1}^{\infty} \frac{(-i)^{n+1}\gamma_n}{\omega_k^n}, \tag{4.1}$$

with $\gamma_n \in \mathbb{R}$. From the first relation in Eq. (3.2), it then follows that, asymptotically,

$$f_2^{\vec{k},(x,y)} = e^{iF_2^{\vec{k},(x,y)}} \sum_{n=0}^{\infty} \frac{(-i)^{n}\tilde{\gamma}_n}{\omega_k^n}, \tag{4.2}$$

with $\tilde{\gamma}_n \in \mathbb{R}$ again, and where the coefficients $\tilde{\gamma}_n$ are defined as

$$\begin{aligned} &\tilde{\gamma}_0 = 1, \qquad \tilde{\gamma}_{2n-1} = 0, \\ &\tilde{\gamma}_{2n} = (-1)^{n+1}\left[\frac{1}{2}\Gamma_{2n} + \sum_{m=2}^{\infty}\frac{(2m-3)!!}{(2^m)m!} \right. \\ &\qquad \left. \times \sum_{i_{m-1}=1}^{n} \dots \sum_{i_1=1}^{i_2} \Gamma_{2n-2i_{m-1}} \dots \Gamma_{2i_1}\right], \qquad \forall n \geq 1, \end{aligned} \tag{4.3}$$

with

$$\Gamma_0 = 0, \quad \Gamma_{2n} = \sum_{i=1}^{2n} (-1)^{n+i}\gamma_i\gamma_{2n-i}, \quad \forall\ n \geq 1, \tag{4.4}$$

and we set $\gamma_0 = 0$.

Substituting these series in the formula for the interaction coefficient $h_I^{\vec{k},(x,y)}$ of $\breve{H}_D$, one finds that

$$h_I^{\vec{k},(x,y)} = e^{-i(J_{\vec{k}}^{(x,y)} - 2F_2^{\vec{k},(x,y)})} \sum_{n=0}^{\infty} \left(\frac{-i}{\omega_k}\right)^n A_{n,0}, \tag{4.5}$$

where

$$\begin{aligned} A_{n,m} = \sum_{l=m}^{n} [&\tilde{\gamma}_{n-l}\partial\gamma_l - \gamma_l\partial\tilde{\gamma}_{n-l} - 2e^{-\alpha}\tilde{\gamma}_l\gamma_{n+1-l} \\ &- \tilde{M}(\gamma_l\gamma_{n-l} + \tilde{\gamma}_l\tilde{\gamma}_{n-l})], \qquad n \geq m, \end{aligned} \tag{4.6}$$

$$A_{n,m} = 0, \qquad n < m. \tag{4.7}$$

It follows that an asymptotic diagonalization of the fermionic contribution to the zero mode of the Hamiltonian constraint is achieved if and only if $A_{n,0} = 0$ for all $n \geq 0$. On the other hand, notice that, if we keep $n \geq 0$ in the formula that gives the coefficients $A_{n,m}$, namely Eq. (4.6), γ_{n+1} only appears in the case with $m = 0$, when one evaluates the contribution corresponding to vanishing label l. In addition, the sum that determines $A_{n,0}$ in Eq. (4.6) can be rewritten as the mentioned contribution with label $l = 0$ plus $A_{n,1}$. With these indications, one can easily deduce that $A_{n,0} = 0$ implies the recursive relation

$$\gamma_{n+1} = -\frac{\tilde{M}e^{\alpha}}{2}\tilde{\gamma}_n + \frac{e^{\alpha}}{2}A_{n,1}. \tag{4.8}$$

Since $\tilde{\gamma}_0 = 1$, the above relation gives us, in particular, the first term of the series (4.1), $\gamma_1 = -\frac{1}{2}\tilde{M}e^{\alpha}$, from which we can univocally obtain the rest of the unknown terms. This is possible because $\tilde{\gamma}_n$ is completely determined via Eq. (4.3) by γ_m with $m \leq n$, and the nonvanishing coefficients $A_{n,1}$ only involve contributions of $\tilde{\gamma}_m$ with $m \leq n$. For instance, a straightforward calculation shows that $\gamma_2 = -\frac{1}{4}e^{-\alpha}\tilde{M}\pi_\alpha$. Thus

$$f_1^{\vec{k},(x,y)} = e^{iF_2^{\vec{k},(x,y)}} \frac{\tilde{M}e^{\alpha}}{2\omega_k} - ie^{iF_2^{\vec{k},(x,y)}} \frac{\tilde{M}e^{-\alpha}}{4\omega_k^2}\pi_\alpha + \mathcal{O}(\omega_k^{-3}), \tag{4.9}$$

an equation that of course is consistent with the previous results of Refs. [20,25].

The asymptotic form of $f_1^{\vec{k},(x,y)}$ severely restricts our choice of creation and annihilationlike variables, leaving all the asymptotic freedom just in the phases $F_2^{\vec{k},(x,y)}$ and $J_{\vec{k}}^{(x,y)}$. With this choice, or rather with this iterative family of choices, we can make the interaction terms $h_I^{\vec{k},(x,y)}$ vanish in the fermionic Hamiltonian at any desired asymptotic order in inverse powers of ω_k.

Let us consider now the rest of fermionic contributions to the zero mode of the Hamiltonian constraint, namely the diagonal fermionic terms. It is convenient to define

$$\begin{aligned} \tilde{f}_1^{\vec{k},(x,y)} &= e^{-iF_2^{\vec{k},(x,y)}} f_1^{\vec{k},(x,y)}, \\ \tilde{f}_2^{\vec{k},(x,y)} &= e^{-iF_2^{\vec{k},(x,y)}} f_2^{\vec{k},(x,y)}, \end{aligned} \tag{4.10}$$

so that

$$\begin{aligned} h_D^{\vec{k},(x,y)} = \Re\Bigg[&\frac{e^{-\alpha}\omega_k}{2}\left(\left|\tilde{f}_2^{\vec{k},(x,y)}\right|^2 - \left|\tilde{f}_1^{\vec{k},(x,y)}\right|^2\right) + \tilde{M}\tilde{f}_1^{\vec{k},(x,y)}\bar{\tilde{f}}_2 \\ &- \frac{i}{2}\left(\bar{\tilde{f}}_1\partial\tilde{f}_1^{\vec{k},(x,y)} + \bar{\tilde{f}}_2\partial\tilde{f}_2^{\vec{k},(x,y)}\right)\Bigg] + \frac{1}{2}\partial F_2^{\vec{k},(x,y)}. \end{aligned} \tag{4.11}$$

Here, we have used that the functions $h_D^{\vec{k},(x,y)}$ are always real.[2] In what follows, we restrict the complex phase $F_2^{\vec{k},(x,y)}$ so that these functions (which provide diagonal fermionic contributions to the Hamiltonian constraint) do not depend on the momentum π_ϕ of the homogeneous inflaton. Notice that the only part in this constraint that contains the coefficients γ_n and $\tilde{\gamma}_n$ is given by

[2]The only term for which this is not obvious is $-i(f_1^{\vec{k},(x,y)} \times \partial\bar{f}_1^{\vec{k},(x,y)} + f_2^{\vec{k},(x,y)}\partial\bar{f}_2^{\vec{k},(x,y)})$. But since $|f_1^{\vec{k},(x,y)}|^2 + |f_2^{\vec{k},(x,y)}|^2 = 1$, the term in parenthesis is indeed imaginary.

$$\check{h}_D^{\vec{k},(x,y)} = h_D^{\vec{k},(x,y)} - \frac{1}{2}\partial F_2^{\vec{k},(x,y)}, \tag{4.12}$$

which, with our asymptotic expansions, takes the specific form

$$\check{h}_D^{\vec{k},(x,y)} = \sum_{n=-1}^{\infty} \frac{\check{\gamma}_n}{\omega_k^n}. \tag{4.13}$$

Finally, a direct calculation shows that the coefficients $\check{\gamma}_n$ turn out to be

$$\check{\gamma}_{-1} = \frac{e^{-\alpha}}{2}, \tag{4.14}$$

$$\check{\gamma}_n = \Re(i^{n+1}) \sum_{l=0}^{n} \left[\frac{(-1)^l}{2} (2\tilde{M}\tilde{\gamma}_l \gamma_{n-l} - 2e^{-\alpha}\gamma_{n+1-l}\gamma_l + \gamma_l \partial\gamma_{n-l} + \tilde{\gamma}_l \partial\tilde{\gamma}_{n-l}) \right], \quad \forall n \geq 0. \tag{4.15}$$

V. HYBRID QUANTIZATION

The results of the previous sections restrict in a physically appealing way the choice of canonical variables for the homogeneous and fermionic parts of the phase space of our truncated cosmology. These canonical variables are the homogeneous pairs (α, π_α) and (ϕ, π_ϕ), and the fermionic annihilation and creationlike variables for particles, $\{(a_{\vec{k}}^{(x,y)}, \bar{a}_{\vec{k}}^{(x,y)})\}_{\vec{k}\neq 0}$, and for antiparticles $\{(b_{\vec{k}}^{(x,y)}, \bar{b}_{\vec{k}}^{(x,y)})\}_{\vec{k}\neq 0}$, all of them determined by relations (3.1)–(3.4). In particular, the homogeneous variables have been defined so that they commute under Poisson brackets with the fermionic variables at our order of perturbative truncation. We have seen that, with asymptotic expansions of the form (4.1) and (4.2), the interaction terms in the fermionic contribution to the zero mode of the Hamiltonian constraint can be rendered as negligible as desired in the ultraviolet sector of large wave numbers. Then, if one decides to restrict all considerations to the context of a fermionic field in linearized cosmology, namely if one ignores the quadratic fermionic backreaction on the classical dynamics of the homogeneous variables, the evolution of the introduced annihilation and creationlike variables becomes asymptotically diagonal. In this respect, the important result is that this diagonalization serves as a valid criterion to select canonical variables for the fermionic degrees of freedom, characterizing them on the entire phase space of our cosmological system. Remarkably, nonetheless, the benefits of using this type of fermionic annihilation and creationlike variables lie beyond the linearized context that we have just commented on. Indeed, their definition is compatible with that of the homogeneous variables in our search for a canonical set, and the resulting expression for the Hamiltonian constraint (at the considered truncation order) asymptotically displays only quadratic combinations of these fermionic variables in a way that is proportional to the number operator, once one adopts a Fock representation with normal ordering. This fact simplifies enormously the task of finding a quantum representation of the constraint operator not just for the fermions, but for the combined system that includes the homogenous variables within the framework of hybrid quantum cosmology. Moreover, as it was argued in Refs. [25,26] and we discuss in this section, there exist quantum states of the entire cosmology such that the resolution of the quantum constraint in a sort of Born-Oppenheimer approximation amounts to the condition that the fermionic part of their wave functions solves a Schrödinger equation. This is similar to the situation found in linearized cosmology, with the very important difference that in our treatment the homogeneous background does not need to correspond to a classical solution or even to an effective trajectory. Rather, the dependence of the linear fermionic equations on this background is given by expectation values of geometric operators in the part of the wave function that describes the homogeneous geometry and, as we have pointed out, in principle it is not necessary that these expectation values evolve as in general relativity or according to any effective dynamics.

In order to proceed to the hybrid quantization of the system, with its phase space already split into different sectors in the way that we have explained, we choose suitable representations for each of those sectors and represent the total system on the tensor product of the partial representation spaces. For the FLRW geometry, corrected with quadratic perturbative contributions according to our comments, we pick out a representation inspired in LQG and specified in Ref. [37] (see also Refs. [38,39]). Therefore, instead of using the canonical variables $\{\alpha, \pi_\alpha\}$ we employ the alternative variable v, proportional to the physical volume of the spatial sections of our cosmological model, together with its canonical momentum $b/2$, which is proportional to the Hubble parameter [40]. More specifically, we have that $|v| = [16\pi/(27 l_0^3 \gamma^2 \Delta_g)]^{3/2} e^{3\alpha}$, where γ is called the Immirzi parameter [41] and Δ_g is the area gap (the minimum allowed nonzero eigenvalue of the area operator in LQG [39]). The sign of v depends on the triad orientation. In addition, the physical spatial volume is $V = 2\pi\gamma\Delta_g^{1/2}|v|$. The new variables v and b contain all the relevant information about the triad and the holonomies of the Asthekar-Barbero connection of the flat FLRW cosmology, within the improved dynamics scheme put forward in Ref. [39]. While fluxes of the triad are functions of the volume v, the interesting holonomies have elements that are complex exponentials of $\pm b/2$. The corresponding Hilbert space $\mathcal{H}_{\text{kin}}^{\text{grav}}$ where the FLRW geometry is represented admits a basis of eigenstates of the volume, provided with the discrete inner product. For each of the states of this basis, the basic holonomy elements simply shift by one the eigenvalue of v. On the other hand, for the homogeneous scalar field we choose the much simpler space of square-integrable functions over the real line, $\mathcal{L}^2(\mathbb{R}, d\phi)$, as the Hilbert space for a standard Schrödinger representation, with canonical variables $\{\phi, \pi_\phi\}$.

For the quantum representation of the gauge-invariant scalar and tensor perturbations, including their contribution to the zero mode of the Hamiltonian constraint, we adopt suitable Fock representations (for more details, see Refs. [29,30,42]). As for the quantum implementation of the linear perturbative constraints, essentially what they imply is that the physical states do not depend on perturbative gauge degrees of freedom. Finally, for the fermionic degrees of freedom, we choose a Fock representation $\mathcal{F}_D$ associated with creation and annihilationlike variables that have an asymptotic behavior in the sector of large ω_k determined by our previous considerations, and hence given by Eqs. (3.2), (4.1), (4.2), and (4.8). These annihilationlike variables are promoted to the annihilation operators $\hat{a}^{(x,y)}_{\vec{k}}$ and $\hat{b}^{(x,y)}_{\vec{k}}$ for particle and antiparticle excitations, respectively, while the creationlike variables are represented by the adjoints of these operators. In the following, we denote this adjoint operation with a dagger.

The complete system formed by all the sectors is subject to the zero mode of the Hamiltonian constraint, which we represent quantum mechanically with some extra prescriptions, additional to the ones fixed by the representation of the elementary variables. In particular, we adopt normal ordering for the products of creation and annihilation operators. The rest of the prescriptions refer to the representations of the functions of the FLRW geometry that appear as coefficients of the quadratic perturbative contributions to the constraint. Since we do not need them explicitly in the rest of our discussion, we refer the reader to Refs. [26,42] for details about these prescriptions.

We impose the zero mode of the Hamiltonian constraint *à la* Dirac [43], with physical states annihilated by its (adjoint) action. Following the strategy of Refs. [26,29,42], we choose an ansatz with separation of variables: The wave functions of the physical states of interest factorize into partial wave functions that depend each on a different sector of the system, namely the FLRW geometry, the gauge-invariant scalar and tensor perturbations, and the fermionic perturbations. We allow that all these partial wave functions depend on the inflaton, which in this way will play the role of a relational time. Additionally, we ask that the part of the wave function that contains the geometric degrees of freedom, which we call $\Gamma(V, \phi)$, is normalized (in the discrete inner product for the volume) and has a unitary evolution in ϕ generated by a positive operator $\hat{\tilde{\mathcal{H}}}_0$, so that

$$-i\partial_\phi \Gamma(V, \phi) = \hat{\tilde{\mathcal{H}}}_0 \Gamma(V, \phi). \tag{5.1}$$

Finally, we restrict our attention to generators for which the action of $\partial_\phi^2 + \hat{\tilde{\mathcal{H}}}_0^2$ on Γ differs from the corresponding action of the constraint of the unperturbed FLRW cosmology at most in a quadratic contribution of the perturbations. In this way, we contemplate the possibility that there exists some kind of quantum backreaction between the perturbations and the homogeneous background.

Furthermore, if we can ignore the transition between states of the FLRW geometry that are mediated by the action of our Hamiltonian constraint, all relevant information about this constraint can be captured by replacing its operator dependence on the homogeneous geometry with expectation values $\langle \cdot \rangle_\Gamma$ on the considered state Γ in $\mathcal{H}^{\text{grav}}_{\text{kin}}$, computed with the discrete inner product. With this approximatiaon and a kind of Born-Oppenheimer one, the imposition of the entire Hamiltonian constraint leads in fact to a set of Schrödinger equations, one for each of the different perturbative sectors of the system [26,29]. For the partial wave function that depends on the fermionic degrees of freedom, which we call $\psi(\mathcal{N}_D, \phi)$,[3] we arrive at the equation

$$\begin{aligned} -i\partial_\phi \psi_D(\mathcal{N}_D, \phi) &= \frac{l_0 \langle \widehat{V^{2/3} e^\alpha \check{H}_D} \rangle_\Gamma - C_D^{(\Gamma)}}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} \psi_D(\mathcal{N}_D, \phi) \\ &\equiv \mathcal{H}_D^{(\Gamma)}(\phi) \psi_D(\mathcal{N}_D, \phi). \end{aligned} \tag{5.2}$$

Here, the hat above a function of the FLRW geometry stands for its representation as a quantum operator. Besides, we have defined $\mathcal{H}_D^{(\Gamma)}(\phi)$, which can be regarded as a time-dependent (i.e., ϕ-dependent) effective fermionic Hamiltonian operator that acts on $\mathcal{F}_D$ and generates the Schrödinger evolution. On the other hand, the term $C_D^{(\Gamma)}$, plus some similar terms in the Schrödinger equations of the gauge-invariant scalar and tensor perturbations, equals the expectation value in Γ of the difference between the action of $\partial_\phi^2 + \hat{\tilde{\mathcal{H}}}_0^2$ and the action of the Hamiltonian constraint of the unperturbed model. It is in this sense that we can call $C_D^{(\Gamma)}$ the fermionic backreaction, as it measures, in average, how much the homogeneous part Γ of the solutions of the perturbed model departs from an unperturbed solution [25,26].

Let us now introduce a change to the time,

$$d\eta_\Gamma = \frac{l_0 \langle \hat{V}^{2/3} \rangle_\Gamma}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} d\phi, \tag{5.3}$$

which is well defined because $\tilde{\mathcal{H}}_0$ is positive and $\hat{V}$ has a strictly positive lower bound (at least in the adopted representation: see Ref. [37]). It should be noted that, if we further restrict $\Gamma(V, \phi)$ to be highly peaked on classical

[3]We use $\mathcal{N}_D$ as an abstract notation for the occupation numbers of the fermionic particles and antiparticles in the chosen Fock representation.

or effective trajectories, this time coincides (up to corrections that are quadratic in perturbations) with the standard conformal time in cosmology as far as we circumscribe it within an interval where the inflaton is monotonic. Nonetheless, our definition of η_Γ is perfectly consistent in the quantum theory beyond such a classical or effective regime, provided that the involved expectation values remain strictly positive and finite. In this sense, η_Γ may be regarded as a relational time for the different parts of the wave function, and one should only attempt to find a correspondence with a standard conformal time within regimes and intervals of the type that we have commented.

Using then Eq. (5.2) and the definition of our creation and annihilationlike variables, we obtain the following Heisenberg relations (in the considered asymptotic regime of large ω_k), evaluated at $\eta_\Gamma = \eta$,

$$d_{\eta_\Gamma}\hat{a}_{\vec{k}}^{(x,y)}(\eta,\eta_0) = -iF_{\vec{k}}^{(\Gamma)}\hat{a}_{\vec{k}}^{(x,y)}(\eta,\eta_0),$$
$$d_{\eta_\Gamma}\hat{b}_{\vec{k}}^{\dagger(x,y)}(\eta,\eta_0) = i(F_{\vec{k}}^{(\Gamma)} + J_{\vec{k}}^{(\Gamma)})\hat{b}_{\vec{k}}^{\dagger(x,y)}(\eta,\eta_0), \quad (5.4)$$

where we have called

$$F_{\vec{k}}^{(\Gamma)} = \frac{2\langle \widehat{V^{2/3}e^{\alpha}h_D^{\vec{k},(x,y)}}\rangle_\Gamma}{\langle \hat{V}^{2/3}\rangle_\Gamma},$$
$$J_{\vec{k}}^{(\Gamma)} = \frac{2\langle \widehat{V^{2/3}e^{\alpha}h_J^{\vec{k},(x,y)}}\rangle_\Gamma}{\langle \hat{V}^{2/3}\rangle_\Gamma}. \quad (5.5)$$

We can integrate these Heisenberg equations to obtain, asymptotically, the following Bogoliubov transformation,

$$\hat{a}_{\vec{k}}^{(x,y)}(\eta,\eta_0) = e^{-iF_{\eta,\vec{k}}^{(\Gamma)}}\hat{a}^{(x,y)},$$
$$\hat{b}_{\vec{k}}^{\dagger(x,y)}(\eta,\eta_0) = e^{i\left(F_{\eta,\vec{k}}^{(\Gamma)}+J_{\eta,\vec{k}}^{(\Gamma)}\right)}\hat{b}^{\dagger(x,y)}, \quad (5.6)$$

where we have defined $\hat{a}_{\vec{k}}^{(x,y)}(\eta_0) = \hat{a}_{\vec{k}}^{(x,y)}$, $\hat{b}_{\vec{k}}^{\dagger(x,y)}(\eta_0) = \hat{b}_{\vec{k}}^{\dagger(x,y)}$ and

$$F_{\eta,\vec{k}}^{(\Gamma)} = \int_{\eta_0}^{\eta} F_{\vec{k}}^{(\Gamma)} d\eta_\Gamma, \qquad J_{\eta,\vec{k}}^{(\Gamma)} = \int_{\eta_0}^{\eta} J_{\vec{k}}^{(\Gamma)} d\eta_\Gamma. \quad (5.7)$$

This Bogoliubov transformation is clearly unitary [44], because it does not mix creation and annihilation operators in the considered asymptotic region, so that the antilinear part of the transformation vanishes asymptotically (or, more precisely, can be made of an asymptotic order as negligible as desired).

Finally, we can construct an operator $\hat{T}$ defined as

$$\hat{T} = \sum_{\vec{k},(x,y)} \hat{T}_{\vec{k}}^{(x,y)},$$
$$\hat{T}_{\vec{k}}^{(x,y)} = iF_{\eta,\vec{k}}^{(\Gamma)}(\hat{a}_{\vec{k}}^{\dagger(x,y)}\hat{a}_{\vec{k}}^{(x,y)} + \hat{b}_{\vec{k}}^{\dagger(x,y)}\hat{b}_{\vec{k}}^{(x,y)}) + iJ_{\eta,\vec{k}}^{(\Gamma)}(\hat{b}_{\vec{k}}^{\dagger(x,y)}\hat{b}_{\vec{k}}^{(x,y)}), \quad (5.8)$$

such that in the regime of large ω_k,

$$e^{\hat{T}}\hat{a}_{\vec{k}}^{(x,y)}e^{-\hat{T}} = \hat{a}_{\vec{k}}^{(x,y)}(\eta,\eta_0), \quad (5.9)$$

$$e^{\hat{T}}\hat{b}_{\vec{k}}^{\dagger(x,y)}e^{-\hat{T}} = \hat{b}_{\vec{k}}^{\dagger(x,y)}(\eta,\eta_0), \quad (5.10)$$

as can be checked using Hadamard's lemma [45]. Hence, $e^{-\hat{T}}$ can be taken as the unitary operator that implements the dynamical Bogoliubov transformation (5.6).

This confirms that, asymptotically, the vacuum (namely the normalized state in the kernel of all the annihilation operators) is stationary under the evolution dictated by this operator. In turn, this implies that the vacuum is annihilated by the left-hand side of Eq. (5.2), up to possibly the contribution of a complex phase. And, since we adopted normal ordering for the representation of the zero mode of the Hamiltonian constraint, the first term of the right-hand side of Eq. (5.2) annihilates the vacuum as well. Hence, with our choice of Fock representation, the fermionic backreaction $C_D^{(\Gamma)}$ for the vacuum (which was only convergent in Ref. [26] after a subtraction of infinities scheme) is not only finite now, but indeed can straightforwardly be set to vanish, at least asymptotically. In this way, the vacuum remains invariant in the evolution. Then, it is clear that its image under the action of the fermionic Hamiltonian is a normalizable state in $\mathcal{F}_D$. As a consequence, we conclude that the fermionic Hamiltonian is properly defined in the dense subset of $\mathcal{F}_D$ spanned by the n-particle/antiparticle states with a finite number of fermionic excitations.

VI. CONCLUSIONS

We have investigated the choice of a vacuum for the Dirac field in an inflationary flat FLRW spacetime by suplementing with extra physical requirements the criterion of invariance under spatial symmetries and unitary Heisenberg evolution that has been explored in the literature recently. More specifically, the additional requirement that we have considered is the diagonalization of the fermionic contribution to the Hamiltonian constraint of the gravitational system when the fermions are treated as perturbative fields on an average (possibly quantum mechanically dressed) background, in the asymptotic regime of large wave numbers, that we identify with the eigenvalues of the Dirac operator on the spatial sections of the cosmology. While the original criterion of spatial symmetry invariance and dynamical unitarity leads to a family of Fock representations that are unitarily equivalent among them, but still leaving an infinite freedom in the choice of a vacuum, the inclusion of the diagonalization requirement has been shown to restrict the available freedom to the choice of two complex phases and terms that are negligible at any desired order in an expansion in inverse powers of the wave number.

In our analysis, we have truncated the Einstein-Dirac action, also in the presence of a scalar field that plays the role of an inflaton, at quadratic order in perturbations, treating as such the nonzero Fourier modes of the metric and the scalar field and all the contributions of the Dirac field. The zero modes of the inflaton and the metric have been treated exactly. Because of this, the action does not get contributions that are linear in our perturbations, including those of the lapse and the shift (actually, this statement holds beyond our quadratic truncation, in higher-order perturbative schemes). Apart from linear perturbative constraints, the system is subject to the zero mode of the Hamiltonian constraint, which contains a term that is formally identical to the global Hamiltonian constraint of the unperturbed model, but in addition includes other contributions that are quadratic in the perturbations, in particular a fermionic term. These perturbations can be described by (an Abelianized version of) the linear perturbative constraints, gauge variables that are momenta of those constraints, and gauge invariants that commute with all the former quantities. For the metric and the inflaton, one can choose as gauge invariants the Mukhanov-Sasaki field and the tensor perturbations, together with their canonical momenta. The fermionic perturbations, on the other hand, are immediately gauge invariants, because the Einstein-Dirac action is quadratic in the Dirac field, so that the latter couples directly to the unperturbed tetrad when we truncate the action in our scheme. The above set of perturbative variables can be completed into a canonical set for the whole system, at the considered truncation order, by including zero modes that are suitably corrected with quadratic perturbative terms [29].

Focusing our discussion on the fermionic sector of the inhomogeneities, one still has considerable liberty in the way in which one can separate the fermionic degrees of freedom from those of the homogeneous background through canonical transformations, with a splitting that maintains the gauge-invariant character of the fermionic variables. Different splittings of the fermionic and the zero-mode sectors of phase space result in different quantum behaviors for the combined system and different quantum dynamics for the fermionic variables, since the separation amounts to a background-dependent (and hence dynamical) redefinition of the basic, creation, and annihilationlike fermionic variables. Instead of regarding this ambiguity as a complication, we have taken advantage of it and looked for a choice of those creation and annihilationlike variables such that the part of the Hamiltonian constraint that rules their evolution has good physical properties. In order to do this, we have considered all possible linear combinations of the fermionic mode coefficients that define creation and annihilationlike variables, allowing these combinations to depend on zero modes. Among all the viable combinations that do not mix fermionic modes, and therefore respect the spatial symmetries of the model, we have then sought for choices that lead to a especially simple fermionic Hamiltonian, without interaction terms that would create and destroy pairs of particles and antiparticles (at least in the ultraviolet sector of large wave numbers). The absence of these interactions amounts to the (asymptotic) diagonalization of the fermionic contribution to the zero mode of the Hamiltonian constraint. We have shown that it is possible to attain this diagonalization at any asymptotic order in inverse powers of the wave number, and that the resulting characterization of fermionic variables is unique up to certain phases at that order and up to terms that are negligible in the asymptotic series of the coefficients that define the creation and annihilationlike variables.

Combining then this Fock representation for the Dirac field, suitable Fock representations for the rest of gauge invariants, and an LQG-inspired quantization for the homogeneous sector, we have considered the hybrid quantization of the system. Given our choice of fermionic creation and annihilation variables, the Fock representation determined by them has a considerably simple quantum dynamics. We have shown this in detail by adopting an ansatz with separation of variables for the physical wave functions and introducing a kind of Born-Oppenheimer approximation in which we neglected changes in the FLRW geometry mediated by the zero mode of the Hamiltonian constraint. The relevant information about this constraint is then captured in its expectation value on the partial wave function that describes the background FLRW cosmology. In this manner, one obtains a Schrödinger equation for the fermionic degrees of freedom that, with our (asymptotic) choice of vacuum, leads to Heisenberg equations that do not mix the creation and annihilation operators of the particles and antiparticles. Thus, the dynamical Bogoliubov transformation of these operators can be implemented trivially as a quantum unitary transformation in the discussed asymptotic regime, because its antilinear part can be made equal to 0 at any desired asymptotic order. We also have constructed an evolution operator that implements this Bogoliubov transformation, and checked that it leaves the vacuum stationary. This property and the fact that the fermionic contribution to the zero mode of the Hamiltonian constraint annihilates the vacuum guarantee that the backreaction term in the Schrödinger equation not only does not diverge, but can be made negligible at any asymptotic order in inverse powers of the wave number, without the need of any regularization scheme.

Let us emphasize that our choice of annihilation and creationlike variables, which leads to an asymptotically diagonal fermionic Hamiltonian, is carried out within a canonical framework that is valid for the entire, truncated, cosmology, with a phase space that describes not only the fermionic perturbations, but also the background variables. In particular, the choice provides a specific splitting between the two sectors of the cosmological system: the homogeneous one and the perturbations. Besides, since the zero mode of the Hamiltonian constraint for this entire cosmology contains a term quadratic in all of the perturbations, the classical dynamics of the selected fermionic variables is only linear if one ignores their backreaction on the homogeneous sector. Nevertheless, the resulting Hamiltonian constraint applies to the entire cosmology even beyond this linearized context, keeping its nice properties for quantization even in that extended scenario. Furthermore, we have seen that it is possible to reach a regime in the quantum dynamics of the entire cosmology where the fermionic wave function effectively obeys a Schrödinger equation. The *effective* Hamiltonian operator that drives this evolution actually corresponds to the Fock representation of the fermionic contribution to the constraint, but with its background dependence replaced with expectation values in the partial wave function that describes the homogeneous geometry. In this sense, the hybrid quantum theory allows for a generalized linearized regime of a fermionic field that propagates over a mean quantum background, which need not follow any classical or effective trajectory and might even allow for some backreaction effects.

Our conclusions support some aspects of a similar study under development for the case of cosmological scalar perturbations in flat FLRW cosmologies, where the requirement of Hamiltonian diagonalization appears to supplement satisfactorily the criterion of spatial symmetry invariance and unitarity of the Heisenberg evolution [46]. It would be interesting to discuss other aspects explored in that work about the properties of the selected vacuum and its relation with adiabatic states, taking into account the results that are known about such states for fermionic fields [47] and extending them with further investigations.

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Fock quantization of the Dirac field in hybrid quantum cosmology: Relation with adiabatic states

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We study the relation between the Fock representations for a Dirac field given by the adiabatic scheme and the unique family of vacua with a unitarily implementable quantum evolution that is employed in hybrid quantum cosmology. This is done in the context of a perturbed flat cosmology that, in addition, is minimally coupled to fermionic perturbations. In our description, we use a canonical formulation for the entire system, formed by the underlying cosmological spacetime and all its perturbations. After introducing an adiabatic scheme that was originally developed in the context of quantum field theory in fixed cosmological backgrounds, we find that all adiabatic states belong to the family of Fock representations that allow a unitarily implementable quantum evolution (although the converse is not generally true). In particular, this unitarity of the dynamics ensures that the vacua defined with adiabatic initial conditions at different times are unitarily equivalent. We also find that, for all adiabatic orders other than 0, these initial conditions allow the definition of annihilation and creation operators for the Dirac field that lead to some finite backreaction in the quantum Hamiltonian constraint and to a fermionic Hamiltonian operator that is properly defined in the span of the n-particle/antiparticle states, in the context of hybrid quantum cosmology.

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I. INTRODUCTION

There exists an inherent difficulty to selecting a vacuum state with acceptable physical properties for fields that propagate in generic curved spacetimes, even when one uses well-known Fock representations in their quantization [1]. This ambiguity is closely related to the fact that the notion of particle, as one defines it in quantum field theory (QFT), is nebulous even in the presence of a large number of symmetries. This problem is often overlooked in standard QFT in Minkowski spacetime because the Poincaré vacuum plays then a privileged role, directly tied up in the observation that flat spacetime is maximally symmetric [2]. In this sense, a central question in any scheme pursuing the Fock quantization of matter fields in a generic spacetime background is the specification of the physical properties that the corresponding vacuum must possess. This issue has been studied at great length for free scalar linear fields [1,3], but much less for fermionic fields, such as the Dirac field [4].

For cosmological spacetimes, a traditional line of attack to the problem of the choice of vacuum is the adiabatic proposal [5–7], which in recent times has found formal support in the algebraic approach to QFT [8]. In this approach, one chooses a series of observables and specifies the relations among them, something that includes the dynamics and the standard commutation (or anticommutation for fermionic fields) relations, in such a way that one constructs an *-algebra. A state is then a normalized positive linear functional from this *-algebra to the complex numbers, which can be interpreted as the result of taking the expectation value of the observables on a physical state. In many cases, a specific Fock representation can be recovered from each algebraic state by means of the so-called Gelfand-Naimark-Segal (GNS) construction [9,10]. A set of states that is traditionally favored in this approach is formed by the Hadamard states, which are characterized by a very specific singularity structure of their two-point function [11,12]. In particular, their associated energy-momentum tensor has good renormalizability properties. The adiabatic scheme aims to provide a strategy to approximate Hadamard states in cosmology by solving the differential equations of motion of the field in an iterative way, with the hope that, if the iteration converges, one would obtain in the end a true Hadamard

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state. Actually, for scalar fields propagating in standard Friedmann-Lemaitre-Robertson-Walker (FLRW) cosmologies it turns out that all adiabatic states are locally quasiequivalent to a Hadamard state [13,14]. The complications that arise in this scheme are well known in the case of scalar fields in cosmological backgrounds, as the iterative relations may not converge for general cosmological evolutions. For Dirac fields in cosmological spacetimes, a similar level of consensus on the definition of adiabatic states and their properties has not been reached [15–18].

Over the last decade, an alternative strategy has been put forward in order to reduce the ambiguities in the choice of a vacuum for fields in cosmological spacetimes [19,20]. In addition to symmetry considerations, this strategy rests primarily on the criterion that the annihilation and creation operators of the Fock quantization display an evolution that is unitarily implementable. This criterion has been shown to select a unique family of vacua, related to each other by unitary transformations, on a multitude of cosmological scenarios [21–24], including the case of Dirac fields in a flat FLRW cosmology [25]. Actually, this criterion is, in turn, motivated in the context of quantum cosmology by the so-called hybrid approach to the quantization of inhomogeneous systems [26,27], which is based on a splitting of the phase space into a homogeneous sector and an inhomogeneous sector, in a way that is specially suitable to obtain a well-behaved dynamics for the complete cosmology. Then, one quantizes the inhomogeneous degrees of freedom (d.o.f.) employing a Fock representation with nice ultraviolet properties, and the homogeneous geometry with techniques inspired by a certain canonical approach to quantum cosmology (for instance, the formalism known as loop quantum cosmology [28], inspired by loop quantum gravity [29]). In this context, one can actually restrict the choice of the Fock vacuum even more, exploiting the freedom allowed by the hybrid approach in a way to split the d.o.f. into the homogeneous and inhomogenous sectors that are to be quantized. Indeed, this was first done for fermionic perturbations in inflationary cosmologies [30] in an attempt to find a representation such that some kind of quantum backreaction on the homogeneous cosmological sector remains finite without the need of a regularization scheme, and that one gets a Hamiltonian constraint that is properly defined on the dense set of the Fock space spanned by the n-particle/antiparticle states [31]. Additionally, it is possible to further refine the description of the inflationary cosmology and arrive at a recurrence relation by which the dynamics of the annihilation and creation operators that describe the fermionic, scalar, and tensor perturbations become diagonal in the asymptotic limit of infinitely large particle/antiparticle wave numbers [32,33].

This paper aims to bridge the gap between the two schemes commented above for the choice of a Fock vacuum in the case of a Dirac field minimally coupled to a flat FLRW cosmology with compact hypersurfaces. For that, we adapt the adiabatic scheme for the fermionic field presented in the Dirac representation in Ref. [17], inspired in turn by Ref. [18], to the Weyl representation employed so far in hybrid quantum cosmology. We compare these adiabatic vacua with those of the family of unitarily equivalent Fock representations that arise from the annihilation and creation operators defined in hybrid quantum cosmology, restricted to the context of QFT in curved spacetimes. The fundamental result that we obtain is that all adiabatic states belong in fact to this equivalence family, and that, for adiabatic orders greater than 0, they allow the definition of annihilation and creation operators in hybrid quantum cosmology that produce finite backreaction terms in the Hamiltonian constraint and give rise to a properly defined Hamiltonian operator. Furthermore, in the context of QFT, the unitary implementability of the dynamics in such Fock quantizations guarantees that the states constructed with adiabatic initial conditions at different times of the cosmological evolution are all unitarily related. Finally, in the appendix, we briefly analyze the adiabatic approach proposed by Hollands in Ref. [16] from an algebraic perspective, and argue that there generally exist obstructions for its implementation to define Fock vacua.

The structure of this paper is organized as follows. In Sec. II we introduce the physical model, which consists of a Dirac field treated as a perturbation around a flat, inflationary FLRW cosmology, and then we summarize the main properties of the choices of annihilation and creation operators for the quantization of this fermionic field in the hybrid approach. In Sec. III we apply the adiabatic scheme to fermions in the Weyl representation. Section IV is devoted to the comparison of these adiabatic states with those associated with the choices of annihilation and creation operators selected in hybrid quantum cosmology. We show that all the adiabatic states determine Fock representations that are unitarily equivalent to those of the hybrid quantization. We summarize our conclusions in Sec. V. The obstructions found in the adiabatic scheme of Ref. [16] are discussed in the appendix. Throughout the paper, we employ units such that $\hbar = c = G = 1$.

II. PHYSICAL SYSTEM AND PROPERTIES OF THE QUANTIZATION

Let us start by describing the spatially homogeneous part of our system. We consider a flat FLRW spacetime geometry specified by a scale factor $\tilde{a}$. The spatial sections that foliate this cosmology are compact and isomorphic to the three-dimensional torus T^3. As the matter content that fuels the dynamics of this cosmological geometry, we minimally couple a homogeneous scalar field (inflaton) $\tilde{\phi}$ subject to a potential $V(\tilde{\phi})$.

In this cosmological model, we include a Dirac field with mass M that is treated entirely as a perturbation (including its homogeneous component, if there is one). In order to obtain a satisfactory Hamiltonian formulation of the entire system, and contemplate the possibility of making canonical transformations that mix the homogeneous and fermionic sectors, we truncate the action at quadratic order in these perturbations [30,34]. One may also include perturbations (of the same magnitude) of the spacetime metric and the inflaton field, describing small anisotropies and inhomogeneities. Nonetheless, we obviate them in our analysis because, at the considered order of truncation, they do not couple to the fermionic contribution that we want to study. The truncated perturbative action supplies the canonical structure and the constraints needed to construct a Hamiltonian description of the whole system.

To work with the Dirac field, we use the Weyl representation of the constant generators γ^b, $b = 0, \ldots, 3$, of the Clifford algebra associated with the four-dimensional Minkowski metric, namely,

$$\gamma^0 = i\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad \vec{\gamma} = i\begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \tag{2.1}$$

where I is the two-dimensional identity matrix, $\vec{\gamma} = (\gamma^1, \gamma^2, \gamma^3)$, and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the tuple formed by the three Pauli matrices. After imposing the time gauge on the tetrad of the homogeneous cosmology (so that the corresponding triad has no internal time components [30]), we rescale the Dirac field by $\tilde{a}^{3/2}$ in order to get constant Dirac brackets between this field and its complex conjugate. In addition, we exploit the symmetries of the homogeneous spatial sections of the cosmological spacetime by expanding each of the two chiral components of the fermionic field in a complete set of eigenespinors of the Dirac operator $-i\vec{\sigma}\vec{\nabla}$ on T^3. These eigenspinors can be divided into two subsets according to their helicity, with label $\lambda = \pm 1$. Since the torus is compact, the spectrum of the Dirac operator is discrete, with eigenvalues $\lambda\omega_k$, where $\omega_k = 2\pi|\vec{k} + \vec{\tau}|/l_0$, $\vec{k} \in \mathbb{Z}^3$, $2\vec{\tau}$ can be any of the vertices of the unit cube and characterizes the spin structure, and l_0 is the compactification length of the torus. The eigenspinor associated with $\lambda\omega_k$ has the form (adopting a diagonal fiducial coordinate system)

$$\xi_\lambda(\vec{k}) \exp{[i2\pi(\vec{k} + \vec{\tau})\vec{x}/l_0]},$$

where $\vec{x}$ are the spatial coordinates on the torus. The bispinor $\xi_\lambda(\vec{k})$ is normalized so that $\xi_\lambda^\dagger \xi_\lambda = 1$. The rescaled Dirac field can then be described by its left-handed and right-handed time-dependent coefficients with helicity λ in an eigenspinor expansion. These coefficients can be handled as ordered pairs of Grasmann variables, respectively describing the left-handed and right-handed components of the field and, up to a constant factor $l_0^{-3/2}$, we call them $(x_{\vec{k},\lambda}, y_{\vec{k},\lambda})$. Each of these mode coefficients displays a nonvanishing Dirac bracket only with its complex conjugate, in that case being equal to $-i$.

We can then introduce annihilationlike variables $a_{\vec{k},\lambda}$ for particles and creationlike variables $\bar{b}_{\vec{k},\lambda}$ for antiparticles by means of a canonical transformation of the form [25]

$$\begin{pmatrix} a_{\vec{k},\lambda} \\ \bar{b}_{\vec{k},\lambda} \end{pmatrix} = \begin{pmatrix} f_1^{k,\lambda} & f_2^{k,\lambda} \\ g_1^{k,\lambda} & g_2^{k,\lambda} \end{pmatrix} \left[I - \frac{1-\lambda}{2}(I - \sigma_1) \right] \begin{pmatrix} x_{\vec{k},\lambda} \\ y_{\vec{k},\lambda} \end{pmatrix}. \tag{2.2}$$

We do not mix different modes of the Dirac operator and only allow mode dependence of the coefficients of the transformation through ω_k, in order to respect the spatial symmetries of the dynamics [25,32]. Besides, we ask that

$$\begin{aligned} f_2^{k,\lambda} &= e^{iF_2^{k,\lambda}} \sqrt{1 - |f_1^{k,\lambda}|^2}, \\ g_1^{k,\lambda} &= e^{iJ_{k,\lambda}} \bar{f}_2^{k,\lambda}, \\ g_2^{k,\lambda} &= -e^{iJ_{k,\lambda}} \bar{f}_1^{k,\lambda}, \end{aligned} \tag{2.3}$$

where $J_{k,\lambda}, F_2^{k,\lambda} \in \mathbb{R}$, so that each annihilation and creationlike variable only displays a nonvanishing Dirac bracket equal to $-i$ with its complex conjugate variable, giving rise in this way to standard canonical anticommutation relations for annihilation and creation operators. In our notation, the overbar indicates complex conjugation. In general, we allow for linear combinations (2.2) that depend on the homogeneous sector, so that $f_l^{k,\lambda} = f_l^{k,\lambda}(\tilde{a}, \pi_{\tilde{a}}, \tilde{\phi}, \pi_{\tilde{\phi}})$, with $l = 1$, 2 and the symbol π (labeled with a subindex) denoting canonical momenta. Following Ref. [30] (see also Ref. [35]), we can complete the above transformation of fermionic variables into a canonical transformation for the whole system, including the FLRW cosmology. For this, we must correct the homogeneous variables in order to arrive at a set $(a, \pi_a, \phi, \pi_\phi)$ that is canonical with the annihilation and creationlike variables defined in Eq. (2.2). Each of these definitions of fermionic variables can then be understood as the selection of a particular dynamical splitting of the homogeneous and fermionic d.o.f. in phase space. In fact, each splitting results in a different identification of the fermionic contribution to the zero mode of the Hamiltonian constraint [31], the only nontrivial constraint to which the system is subject. This contribution is, in general, not diagonal, by which we mean that it contains interacting terms of the sort of $a_{\vec{k},\lambda} b_{\vec{k},\lambda}$. This is especially relevant upon quantization, because a multitude of important features depend on the behavior of the nondiagonal part of the fermionic contribution to the Hamiltonian constraint in the asymptotic limit of infinitely large ω_k. Indeed, choices of canonical annihilation and creationlike variables that result in a decrease of asymptotic order for the coefficients of these interacting terms turn out to display much better physical properties.

The conclusions about of the consequences of the selection of variables for the fermionic perturbations proven in previous works [25,31,32] can be summarized as follows:

(i) After one chooses a standard convention for particles and antiparticles, the annihilation and creationlike variables undergo an evolution that is unitarily implementable in the context of QFT in a fixed FLRW cosmology if and only if, in the asymptotic limit of large ω_k [25],

$$f_1^{k,\lambda} = \frac{Ma}{2\omega_k} e^{iF_2^{k,\lambda}} + \theta^{k,\lambda}, \qquad \sum_{\vec{k}\in\mathbb{Z}^3} |\theta^{k,\lambda}|^2 < \infty. \tag{2.4}$$

This condition ensures that the interacting fermionic part of the Hamiltonian has asymptotic order $\mathcal{O}(\omega_k^{-1})$ [30]. Furthermore, all possible families of annihilation and creation operators defined by means of coefficients of the form (2.4) define unitarily equivalent Fock representations [25].

(ii) With a hybrid quantization of the entire system, it is possible to identify a quantity, interpretable as a backreaction, which appears in the quantum dynamical equation of the fermionic states and that measures the average difference between the quantum evolution of the perturbed and unperturbed cosmology. Unfortunately, this quantity generally fails to be finite. In this case, rather than regularize by performing a "substraction of infinities," one can further restrict the choice of fermionic variables (and therefore the way to split the d.o.f. in phase space) so that, asymptotically [31],

$$\theta^{k,\lambda} = -i\frac{\pi M \pi_a}{3l_0^3\omega_k^2} e^{iF_2^{k,\lambda}} + \vartheta^{k,\lambda}, \qquad \sum_{\vec{k}\in\mathbb{Z}^3} \omega_k |\vartheta^{k,\lambda}|^2 < \infty. \tag{2.5}$$

(iii) One can go one step beyond and demand that the interacting fermionic part of the Hamiltonian be square summable. This happens to be the necessary and sufficient condition for the Hamiltonian constraint to be properly defined in the dense set spanned by the n-particle/antiparticle states within Fock space, and amounts to requiring that the following sequence be summable as well [31]:

$$\{\omega_k^2 |\vartheta^{k,\lambda}|^2\}_{\vec{k}\in\mathbb{Z}^3}. \tag{2.6}$$

(iv) The last step in this improvement of the properties of the fermionic Hamiltonian upon quantization is a recursive procedure to diminish, as much as desired, the asymptotic order of its interacting part [32]. This method of "asymptotic diagonalization" restricts almost completely the choice of fermionic canonical variables in the ultraviolet regime, leaving all the possible remaining freedom in the determination of the phases $J_{k,\lambda}$ and $F_2^{k,\lambda}$. More specifically, let us start with the ansatz

$$f_1^{k,\lambda} = e^{iF_2^{k,\lambda}} \sum_{n=1}^{\infty} \frac{(-i)^{n+1}\Gamma_n}{\omega_k^n}, \qquad f_2^{k,\lambda} = e^{iF_2^{k,\lambda}} \sum_{n=0}^{\infty} \frac{(-i)^{n}\tilde{\Gamma}_n}{\omega_k^n}, \qquad \Gamma_n, \tilde{\Gamma}_n \in \mathbb{R}, \tag{2.7}$$

where $\tilde{\Gamma}_0 = 1$ and the coefficients $\tilde{\Gamma}_n = \tilde{\Gamma}_n(\Gamma_1, \ldots, \Gamma_{n-1})$ are fixed by the first condition in Eq. (2.3). Then, for any $n \geq 0$, the nondiagonal part of the Hamiltonian is of order $\mathcal{O}(\omega_k^{-n-1})$ if [32]

$$\Gamma_{n+1} = -\frac{Ma}{2}\tilde{\Gamma}_n + \frac{a}{2}\sum_{l=1}^{n}\Big[\Gamma_l\{\tilde{\Gamma}_{n-l}, H_{|0}\} - \tilde{\Gamma}_{n-l}\{\Gamma_l, H_{|0}\} - \frac{2}{a}\tilde{\Gamma}_l\Gamma_{n+1-l} - M(\Gamma_l\Gamma_{n-l} + \tilde{\Gamma}_l\tilde{\Gamma}_{n-l})\Big]. \tag{2.8}$$

In all of these results, $\{\cdot,\cdot\}$ are the Poisson brackets of our truncated system and $H_{|0}$ is the Hamiltonian constraint of the unpertubed FLRW cosmology. Recall also that M is the bare mass of the Dirac field.

III. ADIABATIC FERMIONIC STATES IN THE WEYL REPRESENTATION

In order to introduce the adiabatic scheme, we first limit our attention to situations in which the background variables are treated as classical functions of time that follow the Hamilton trajectories dictated by $H_{|0}$ (namely, by the Einstein equations in the linearized theory). In this way, we can express all of our fermionic variables in terms of a conformal time η, and work in the framework of QFT in a fixed FLRW cosmology. In addition, we restrict all considerations from now on to the trivial spin structure $\vec{\tau} = 0$, as this is the choice that can be naturally extended to the case of noncompact spatial sections, which is precisely the scenario contemplated in Ref. [17] for the construction of adiabatic states in the Dirac representation that we parallel here, although now adopting the Weyl representation. Then, given a choice of initial time η_0, any set of annihilation and creationlike variables defined by Eqs. (2.2) and (2.3) selects a decomposition of the Dirac field of the form

$$\psi(\eta,\vec{x}) = \sum_{\vec{k}\in\mathbb{Z}^3}\sum_{\lambda=\pm1}[u_{\vec{k},\lambda}(\eta,\vec{x})A_{\vec{k},\lambda} + v_{\vec{k},\lambda}(\eta,\vec{x})\bar{B}_{\vec{k},\lambda}], \tag{3.1}$$

where we have defined the annihilation and creationlike constant coefficients

$$A_{\vec{k},\lambda} = a_{\vec{k},\lambda}(\eta_0), \qquad \bar{B}_{\vec{k},\lambda} = \bar{b}_{-\vec{k},\lambda}(\eta_0), \tag{3.2}$$

and

$$u_{\vec{k},\lambda}(\eta,\vec{x}) = \frac{e^{i2\pi\vec{k}\,\vec{x}/l_0}}{\sqrt{l_0^3 a^3}} \begin{pmatrix} h^I_{k,\lambda}(\eta)\xi_\lambda(\vec{k}) \\ \lambda h^{II}_{k,\lambda}(\eta)\xi_\lambda(\vec{k}) \end{pmatrix},$$
$$v_{\vec{k},\lambda}(\eta,\vec{x}) = -e^{-iJ_{k,\lambda}(\eta_0)}\lambda\gamma^2\bar{u}_{\vec{k},\lambda}(\eta,\vec{x}). \tag{3.3}$$

The functions $(h^I_{k,\lambda}, h^{II}_{k,\lambda})$ are a basis of mode solutions of the Dirac equation, and they are normalized so that $|h^I_{k,\lambda}|^2 + |h^{II}_{k,\lambda}|^2 = 1$ (this normalization is just a consequence of the canonical anticommutation relations). Their explicit form in terms of the time-dependent coefficients that define the annihilation and creationlike variables in Eqs. (2.2) and (2.3) is not needed yet, and hence we postpone specifying it until the next section. We note that the spinors $v_{\vec{k},\lambda}$, that contain the information about antiparticles in the decomposition of the Dirac field are the charge conjugate of those that describe the particles, $u_{\vec{k},\lambda}$, only if we fix $J_{k,\lambda}(\eta_0)$ so that $v_{\vec{k},\lambda} = -\gamma^2\bar{u}_{\vec{k},\lambda}$. Although this is not necessary in principle, we choose to do so in order to maintain this charge conjugation symmetry in the selected Fock representation.

The identification of adiabatic states proposed in Ref. [17] for cosmological spacetimes was implemented in the Dirac representation of the Clifford algebra. Here we instead obtain these states in the Weyl representation following the same line of reasoning that we summarize below. Since the field ψ is a solution to the Dirac equation, the variables $(h^I_{k,\lambda}, h^{II}_{k,\lambda})$ in the decomposition (3.1)–(3.3) satisfy the Schrödinger-like equation [25]

$$i\partial_\eta \boldsymbol{h} = \boldsymbol{H}(\eta)\boldsymbol{h}, \qquad \boldsymbol{h} = \begin{pmatrix} h^I_{k,\lambda} \\ h^{II}_{k,\lambda} \end{pmatrix},$$
$$\boldsymbol{H} = \lambda \begin{pmatrix} -\omega_k & Ma \\ Ma & \omega_k \end{pmatrix}. \tag{3.4}$$

The construction of adiabatic states starts by diagonalizing the time-dependent Schrödinger Hamiltonian $\boldsymbol{H}(\eta)$. For this, one performs an explicitly time-dependent change of variables by means of a unitary matrix $\boldsymbol{U}_0$, such that the new variables $\boldsymbol{h}_0 = \boldsymbol{U}_0^\dagger \boldsymbol{h}$ satisfy a similar equation, but with a lower dominant asymptotic order in (inverse) powers of ω_k in the nondiagonal part. A valid choice is the unitary matrix that brings $\boldsymbol{H}$ into its diagonal form $\boldsymbol{D}_0$. In this way, one obtains

$$i\partial_\eta \boldsymbol{h}_0 = \boldsymbol{H}_0 \boldsymbol{h}_0, \qquad \boldsymbol{H}_0 = \boldsymbol{D}_0 - i\boldsymbol{U}_0^\dagger \partial_\eta \boldsymbol{U}_0. \tag{3.5}$$

This process can be repeated iteratively. At each step one gets the following new variables and Hamiltonian:

$$\boldsymbol{h}_{j+1} = \boldsymbol{U}_{j+1}^\dagger \boldsymbol{h}_j, \qquad \boldsymbol{H}_{j+1} = \boldsymbol{D}_{j+1} - i\boldsymbol{U}_{j+1}^\dagger \partial_\eta \boldsymbol{U}_{j+1}. \tag{3.6}$$

The diagonal matrix $\boldsymbol{D}_{j+1}$ and the unitary matrix $\boldsymbol{U}_{j+1}$ are found diagonalizing $\boldsymbol{H}_j$, and then $i\partial_\eta \boldsymbol{h}_{j+1} = \boldsymbol{H}_{j+1}\boldsymbol{h}_{j+1}$. The important point for the adiabatic scheme is that the dominant asymptotic order in the nondiagonal part of $\boldsymbol{H}_j$ decreases at each iterative step, in the limit $\omega_k \to \infty$. Therefore, the approximation of $\boldsymbol{h}_n$ by a solution $\tilde{\boldsymbol{h}}_n$ to the diagonal dynamics dictated by $\boldsymbol{D}_n$ gets more and more accurate for large ω_k as we increase the order n of our adiabatic iteration. A straightforward integration of the diagonal evolution gives

$$\tilde{\boldsymbol{h}}_n(\eta) = \tilde{\boldsymbol{U}}_n(\eta,\tilde{\eta}_0)\mathfrak{h}(\tilde{\eta}_0),$$
$$\tilde{\boldsymbol{U}}_n = \mathrm{diag}\left(\exp\left(-i\int_{\tilde{\eta}_0}^{\eta}\Omega_n\right), \exp\left(i\int_{\tilde{\eta}_0}^{\eta}\Omega_n\right)\right),$$
$$\mathfrak{h}(\tilde{\eta}_0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{3.7}$$

where $\tilde{\boldsymbol{U}}_n$ is a diagonal matrix and $\pm\Omega_n$ are the diagonal elements of $\boldsymbol{D}_n$. This frequency Ω_n is manifestly positive in the asymptotic regime of infinitely large ω_k. Besides, the initial condition $\mathfrak{h}(\tilde{\eta}_0)$ was motivated in Ref. [17] in order to select positive frequencies. With this choice, an adiabatic Fock representation of order n is characterized as follows by a specific basis of solutions $\boldsymbol{h}_{|n}(\eta)$ of Eq. (3.4), which we define in a similar way as for scalar fields [13]. They are determined precisely by the initial conditions at time η_0 obtained from the approximate solution at order n after undoing all the changes of variables involved in the iterative process,

$$\boldsymbol{h}_{|n}(\eta_0) = \left(\prod_{i=0}^{n}\boldsymbol{U}_i(\eta_0)\right)\tilde{\boldsymbol{U}}_n(\eta_0,\tilde{\eta}_0)\mathfrak{h}(\tilde{\eta}_0). \tag{3.8}$$

Given the specific form of $\mathfrak{h}(\tilde{\eta}_0)$, different choices of initial time for the integration of the diagonal dynamics only yield different constant global phases in the expansion of the Dirac field ψ in terms of annihilation and creation operators. Actually, these phases carry no relevant information about the quantum properties of the field, and so we can choose them freely and set $\eta_0 = \tilde{\eta}_0$ for simplicity.

In the above discussion, we have applied the adiabatic procedure directly to the decomposition (3.1)–(3.3) of the fermionic field in the Weyl representation of the Clifford algebra. Let us now show that the result coincides indeed with that obtained in Ref. [17] employing the same type of decomposition in the Dirac representation (and, therefore, starting with a different Schrödinger Hamiltonian). The change to the unitarily related Weyl representation can be carried out as follows:

$$T\gamma_D^b T^\dagger = \gamma_W^b, \qquad T = \frac{1}{\sqrt{2}}\begin{pmatrix} I & -I \\ I & I \end{pmatrix}. \tag{3.9}$$

In the rest of this section, the sub/superscripts D and W indicate spinors in the Dirac or the Weyl representation, respectively. Thus, for the fermionic field, we have $\psi^W = T\psi^D$ or, in terms of the basis of mode solutions associated with a certain vacuum,

$$\boldsymbol{h}^W = \tilde{T}\boldsymbol{h}^D, \qquad \tilde{T} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -\lambda \\ \lambda & 1 \end{pmatrix}, \tag{3.10}$$

where $\tilde{T}$ is clearly unitary, because $\lambda^2 = 1$. The Schrödinger Hamiltonians in both representations are then unitarily related by $\boldsymbol{H}^W = \tilde{T}\boldsymbol{H}^D\tilde{T}^\dagger$, and therefore they have the same diagonal form $\boldsymbol{D}_0$. It follows that the zeroth-order step in the adiabatic iterative procedure is the same when applied to both representations, except for the unitary matrix that diagonalizes the Hamiltonian, which changes as $\boldsymbol{U}_0^W = \tilde{T}\boldsymbol{U}_0^D$. Since this transformation is unitary and constant, the Schrödinger Hamiltonian $\boldsymbol{H}_0$ needed for the next adiabatic step is already the same at zeroth order, regardless of whether one applies the procedure in the Dirac or the Weyl representation. Hence, the same quantities must appear as well in both representations for all the higher-order steps up to the desired order n, including the conditions (3.7) on $\mathfrak{h}(\tilde{\eta}_0)$. It is then straightforward to conclude what we wanted to check, namely, that, for an adiabatic state of order n, one obtains the same set of solutions independently of whether one first performs the adiabatic construction in the Dirac representation and then transforms to the Weyl representation, or alternatively one applies the construction directly in the latter of these representations, with the change between them given by the transformation $\boldsymbol{h}^W_{|n} = \tilde{T}\boldsymbol{h}^D_{|n}$.

IV. UNITARY EQUIVALENCE AND CHOICE OF INITIAL TIME

The family of Fock representations for the Dirac field presented in Sec. II is completely characterized by certain background-dependent (or time-dependent, in the context of QFT in the linearized theory) functions $f_1^{k,\lambda}, f_2^{k,\lambda}$, and $J_{k,\lambda}$, subject to the conditions (2.3). In terms of them, the basis of mode solutions for the field decomposition (3.1)–(3.3) adopts the expression

$$\boldsymbol{h}(\eta) = \left[I - \frac{1-\lambda}{2}(I - i\sigma_2)\right] \times \begin{pmatrix} \bar{f}_1^{k,\lambda}(\eta)\alpha_{k,\lambda}(\eta,\eta_0) - f_2^{k,\lambda}(\eta)e^{-iJ_{k,\lambda}(\eta_0)}\bar{\beta}_{k,\lambda}(\eta,\eta_0) \\ \bar{f}_2^{k,\lambda}(\eta)\alpha_{k,\lambda}(\eta,\eta_0) + f_1^{k,\lambda}(\eta)e^{-iJ_{k,\lambda}(\eta_0)}\bar{\beta}_{k,\lambda}(\eta,\eta_0) \end{pmatrix}, \tag{4.1}$$

where we have taken into account that, for QFT in curved spacetimes, the evolution of the variables defined in Eqs. (2.2) and (2.3) comes from the dynamics dictated by the Dirac equation, and is given by a Bogoliubov transformation of the form [24,25]

$$\begin{aligned} a_{\vec{k},\lambda}(\eta) &= \alpha_{k,\lambda}(\eta,\eta_0)a_{\vec{k},\lambda}(\eta_0) + \beta_{k,\lambda}(\eta,\eta_0)\bar{b}_{\vec{k},\lambda}(\eta_0), \\ \bar{b}_{\vec{k},\lambda}(\eta) &= e^{i[J_{k,\lambda}(\eta)-J_{k,\lambda}(\eta_0)]}\bar{\alpha}_{k,\lambda}(\eta,\eta_0)\bar{b}_{\vec{k},\lambda}(\eta_0) \\ &\quad - e^{i[J_{k,\lambda}(\eta)-J_{k,\lambda}(\eta_0)]}\bar{\beta}_{k,\lambda}(\eta,\eta_0)a_{\vec{k},\lambda}(\eta_0), \end{aligned} \tag{4.2}$$

with $|\alpha_{k,\lambda}|^2 + |\beta_{k,\lambda}|^2 = 1$. From these relations, it is then clear that any adiabatic state defined by the initial conditions (3.8) for $\boldsymbol{h}_{|n}(\eta)$ at time η_0 (equal to $\tilde{\eta}_0$, for simplicity) is associated to a choice of functions $f_{1|n}^{k,\lambda}$ and $f_{2|n}^{k,\lambda}$ such that

$$\begin{pmatrix} \bar{f}_{1|n}^{k,\lambda}(\eta_0) \\ \bar{f}_{2|n}^{k,\lambda}(\eta_0) \end{pmatrix} = \left[I - \frac{1-\lambda}{2}(I + i\sigma_2)\right]\left(\prod_{i=0}^{n}\boldsymbol{U}_i(\eta_0)\right)\mathfrak{h}(\eta_0). \tag{4.3}$$

Here, we have used that $\alpha_{k,\lambda}(\eta_0,\eta_0) = 1$ and $\beta_{k,\lambda}(\eta_0,\eta_0) = 0$. The quantities $f_{1|n}^{k,\lambda}(\eta_0)$ and $f_{2|n}^{k,\lambda}(\eta_0)$ depend, in general, on the scale factor of the homogeneous cosmological background and its derivatives, evaluated at time η_0. Extending the dependence of these homogeneous variables on the initial time η_0 to the whole time domain indeed defines a set of annihilation and creationlike variables in the same way as in Eqs. (2.2) and (2.3), up to the choice of the time-dependent phases $J_{k,\lambda}$ and $F_2^{k,\lambda}$. Actually, it is worth noting that the initial value of these phases at time η_0 is already fixed, respectively, by imposing charge conjugation symmetry and by relation (4.3).

Let us now analyze the properties of the resulting adiabatic quantization and its associated annihilation and creation operators. With respect to the asymptotic expansion in the limit $\omega_k \to \infty$, the adiabatic construction is such that $f_{1|n}^{k,\lambda}$ maintains, for each $n \geq 1$, the same dominant terms that appear in $f_{1|n-1}^{k,\lambda}$ up to order $\mathcal{O}(\omega_k^{-n-1})$. Computing just the two first adiabatic orders, one observes that

$$f_{1|0}^{k,\lambda}(\eta) = \frac{Ma(\eta)}{2\omega_k} + \mathcal{O}(\omega_k^{-2}), \tag{4.4}$$

$$\begin{aligned} f_{1|1}^{k,\lambda}(\eta) &= \frac{Ma(\eta)}{2\omega_k} + \frac{iMa'(\eta)}{4\omega_k^2} + \mathcal{O}(\omega_k^{-3}) \\ &= \frac{Ma(\eta)}{2\omega_k} - i\frac{\pi M\pi_a(\eta)}{3l_0^3\omega_k^2} + \mathcal{O}(\omega_k^{-3}). \end{aligned} \tag{4.5}$$

In the last line we have denoted with a prime the total derivative with respect to the conformal time, and used Hamilton equations for the homogeneous cosmology in the linearized theory in order to express the result in terms of canonical variables. The dominant terms in these expressions (that are written explicitly) remain in higher-order adiabatic states, according to our comments. Recalling then the results listed in Sec. II, and, in particular, condition (2.4), we can see just from the zeroth-order shown in Eq. (4.4) that all the adiabatic states live in the family of unitarily equivalent vacua that are determined by the annihilation and creationlike variables (2.2) and (2.3), for which the quantum Heisenberg evolution is unitarily implementable. Furthermore, for adiabaticity order greater than 0, the Fock quantization of these annihilation and creationlike variables leads to a finite mean backreaction in hybrid quantum cosmology (in the sense explained in Sec. II) and their contribution to the total Hamiltonian constraint of the system is well defined on the dense set of Fock space spanned by the states with a definite number of particles/antiparticles.

Finally, let us comment on the relevance of the choice of initial time η_0 in the discussed construction of fermionic adiabatic states. Indeed, each of these adiabatic representations of the Dirac field depends on the time at which one sets initial conditions of the form (3.8) for the basis of mode solutions. Let us specifically call $\boldsymbol{h}^{\eta_0}_{|n}$ the basis of adiabatic solutions obtained with initial conditions at time η_0. Imagine that, rather than at η_0, we imposed adiabatic initial conditions at another time η_1, getting in that way a new basis of mode solutions $\boldsymbol{h}^{\eta_1}_{|n}$. According to our discussion above [and, in particular, to formula (4.1)], the two sets of solutions, evaluated at the same time η_0, are related by

$$\boldsymbol{h}^{\eta_1}_{|n}(\eta_0) = \left[I - \frac{1-\lambda}{2}(I - i\sigma_2)\right][\alpha_{k,\lambda}(\eta_0,\eta_1)\boldsymbol{h}^{\eta_0}_{|n}(\eta_0) - i\lambda\sigma_2\bar{\beta}_{k,\lambda}(\eta_0,\eta_1)\bar{\boldsymbol{h}}^{\eta_0}_{|n}(\eta_0)], \tag{4.6}$$

where we have fixed $J_{k,\lambda}(\eta_1) = (3+\lambda)\pi/2$ by requiring charge conjugation symmetry. This relation between the two sets of data at η_0 is a Bogoliubov transformation, and its unitary implementability in the quantum theory depends exclusively on the square summability of the beta coefficients, over all $\vec{k} \in \mathbb{Z}^3$. But we note that, in norm, these coefficients are precisely the same that characterize the dynamical transformations of the annihilation and creationlike variables, whose evolution that we have seen is indeed unitarily implementable. Hence, we conclude that any two adiabatic representations that differ on the value of the initial time at which one imposes the conditions (3.8) are unitarily equivalent. Furthermore, this equivalence is directly related to the fact that the representations allow the definition of families of annihilation and creation operators that can evolve unitarily.

V. CONCLUSIONS

In this work, we have investigated the relation between the adiabatic construction and the criterion employed in hybrid quantum cosmology to select Fock states that can play the role of vacua for the Dirac field, treated as a fermionic perturbation of an inflationary flat FLRW universe. Specifically, we have found that all adiabatic states belong to the family of unitarily equivalent Fock vacua employed in hybrid quantum cosmology, characterized by the invariance under the isometries of the spatial sections and by a unitarily implementable Heisenberg evolution of the corresponding annihilation and creation operators when the FLRW cosmology is regarded as a curved background. Moreover, for adiabatic orders other than 0, they allow quantizations with other desirable ultraviolet properties, such as a finite backreaction term in the only nontrivial constraint of the system and a properly defined fermionic Hamiltonian operator.

Given a mode decomposition of a solution to the Dirac equation, its coefficients determine a set of annihilation and creation constant operators. The adiabatic scheme that we have discussed makes use of this fact, selecting a particular set of mode solutions. More specifically, any decomposition is characterized by functions that satisfy a Schrödinger-like equation with a time-dependent Hamiltonian matrix. One can introduce a series of time-dependent transformations on these functions that decrease the asymptotic order of the nondiagonal part of their Hamiltonian in the ultraviolet regime of large wave numbers. If one neglects this nondiagonal part once a certain asymptotic order is reached, it is straightforward to construct a set of approximate solutions and, in this way, specify a mode decomposition. In this work, we have adapted this procedure to the Weyl representation of the Clifford algebra. The implementation in the Dirac representation had been studied in Ref. [17]. We have provided the transformation between these two representations and shown that the conclusions obtained in both cases are consistent.

We have computed explicitly the approximate mode solutions at the two lowest adiabatic orders and, with them, we have identified the dominant and first subdominant asymptotic terms for large ω_k in the functions that define the corresponding dynamical sets of annihilation and creationlike variables. Comparing these asymptotic terms with those that are characteristic of the family of Fock quantizations admissible in hybrid quantum cosmology, we have proven that all adiabatic vacua belong indeed to this family and, furthermore, that for adiabatic orders other than 0, those vacua can be associated with annihilation and creation operators that lead to well-defined mean backreaction contribution and fermionic quantum Hamiltonian in the only nontrivial constraint of the system. These results also ensure that the alternative adiabatic vacua constructed with different choices of initial time for the integration of the approximate mode solutions are all unitarily related.

In spite of the proven unitary equivalence between the two considered quantization schemes, it is worth commenting that the approach followed in hybrid quantum cosmology possesses a useful feature that, in principle, is missing in the adiabatic proposal. Indeed, in the former approach one starts by characterizing the set of admissible annihilation and creationlike variables, including their dynamical behavior, and therefore the genuine quantum fermionic excitations that have desirable physical properties. On the other hand, the adiabatic approach only defines a Fock representation of the Dirac field in terms of constant annihilation and creation operators. Without further information, there is no unambiguous way of isolating, from the evolution of the field, a Heisenberg dynamics with nice quantum behavior that dictates exclusively the dynamical transformations of those fermionic operators, separating them from the background dependence. Clearly, after one has introduced a dynamical family of annihilation and creationlike variables in the hybrid approach, one can also make the corresponding identification of adiabatic states. This advantage of the hybrid strategy in specifying quantum excitations of the field that are dynamically well behaved can be a potential help to understand the origin of the plausibly good ultraviolet properties of adiabatic states. In fact, we have already seen here that the unitarity of the Heisenberg dynamics of the fermionic operators in the hybrid approach is capable of explaining the equivalence (up to unitary transformations) of all the adiabatic states, irrespectively of the time selected to set their initial conditions. Finally, the splitting of the phase space into a homogeneous and an inhomogeneous sector, which is induced by the choice of variables in hybrid quantum cosmology, is crucial for the later quantization of the entire truncated cosmological system. In fact, this choice may potentially be useful at higher orders of perturbative truncation in the action, where the selected fermionic variables could constitute a starting point in the search for a new refined splitting of this kind that takes into account the nonlinearities present in the higher-order system.

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APPENDIX: SOME COMMENTS ABOUT THE ADIABATIC SCHEME PROPOSED BY HOLLANDS

An alternative construction of adiabatic states has been proposed by Hollands in Ref. [16]. The first step in this procedure is to find a pseudodifferential operator (see e.g., Refs. [36,37]) T that factorizes the spinorial Klein-Gordon operator, namely,

$$\begin{aligned} &-(in^\mu\nabla_\mu + iK + H)(in^\mu\nabla_\mu - H) \\ &\quad = -(in^\mu\nabla_\mu + iK + T)(in^\mu\nabla_\mu - T), \end{aligned} \tag{A1}$$

modulo an operator with smooth kernel. In this relation, H is the one-particle Dirac Hamiltonian, $K = \nabla^\nu n_\nu$ is the extrinsic curvature of the spatial sections, and the operator T has principal symbol $\sigma_1(T)(\vec{x},\vec{\xi}) = \sqrt{h_{ij}(\vec{x})\xi^i\xi^j}$, where h_{ij} is the metric of the spatial sections. Although finding T is a hard problem in general, one can construct approximate solutions by means of an iterative method. We call T_n the resulting operator after n steps. One then defines $L_{n,\pm} = T_n \pm H$ and looks for a positive Hermitic operator Q_n such that

$$L_{n,+}Q_nL_{n,+}^* + L_{n,-}^*Q_nL_{n,-} = 1. \tag{A2}$$

With this, one can define the following operators:

$$B_n = L_{n,+}Q_nL_{n,+}^*, \qquad B_{n,-} = L_{n,-}^*Q_nL_{n,-}, \tag{A3}$$

which must be symmetric and positive. These operators determine the algebraic state desired for the quantization of the Dirac field [16]. In fact, such a state corresponds to a Fock representation if and only if B_n is a projector [38]. In practice, to find these operators, it is convenient to introduce their mode decomposition. This was done in Ref. [16] by using the Dirac representation of the Clifford algebra and a basis of spinors for which the one-particle Hamiltonian is instantaneously diagonal,

$$\begin{aligned} u^+_{\vec{k},\lambda} &= \frac{\mathcal{U}_{k,\lambda}}{\sqrt{l_0^3a^3}}\begin{pmatrix}\xi_\lambda(\vec{k})\\ 0\end{pmatrix}e^{i2\pi(\vec{k}+\vec{\tau})\vec{x}/l_0}, \\ u^-_{\vec{k},\lambda} &= \frac{\mathcal{U}_{k,\lambda}}{\sqrt{l_0^3a^3}}\begin{pmatrix}0\\ \xi_\lambda(\vec{k})\end{pmatrix}e^{i2\pi(\vec{k}+\vec{\tau})\vec{x}/l_0}, \end{aligned} \tag{A4}$$

where, defining $\Delta_k(a) = \sqrt{\omega_k^2 + M^2a^2}$, we have called

$$\mathcal{U}_{k,s} = \frac{1}{\sqrt{2\Delta_k(a)}}\begin{pmatrix}\sqrt{\Delta_k(a)+Ma} & -\lambda\sqrt{\Delta_k(a)-Ma}\\ \lambda\sqrt{\Delta_k(a)-Ma} & \sqrt{\Delta_k(a)+Ma}\end{pmatrix}. \tag{A5}$$

With this basis one may define the mode decomposition of any differential operator B on the spatial sections by the formulas

$$\begin{aligned} a^3\int_{T^3}d^3\vec{x}f_1^\dagger Bf_2 &= \sum_{\vec{k},s,pq}b^{pq}_{\vec{k},s}\bar{\tilde{f}}^p_{1,\vec{k},\lambda}\tilde{f}^q_{2,\vec{k},\lambda}, \\ \tilde{f}^p_{\vec{k},\lambda} &= a^3\int_{T^3}d^3\vec{x}(u^p_{\vec{k},\lambda})^\dagger f, \end{aligned} \tag{A6}$$

for any two spinors f_1 and f_2, with $p, q = \pm$. In essence, this decomposition maps operators (and pseudodifferential operators) into 2×2 complex matrices while respecting products and the adjoint operation.

In the following, to simplify our notation, we drop from it the dependence on $\vec{k}$ and λ unless explicitly stated. In addition, we use lowercase letters to refer to the mode decomposition of the operators, with the correspondence $T_n \to \tau_n$, $H \to h$, $Q_n \to q_n$, $L_n \to \ell_n$, and $B_n \to b_n$. Besides, we recall that the prime symbol denotes the total derivative with respect to the conformal time. The decomposition (A1), as given by Eq. (A6), can then be reexpressed as

$$i\tau' + \frac{3ia'}{2a}\tau + [\tau, d] + a\tau^2 = ih' + \frac{3ia'}{2a}h + [h, d] + ah^2, \tag{A7}$$

where

$$d = i\mathcal{U}^*(\partial_\eta \mathcal{U}) = \frac{\lambda\omega_k M a'}{2(\omega_k^2 + M^2 a^2)}\sigma_2. \tag{A8}$$

The procedure to determine τ_n goes as follows. Starting from the ansatz $\tau_n = \sum_{j=0}^{n} \vartheta_j$, with $\vartheta_j = \mathcal{O}(\omega_k^{1-j})$, and setting $\tau_0 = \mathrm{diag}[\sqrt{a^{-2}\omega_k^2 + M^2}, \sqrt{a^{-2}\omega_k^2 + M^2}]$, one solves (A7) iteratively, obtaining

$$\vartheta_{n+1} = \frac{1}{2\sqrt{\omega_k^2 + M^2 a^2}}[F(h) - F(\tau_n)], \tag{A9}$$

where we have defined $F(o) = io' + 3i(\ln a)'o/2 + [o, d] + ao^2$. The mode versions of Eqs. (A2) and (A3) are then used to construct b_n. In order for the algebraic state resulting from the operator B_n to correspond to a Fock representation, that operator must be a nontrivial projector, something that requires that b_n be singular. Unfortunately this turns out not to be the case in the system that we are considering, as can be checked by noticing that, for all $n \geq 1$,

$$\ell_{n,+} = \mathrm{diag}\left[\frac{2\omega_k}{a}, -\frac{ia'}{2a}\right] + \mathcal{O}(\omega_k^{-1}),$$
$$q_n = \mathrm{diag}\left[\frac{a^2}{4\omega_k^2}, \frac{a^2}{4\omega_k^2}\right] + \mathcal{O}(\omega_k^{-3}). \tag{A10}$$

This result implies that, except for the trivial case of a constant scale factor, $\det(b_n)$ is always of asymptotic order ω_k^{-2}, and thus dominant over $\mathcal{O}(\omega_k^{-n})$ for all $n \geq 3$. Therefore, at each order $n \geq 3$, the operator B_n fails to be singular (even if one truncates it at asymptotic order ω_k^{1-n}), and so it cannot be a projector. The corresponding algebraic states are thus not suitable to be employed in hybrid quantum cosmology, inasmuch as they do not define Fock representations, and hence they cannot be compared with our family of unitarily equivalent Fock vacua.

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Unique fermionic vacuum in de Sitter spacetime from hybrid quantum cosmology

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In this work we show how the criterion of asymptotic Hamiltonian diagonalization originated in hybrid quantum cosmology serves to pick out a unique vacuum for the Dirac field in de Sitter, in the context of quantum field theory in curved spacetimes. This criterion is based on the dynamical definition of annihilation and creationlike variables for the fermionic field, which obey the linearized dynamics of a Hamiltonian that has been diagonalized in a way that is adapted to its local spatial structure. This leads to fermionic variables that possess a precise asymptotic expansion in the ultraviolet limit of large wave numbers. We explicitly show that, when the cosmological background is fixed as a de Sitter solution, this expansion uniquely selects the choice of fermionic annihilation and creationlike variables for all spatial scales, and thus picks out a unique privileged Fock representation and vacuum state for the Dirac field in de Sitter. The explicit form of the basis of solutions to the Dirac equation associated with this vacuum is then computed.

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I. INTRODUCTION

One of the solutions of general relativity (GR) that deserves special attention in modern cosmology is de Sitter spacetime. This is because, in the context of primordial cosmology, this solution approximates quite well the expected behaviour of an inflationary period in the evolution of the Universe. The practical benefits of this approximation are numerous, among which it is remarkable the application to the quantum field theory (QFT) description of cosmological perturbations. Indeed, for cosmological inflationary models driven by a spin-0 matter field (the inflaton), the standard theoretical guideline for the choice of an initial quantum state of the inhomogeneous perturbations in the metric and the inflaton at the onset of inflation is to select an analogue of the Bunch-Davies (BD) vacuum [1,2]. This is, in turn, the preferred Fock vacuum of a quantum scalar field propagating in de Sitter, that is picked out as the unique Hadamard state among those that are invariant under the isometry group of de Sitter spacetime, that is maximally symmetric [3–5]. Interestingly, the power spectra of cosmological perturbations that is predicted in GR with such a choice of BD vacuum agrees, to a high degree of accuracy, with the current experimental observations of the cosmic microwave background [6–9].

The physical and mathematical properties of the BD vacuum (and its associated Fock representation) for scalar fields have been thoroughly studied in the literature (see, e.g., Refs. [10–17]). For higher spin fields, and in particular for the case of the spin-$1/2$ Dirac field, generalizations of the notion and features of the BD vacuum have also been widely discussed in the literature [18–21], even though the uniqueness of the resulting state might not be as broadly established as for scalar fields. The aim of this paper is to justify a physically natural choice of Fock vacuum state in de Sitter spacetime, for a minimally coupled Dirac field, that displays BD-like properties and that finds its motivation in the context of quantum cosmology. More specifically, we will explicitly derive the unique Fock representation that turns out to be selected by the criterion of asymptotic Hamiltonian diagonalization, recently introduced for the so-called hybrid approach to canonical quantum cosmology [22].

Hybrid quantum cosmology [23,24] is an strategy for the canonical quantization of spacetimes that contain inhomogeneities, but also possess some notion of symmetry. Such is the case, for instance, of the system formed by matter and metric perturbations over an otherwise homogeneous and isotropic inflationary cosmology of the Friedmann-Lemaître-Robertson-Walker (FLRW) type [25–30]. In particular, the quantization strategy is based on the use of

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different representation techniques for the canonical algebra that describes the homogeneous degrees of freedom, on the one hand, and for the algebra that contains the inhomogeneous fields, on the other hand. The homogeneous algebra is represented with techniques imported from a theory of quantum gravity or quantum cosmology, e.g., loop quantum gravity [31], while the inhomogeneous fields are given a more conventional Fock representation. From a theoretical point of view, the first important condition that one should require from this approach is that the combination of the two different quantum representations consistently leads to nicely defined operator versions of the constraints of the gravitational system. To that end, it becomes necessary to carry out a sensible choice of canonical splitting between the homogeneous and inhomogeneous sectors of phase space, in view of their posterior quantization, taking into account the qualitatively different quantum descriptions that are going to be adopted for them.

Declaring which part of the phase space should correspond to the inhomogeneous fields in hybrid quantum cosmology has been the central point of several investigations. Actually, this ambiguity can be codified altogether with the freedom in the choice of a Fock representation for them, by means of families of variables that are the classical counterpart of the annihilation and creation operators, obtained through canonical transformations in the entire phase space that respect the basic symmetries of the homogeneous sector. The first physical criterion for any admissible Fock representation in hybrid quantum cosmology should then be that, in the context of QFT in curved spacetimes (and hence regarding the homogeneous sector as classical), the annihilation and creation operators undergo an evolution that can be implemented by a quantum unitary transformation [32–40]. This criterion of choice has been further restricted in the context of fermionic perturbations in hybrid quantum cosmology, in such a way that certain effective backreaction to the Hamiltonian constraint does not develop divergences, without the need of introducing any regularization procedure [41]. Finally, and motivated by these previous conditions, the most recent works on the theoretical formulation of the hybrid quantization of both fermionic and scalar cosmological perturbations have proposed an approach that aims to remove all the ambiguities (up to irrelevant phases) in the choice of the canonical algebra associated with the perturbations, that is going to be quantized *à la* Fock [22,42]. The approach tries and constructs a quantum description of the inhomogeneities such that the local structure of the Hamiltonian contains no self-interaction contributions in terms of the annihilation and creation operators, and thus it is asymptotically diagonalized in the ultraviolet regime of short scales. Such a criterion turns out to completely fix, in an asymptotic expansion, the dynamical definition of those operators, expansion from which one may hope to uniquely determine them globally. In the restricted context of QFT in a de Sitter background cosmology, this hope was actually realized for the scalar perturbations, resulting in the specification of the well-known BD vacuum [42]. In this paper, we show in detail how the criterion of asymptotic diagonalization also serves to uniquely fix the choice of vacuum in de Sitter for fermionic perturbations of the Dirac type. The result provides a privileged Fock representation of the Dirac field in de Sitter spacetime for which the selection criterion is univocally characterized and well understood.

The structure of this paper is as follows. In Sec. II we introduce the fermionic perturbations for a general FLRW cosmological background, and the fermionic variables that are going to be promoted to annihilation and creation operators that display a dynamical evolution that is dictated by a diagonal Hamiltonian. We summarize the procedure to construct these variables, that is based on an asymptotic diagonalization. In Sec. III we explicitly solve the problem of finding the most general family of annihilation and creation operators that evolve without self-interaction in a fixed de Sitter background. We then show how the method of asymptotic diagonalization of the Hamiltonian, adapted to its local structure, serves to fix a unique set of annihilation and creation operators, and give the specific form of the corresponding privileged Fock representation. Finally, in Sec. IV we summarize our results.

Throughout the text, we employ natural units, so that $G = c = \hbar = 1$.

II. FERMIONIC VACUUM IN HYBRID QUANTUM COSMOLOGY

In this paper we focus our attention on a system that has been extensively studied in hybrid quantum cosmology: a spatially flat homogeneous FLRW spacetime which is minimally coupled to a homogeneous scalar field with a certain potential, as well as to an inhomogeneous Dirac field. The spatial hypersurfaces of this cosmology are taken to be compact, isomorphic to the three torus T^3. The FLRW metric can be described in terms of a scale factor $\tilde{a}$. On the other hand, we treat the Dirac field entirely as a perturbation of the system. Moreover, whenever we consider canonical transformations that mix the fermionic degrees of freedom with the homogeneous background, we adopt a truncation scheme in which we only preserve contributions to the Einstein-Dirac action that are at most quadratic in the perturbations. The transformations are viewed as canonical within the framework of this perturbative truncation, including the symplectic structure of the system. Potentially, one may also introduce perturbations of the metric and the scalar field, and work consistently within our truncation scheme and a canonical framework for the entire cosmological system [28–30].

For the description of the Dirac field ψ, we use the Weyl representation of the constant Clifford algebra associated with the four-dimensional flat metric,

$$\gamma^0 = i\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \qquad \vec{\gamma} = i\begin{pmatrix} 0 & \vec{\sigma} \\ -\vec{\sigma} & 0 \end{pmatrix}, \tag{2.1}$$

where I denotes the identity matrix (here, in two dimensions), $\vec{\gamma} = (\gamma^1, \gamma^2, \gamma^3)$, and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is the triple formed by the three Pauli matrices. In addition, we fix the gauge time direction of the tetrads so that it coincides with the (future-directed) normal vector to the homogeneous spatial hypersurfaces, in order to simplify the Dirac brackets of the field [43] and so that, with respect to its local Lorentz transformation properties, we can regard it as two representation spaces of $SU(2)$, rather than $SL(2,\mathbb{C})$ [39]. Then, we exploit the high symmetry and compactness of the flat homogeneous spatial hypersurfaces in order to decompose the Dirac field in terms of a complete set of modes [30,39,40],

$$\psi(t,\vec{x}) = \sum_{\vec{k}\in\mathbb{Z}^3}\sum_{\lambda=\pm1}\frac{e^{i2\pi\vec{k}\,\vec{x}/l_0}}{\sqrt{l_0^3\tilde{a}^3}}\begin{pmatrix} x_{\vec{k},\lambda}(t)\xi_\lambda(\vec{k}) \\ y_{\vec{k},\lambda}(t)\xi_\lambda(\vec{k}) \end{pmatrix},$$
$$-i\vec{\sigma}\,\vec{\nabla}[\xi_\lambda(\vec{k})e^{i2\pi\vec{k}\,\vec{x}/l_0}] = \lambda\omega_k\xi_\lambda(\vec{k})e^{i2\pi\vec{k}\,\vec{x}/l_0}. \tag{2.2}$$

Here, l_0 is the compactification length of the torus, $\lambda\omega_k$ are the eigenvalues of the Dirac operator $-i\vec{\sigma}\,\vec{\nabla}$ on T^3, where $\lambda = \pm 1$ represents the helicity, the two-component objects $\xi_\lambda(\vec{k})\exp(i2\pi\vec{k}\,\vec{x}/l_0)$ are its eigenspinors, and $\omega_k = 2\pi|\vec{k}|/l_0$ with $\vec{k}\in\mathbb{Z}^3$. In addition, we are imposing spatially periodic boundary conditions to the Dirac field, restricting ourselves in this way to the trivial choice of spin structure in T^3 [44]. The time-dependent coefficients $(x_{\vec{k},\lambda}, y_{\vec{k},\lambda})$ are Grassmann variables that only display nonvanishing Dirac brackets with their complex conjugates, each of these nontrivial brackets being equal to $-i$.

In the truncation scheme that we have adopted, these fermionic variables contribute to the total Hamiltonian of the system only through the zero-mode of the Hamiltonian constraint. Explicitly, this fermionic contribution to the Hamiltonian is given by [30]

$$\tilde{H}_D = N_0\sum_{\vec{k},\lambda}[M(\bar{y}_{\vec{k},\lambda}x_{\vec{k},\lambda} + \bar{x}_{\vec{k},\lambda}y_{\vec{k},\lambda}) - \tilde{a}^{-1}\lambda\omega_k(\bar{x}_{\vec{k},\lambda}x_{\vec{k},\lambda} - \bar{y}_{\vec{k},\lambda}y_{\vec{k},\lambda})], \tag{2.3}$$

where M is the bare mass of the Dirac field, N_0 is the lapse function of the homogeneous FLRW background, and an overbar indicates complex conjugation. We exclude from all of our considerations and sums the terms with $\vec{k} = 0$, namely the fermionic zero-modes, since they contribute to the Hamiltonian in a slightly different manner and can be isolated and quantized separately. For instance, one could directly adopt a standard holomorphic representation for the (finitely many) anticommuting variables that describe these zero-modes (for details on this type of quantization, see, e.g., Ref. [45]). On the other hand, let us notice that modes corresponding to different values of $\vec{k}$ and λ completely decouple in $\tilde{H}_D$, and that the coefficients of the fermionic variables only depend on $\lambda\omega_k$, but not on the degeneracy of these eigenvalues of the Dirac operator (i.e., they only depend on the helicity and on the norm of $\vec{k}$). This is mostly a manifestation of the spatial symmetries of the spatial sections, together with the conservation of the helicity of the field in FLRW cosmologies [40].

The freedom that exists in hybrid quantum cosmology in the way to split the phase space into a homogeneous sector and an inhomogeneous sector can be captured in the choice of a background-dependent family of variables of annihilation and creation type for the description of the dynamical Dirac field, respecting the symmetries of the Hamiltonian that we have commented in the above paragraph. These families of variables are of the general form

$$\begin{pmatrix} a_{\vec{k},\lambda} \\ \bar{b}_{-\vec{k},\lambda} \end{pmatrix} = \begin{pmatrix} f_1^{k,\lambda} & f_2^{k,\lambda} \\ g_1^{k,\lambda} & g_2^{k,\lambda} \end{pmatrix}\left[I - \frac{1-\lambda}{2}(I - \sigma_1)\right]\begin{pmatrix} x_{\vec{k},\lambda} \\ y_{\vec{k},\lambda} \end{pmatrix}. \tag{2.4}$$

As we have indicated, the coefficients $f_l^{k,\lambda}$ and $g_l^{k,\lambda}$, with $l = 1,\ 2$, are in principle allowed to depend on the canonical variables that determine the homogeneous cosmological background: the scale factor $\tilde{a}$, the homogeneous scalar field, and their canonical momenta. These coefficients are subject to the following relations:

$$f_2^{k,\lambda} = e^{iF_2^{k,\lambda}}\sqrt{1 - |f_1^{k,\lambda}|^2}, \qquad g_1^{k,\lambda} = e^{iJ_{k,\lambda}}\bar{f}_2^{k,\lambda},$$
$$g_2^{k,\lambda} = -e^{iJ_{k,\lambda}}\bar{f}_1^{k,\lambda}, \tag{2.5}$$

that ensure that the transformation of the pair $(x_{\vec{k},\lambda}, y_{\vec{k},\lambda})$ to $(a_{\vec{k},\lambda}, \bar{b}_{-\vec{k},\lambda})$ is canonical with respect to the symplectic structure restricted to the fermionic sector of phase space. Here, $F_2^{k,\lambda}$ and $J_{k,\lambda}$ are unspecified phases. The standard convention is then to regard $a_{\vec{k},\lambda}$ as the prequantum version of annihilation operators of particles, and $\bar{b}_{\vec{k},\lambda}$ as the variables that are going to be promoted to creation operators of antiparticles. Every single specification of such variables for all wave vectors $\vec{k}$ defines a different Fock quantization of the fermionic field.

We notice that, since the coefficients $f_l^{k,\lambda}$ and $g_l^{k,\lambda}$ that define them depend generally on the homogeneous cosmological background or, from a classical perspective, on time, the Hamiltonian that dictates the linearized classical dynamics of these annihilation and creationlike variables is different from $\tilde{H}_D$ in Eq. (2.3). In the linearized classical scenario, where the homogeneous background is fixed as a cosmological FLRW solution in GR, the difference between both Hamiltonian functions is just the time derivative of the generating function of the canonical transformation given by Eqs. (2.4) and (2.5). This change in the Hamiltonian can be realized within the canonical framework of the entire system, that is employed in hybrid quantum cosmology, by completing our change of fermionic variables into a canonical transformation for the full cosmology, that also includes the homogeneous background. This is achieved, at the considered order of perturbative truncation, by correcting the variables of the homogeneous sector with the addition of very specific terms that are quadratic in the fermionic perturbations. In particular, we denote by a the resulting new scale factor. We refer the reader to Refs. [22,28,30,41] for the specific details of this procedure. Expressing the total Hamiltonian in terms of the new canonical set of variables for the complete system gives rise to the following contribution [22]:

$$H_D = N_0\sum_{\vec{k},\lambda}[2h_D^{k,\lambda}(\bar{a}_{\vec{k},\lambda}a_{\vec{k},\lambda}+\bar{b}_{\vec{k},\lambda}b_{\vec{k},\lambda})+\{J_{k,\lambda},H_{|0}\}\bar{b}_{\vec{k},\lambda}b_{\vec{k},\lambda} + \bar{h}_I^{k,\lambda}a_{\vec{k},\lambda}b_{-\vec{k},\lambda} - h_I^{\vec{k},(x,y)}\bar{a}_{\vec{k},\lambda}\bar{b}_{-\vec{k},\lambda}], \tag{2.6}$$

where we have imposed normal ordering of the Grassmann variables, and

$$h_D^{k,\lambda} = \frac{\omega_k}{2a}(|f_2^{k,\lambda}|^2-|f_1^{k,\lambda}|^2)+M\mathrm{Re}(f_1^{k,\lambda}\bar{f}_2^{k,\lambda}) + \frac{i}{2}(\bar{f}_1^{k,\lambda}\{f_1^{k,\lambda},H_{|0}\}+\bar{f}_2^{k,\lambda}\{f_2^{k,\lambda},H_{|0}\}), \tag{2.7}$$

$$h_I^{k,\lambda} = e^{-iJ_{k,\lambda}}[if_1^{k,\lambda}\{f_2^{k,\lambda},H_{|0}\}-if_2^{k,\lambda}\{f_1^{k,\lambda},H_{|0}\} + 2\omega_k a^{-1}f_1^{k,\lambda}f_2^{k,\lambda}+M(f_1^{k,\lambda})^2-M(f_2^{k,\lambda})^2]. \tag{2.8}$$

In all of these expressions, $\{.,H_{|0}\}$ denotes the Poisson bracket with the Hamiltonian constraint $H_{|0}$ of the homogeneous FLRW inflationary cosmology, evaluated at the new background variables. For concreteness, let us note that this is the cosmological model that can be obtained from ours by ignoring or eliminating the perturbations. Its Hamiltonian is given by $N_0H_{|0}$. Hence, the considered Poisson bracket is just the derivative with respect to the proper time in the context of linearized classical cosmology. In addition, all the functions of the background in Eq. (2.6) are functionally evaluated on the new canonical variables for the description of this homogeneous sector. The symbol Re(·) stands for the real part. Finally, in what follows we will restrict $J_{k,\lambda}$ to be constant, in order not to introduce any artificial asymmetry in the dynamics of the annihilation and creationlike variables for particles and antiparticles [see Eq. (2.6)].

A. Asymptotic diagonalization

A look at the Hamiltonian (2.6) immediately shows that, dynamically, the creation and annihilation of pairs of particles and antiparticles is ruled by the function $h_I^{k,\lambda}$ of the homogeneous background. Importantly, it is this self-interactive part of the fermionic Hamiltonian what can produce the most severe QFT-type of divergences in the quantum theory [30,41]. The issue is directly related to the asymptotic behavior of this function, in the ultraviolet limit of large wave numbers ω_k. Remarkably, this ultraviolet behavior is greatly tamed by the criteria put forward in hybrid quantum cosmology of (i) requiring that the fermionic annihilation and creation operators can evolve unitarily in the context of QFT in curved spacetimes [30,40]; and (ii) asking that the Fock representation of the fermionic contribution to the Hamiltonian constraint (2.6) is well defined on the vacuum, something that actually guarantees that certain backreaction effects in the hybrid quantum theory are nondivergent without the need of any regularization [41]. Technically, these criteria succeed in eliminating the first few dominant asymptotic contributions of $h_I^{k,\lambda}$ (in powers of the scale ω_k). Furthermore, by imposing these criteria one derives the additional benefit of restricting the asymptotic form of the annihilation and creationlike variables (2.4), and thus the choice of their Fock representation.

Motivated by these results, a more restrictive criterion, intended for the complete determination of the Fock quantization of the fermionic perturbations, has been recently proposed [22]. It aims to diminish as much as possible the interaction terms in their Hamiltonian, in the ultraviolet regime of large ω_k. For that, one starts with annihilation and creationlike variables that admit a unitarily implementable dynamics in QFT, within the unique family of unitarily equivalent representations that possess such property, adhering to a standard convention for particles and antiparticles [40]. Then, an iterative procedure (that we call asymptotic diagonalization), applied order by order in inverse powers of the Fourier scale ω_k, univocally leads to a complete asymptotic elimination of the interaction terms $h_I^{k,\lambda}$, requiring that [22]

$$f_1^{k,\lambda} = f_2^{k,\lambda}\varphi_{k,\lambda}, \qquad \varphi_{k,\lambda}\sim\frac{1}{2\omega_k}\sum_{n=0}^{\infty}\left(-\frac{i}{2\omega_k}\right)^n\gamma_n, \tag{2.9}$$

where

$$\gamma_0 = Ma, \qquad \gamma_{n+1} = a\{H_{|0},\gamma_n\}+Ma\sum_{m=0}^{n-1}\gamma_m\gamma_{n-(m+1)}, \qquad \forall\ n\geq 0. \tag{2.10}$$

We note that, up to the phases $F_2^{k,\lambda}$ and $J_{k,\lambda}$, relations (2.5), (2.9), and (2.10) uniquely provide asymptotic expansions of the coefficients that define the annihilation and creation-like variables for the fermionic perturbations. Specifically, relations (2.5) directly imply that

$$|f_2^{k,\lambda}|^2 = \frac{1}{1+|\varphi_{k,\lambda}|^2}, \tag{2.11}$$

so, as an asymptotic expansion, $f_2^{k,\lambda} \neq 0$ in our characterization.

The actual hope in hybrid quantum cosmology is that, even if in the form of as an asymptotic expansion, the diagonalization explained above can be used to select (up to the mentioned phases) a complete set of fermionic annihilation and creation operators for all wave vectors $\vec{k} \neq 0$, and hence a specific Fock quantization of the fermionic excitations. In fact, assuming that $f_2^{k,\lambda} \neq 0$, as it is required by the standard convention of particles and antiparticles [40], the elimination of interaction terms $h_I^{k,\lambda}$ in the fermionic Hamiltonian for all $\omega_k \neq 0$ is attained if and only if

$$a\{\varphi_{k,\lambda}, H_{|0}\} + 2i\omega_k\varphi_{k,\lambda} + iaM\varphi_{k,\lambda}^2 - iaM = 0. \tag{2.12}$$

This is a semilinear partial differential equation for $\varphi_{k,\lambda}$, and the current concern regarding the asymptotic diagonalization criterion in hybrid quantum cosmology is whether the asymptotic expansion (2.9) uniquely characterizes a solution. In the upcoming section, we argue that this is indeed the case when the homogeneous background describes a de Sitter spacetime, and the fermionic perturbations are considered within the linearized context of QFT in curved spacetimes.

III. UNIQUE VACUUM IN DE SITTER

We now restrict all our attention to the scenario of cosmological models with negligible backreaction of the perturbations on the homogeneous background, situation in which this background follows the classical dynamics of an FLRW spacetime fuelled with a homogeneous scalar field. In practice, this means that the old and new variables that describe the homogeneous cosmology can be identified (in particular, we have $a = \tilde{a}$), and that the Poisson bracket $a\{., H_{|0}\}$ is the derivative with respect to conformal time, η. The metric that describes the de Sitter spacetime is a particular solution of the considered, classical flat FLRW cosmologies, expressed in coordinates that correspond to its flat slicing [2]. Specifically, this solution can be reached with a constant potential for the scalar field. In conformal time, the scale factor then behaves as

$$a = -(\eta H_\Lambda)^{-1}, \qquad -\infty < \eta < 0, \tag{3.1}$$

where H_Λ is the Hubble constant. In this de Sitter background, the general condition (2.12) that cancels the interaction terms in the fermionic Hamiltonian becomes the following Riccati equation

$$\varphi_{k,\lambda}' + 2i\omega_k\varphi_{k,\lambda} - iM(\eta H_\Lambda)^{-1}\varphi_{k,\lambda}^2 + iM(\eta H_\Lambda)^{-1} = 0, \tag{3.2}$$

where the prime denotes the derivative with respect to η. In order to eventually find the general solution to this equation, we introduce the standard change of variable

$$\varphi_{k,\lambda} = i\eta M^{-1}H_\Lambda(\log u_{k,\lambda})', \tag{3.3}$$

which leads to the second-order linear equation

$$u_{k,\lambda}'' + (2i\omega_k + \eta^{-1})u_{k,\lambda}' + (M^{-1}H_\Lambda\eta)^{-2}u_{k,\lambda} = 0. \tag{3.4}$$

We can bring this equation to a well-known ordinary differential equation if we redefine $u_{k,\lambda} = e^{iMt}v_{k,\lambda}$, where t is the comoving cosmological time, in terms of which the scale factor is $a = \exp(H_\Lambda t)$. In this way, and introducing the mode-dependent complex time $T_k = -2i\omega_k\eta$, we finally arrive at

$$T_k\frac{d^2v_{k,\lambda}}{dT_k^2} + (1 - 2iMH_\Lambda^{-1} - T_k)\frac{dv_{k,\lambda}}{dT_k} + iMH_\Lambda^{-1}v_{k,\lambda} = 0. \tag{3.5}$$

This is a confluent hypergeometric equation in the complex variable T_k [46]. Its general solution is given by the following linear combination of convergent hypergeometric functions:

$$\begin{aligned} v_{k,\lambda} = {} & A\,{}_1F_1(-iMH_\Lambda^{-1}; 1 - 2iMH_\Lambda^{-1}; T_k) \\ & + BT_k^{2iMH_\Lambda^{-1}}\,{}_1F_1(iMH_\Lambda^{-1}; 1 + 2iMH_\Lambda^{-1}; T_k), \end{aligned} \tag{3.6}$$

where A and B are arbitrary complex integration constants that may in general depend on ω_k and λ, even if we have not indicated explicitly this possibility. For concreteness, we recall the definition of the hypergeometric function of type (p, q), as a formal power series,

$$\begin{aligned} {}_pF_q(b_1, \ldots, b_p; c_1, \ldots, c_q; z) &= \sum_{n=0}^{\infty} \frac{(b_1)_n \ldots (b_p)_n}{(c_1)_n \ldots (c_q)_n}\frac{z^n}{n!}, \\ (b)_n &= \begin{cases} 1 & \text{if } n = 0, \\ b(b+1)\ldots(b+n-1) & \text{if } n > 0, \end{cases} \end{aligned} \tag{3.7}$$

for b equal to any of the complex numbers $b_1, \ldots, b_p, c_1, \ldots, c_q$. Let us point out that this series converges absolutely for all z if $p \leq q$, while it has a vanishing radius of convergence if $p > q + 1$ [46].

A. Uniqueness from asymptotic diagonalization

In the de Sitter background, formula (3.6) can be used to obtain the form of the general solution $\varphi_{k,\lambda} = f_1^{k,\lambda}(f_2^{k,\lambda})^{-1}$ to Eq. (3.2) and, by means of relation (2.11), the coefficients for the definition of fermionic annihilation and creationlike variables that display no dynamical self-interaction. In what follows, we show that the criterion of asymptotic diagonalization, that leads to the asymptotic expansion given in Eqs. (2.9) and (2.10), uniquely determines a pair of integration constants A and B in Eq. (3.6) (up to a global multiplicative factor), and hence a unique solution $\varphi_{k,\lambda}$.

Let us start by studying the iterative relation (2.10) for the coefficients γ_n that appear in the asymptotic diagonalization expansion, for the classical de Sitter cosmological background. In the considered linearized context, it reads

$$\gamma_0 = -M(H_\Lambda\eta)^{-1},$$
$$\gamma_{n+1} = -\gamma_n' - M(H_\Lambda\eta)^{-1}\sum_{m=0}^{n-1}\gamma_m\gamma_{n-(m+1)}, \qquad \forall\ n \geq 0. \tag{3.8}$$

It is not hard to check that its solution leads to an asymptotic expansion for $\varphi_{k,\lambda}$ of the form

$$\varphi_{k,\lambda} \sim iT_k^{-1}\sum_{n=0}^{\infty}(-T_k)^{-n}C_n,$$
$$C_0 = MH_\Lambda^{-1},$$
$$C_{n+1} = (n+1)C_n + MH_\Lambda^{-1}\sum_{m=0}^{n-1}C_mC_{n-(m+1)}, \qquad \forall\ n \geq 0. \tag{3.9}$$

We do not need to solve the complicated iterative equation for these coefficients, as all the relevant information is contained in the associated expansion of $v_{k,\lambda}$, that we explicitly determine below. In fact, the deduced expression greatly constrains the asymptotic behavior of the corresponding, particular solution $v_{k,\lambda}$ of the confluent hypergeometric equation (3.5). Indeed, since

$$\varphi_{k,\lambda} = 1 + iM^{-1}H_\Lambda T_k\frac{d}{dT_k}(\log v_{k,\lambda}), \tag{3.10}$$

the asymptotic expansion in inverse powers of T_k that we have obtained for $\varphi_{k,\lambda}$ implies that, necessarily,

$$v_{k,\lambda} \sim T_k^{iMH_\Lambda^{-1}}\sum_{n=0}^{\infty}(-T_k)^{-n}v_n, \quad \text{with} \quad v_1 = (MH_\Lambda^{-1})^2v_0. \tag{3.11}$$

The imaginary power of T_k that appears in the above expression in fact is needed to eliminate the term of order 1 in $\varphi_{k,\lambda}$, so that the function $T_k\varphi_{k,\lambda}$ dominantly behaves like iMH_Λ^{-1} when $\omega_k \to \infty$, as it is required by Eq. (3.9). If we introduce this asymptotic expansion for $v_{k,\lambda}$ in the confluent hypergeometric equation that it must satisfy, we find a recursion relation for its constant coefficients v_n,

$$v_{n+1} = \frac{(n + iMH_\Lambda^{-1})(n - iMH_\Lambda^{-1})}{n+1}v_n. \tag{3.12}$$

The solution is clearly

$$v_n = \frac{v_0}{n!}(iMH_\Lambda^{-1})_n(-iMH_\Lambda^{-1})_n \tag{3.13}$$

for an arbitrary constant v_0, and where we have used the notation introduced in Eq. (3.7). So, the asymptotic expansion selected for $v_{k,\lambda}$ by our Hamiltonian diagonalization corresponds to the hypergeometric function

$$v_{k,\lambda} \sim v_0T_k^{iMH_\Lambda^{-1}}\,{}_2F_0(iMH_\Lambda^{-1}, -iMH_\Lambda^{-1}; -; -T_k^{-1}), \tag{3.14}$$

that has a vanishing radius of convergence. Here, the hyphen between semicolons in the argument of the hypergeometric function just indicates the case $q = 0$ of its definition, case for which the denominator in Eq. (3.7) becomes the factorial of n. Even though it is formally divergent, this is precisely the asymptotic expansion (up to the global factor v_0) of a very particular recessive solution of the confluent equation, known as the Tricomi solution [46,47]. We now explicitly prove that this solution is actually the only one that admits such an asymptotic behavior. To do so, we first need the asymptotic expansion of the general solution (3.6) for arbitrary constants A and B. Actually, for $-\pi/2 < \arg(z) < 3\pi/2$, it holds that [47]

$${}_1F_1(b;c;z) \sim \frac{\Gamma(c)}{\Gamma(c-b)}z^{-b}e^{i\pi b}\,{}_2F_0(b, 1+b-c; -; -z^{-1}) + \frac{\Gamma(c)}{\Gamma(b)}z^{b-c}e^{z}\,{}_2F_0(c-b, 1-b; -; z^{-1}), \tag{3.15}$$

so the general solution (3.6) of our confluent equation has the following asymptotic expansion with respect to T_k:

$$v_{k,\lambda} \sim T_k^{iMH_\Lambda^{-1}} {}_2F_0(iMH_\Lambda^{-1}, -iMH_\Lambda^{-1}; -; -T_k^{-1}) \left[A \frac{\Gamma(1-2iMH_\Lambda^{-1})}{\Gamma(1-iMH_\Lambda^{-1})} e^{\pi MH_\Lambda^{-1}} + B \frac{\Gamma(1+2iMH_\Lambda^{-1})}{\Gamma(1+iMH_\Lambda^{-1})} e^{-\pi MH_\Lambda^{-1}} \right]$$
$$+ e^{T_k} T_k^{-1+iMH_\Lambda^{-1}} {}_2F_0(1-iMH_\Lambda^{-1}, 1+iMH_\Lambda^{-1}; -; T_k^{-1}) \left[A \frac{\Gamma(1-2iMH_\Lambda^{-1})}{\Gamma(-iMH_\Lambda^{-1})} + B \frac{\Gamma(1+2iMH_\Lambda^{-1})}{\Gamma(iMH_\Lambda^{-1})} \right]. \quad (3.16)$$

The two terms on the right-hand side of this expression clearly represent (even if only formally) two linearly independent functions of T_k, whereas just one of them appears in the expansion (3.14) that is selected by the asymptotic diagonalization criterion. Therefore, a necessary condition imposed by this criterion is that

$$B = -\frac{\Gamma(iMH_\Lambda^{-1})\Gamma(1-2iMH_\Lambda^{-1})}{\Gamma(1+2iMH_\Lambda^{-1})\Gamma(-iMH_\Lambda^{-1})} A. \quad (3.17)$$

Introducing this value of B in the general formula (3.16), and using the general property of the Gamma function $\Gamma(1+z) = z\Gamma(z)$, with $z \in \mathbb{C}$ [47], we obtain

$$v_{k,\lambda} \sim A T_k^{iMH_\Lambda^{-1}} 4\cosh(\pi MH_\Lambda^{-1}) \times \frac{\Gamma(-2iMH_\Lambda^{-1})}{\Gamma(-iMH_\Lambda^{-1})} {}_2F_0(iMH_\Lambda^{-1}, -iMH_\Lambda^{-1}; -; -T_k^{-1}). \quad (3.18)$$

Comparing once again with the asymptotic expansion (3.14) of our desired solution, we can determine the value of A. In this way, we are univocally led to conclude that

$$A = v_0 \frac{\Gamma(2iMH_\Lambda^{-1})}{\Gamma(iMH_\Lambda^{-1})}, \qquad B = v_0 \frac{\Gamma(-2iMH_\Lambda^{-1})}{\Gamma(-iMH_\Lambda^{-1})}, \quad (3.19)$$

where we have employed the general identity [47]

$$\frac{1}{4\cosh(\pi y)} = \frac{\Gamma(2iy)\Gamma(-2iy)}{\Gamma(iy)\Gamma(-iy)}, \qquad y \in \mathbb{R}.$$

We have henceforth proven that, in a de Sitter background, our asymptotic characterization inspired by hybrid quantum cosmology uniquely picks out a particular solution of the confluent hypergeometric equation (3.5) (up to the irrelevant factor v_0), and therefore a particular function $\varphi_{k,\lambda}$ [cf. Eq. (3.10)] that eliminates the self-interaction in the fermionic Hamiltonian for all $\vec{k} \neq 0$. The specification of $\varphi_{k,\lambda}$, in turn, corresponds to a precise choice of the fermionic annihilation and creationlike variables (2.4), up to the two phases $F_2^{k,\lambda}$ and $J_{k,\lambda}$, and thus to a unique Fock representation (with its associated vacuum state) of the Dirac field. In particular, the selected solution $v_{k,\lambda}$ is given by Eq. (3.6) after substituting the constant coefficients A and B by the values given in Eq. (3.19). Up to the constant factor v_0, the result is then the recessive solution of the confluent hypergeometric equation commonly known as the Tricomi function, usually expressed as $U(-iMH_\Lambda^{-1}, 1-2iMH_\Lambda^{-1}, T_k)$ [46,47].

B. Field decomposition

In this final subsection we explicitly compute the basis of solutions of the Dirac equation in de Sitter cosmology that is associated with the choice of Fock representation selected by the asymptotic diagonalization criterion. It is in terms of this basis that the quantum representation of the Dirac field, viewed as an operator valued distribution, can be decomposed, and the coefficients in such decomposition are the annihilation and creation operators for particles and antiparticles. The fermionic vacuum state in the resulting Fock space is then uniquely specified (up to a phase) as the state that vanishes upon the action of all of the annihilation operators.

In order to obtain this field decomposition, let us first notice that, combining Eqs. (2.2), (2.4), and (2.5), one can express the Dirac field in terms of any canonical set of annihilation and creationlike variables. In the context of QFT in classical cosmological spacetimes, these variables obey the dynamics dictated by the Hamiltonian (2.6)–(2.8) (where the Poisson brackets must be replaced with the corresponding time derivatives). Then, for variables that display no dynamical self-interaction, namely for coefficients $f_1^{k,\lambda}$ and $f_2^{k,\lambda}$ such that Eq. (2.12) holds, we can write the Dirac field as

$$\psi(\eta, \vec{x}) = \sum_{\vec{k},\lambda} [u_{\vec{k},\lambda}(\eta, \vec{x}) A_{\vec{k},\lambda} + w_{\vec{k},\lambda}(\eta, \vec{x}) \bar{B}_{\vec{k},\lambda}], \quad (3.20)$$

where $A_{\vec{k},\lambda} = a_{\vec{k},\lambda}(\eta_0)$ and $B_{\vec{k},\lambda} = b_{\vec{k},\lambda}(\eta_0)$ are the constant annihilation coefficients for particles and antiparticles (to be promoted to the corresponding operators in the Schrödinger picture) and η_0 is an arbitrary choice of initial time employed for their definition. In addition, the basis elements are

$$u_{\vec{k},\lambda}(\eta, \vec{x}) = \frac{e^{i2\pi \vec{k}\vec{x}/l_0}}{\sqrt{l_0^3 a^3}} \left[I - \frac{1-\lambda}{2}(I + i\gamma^0) \right] \bar{f}_2^{k,\lambda} e^{-i\Omega_k(\eta,\eta_0)} \times \begin{pmatrix} \bar{\varphi}_{k,\lambda}(\eta)\xi_\lambda(\vec{k}) \\ \xi_\lambda(\vec{k}) \end{pmatrix}, \quad (3.21)$$

$$w_{\vec{k},\lambda}(\eta,\vec{x}) = -e^{-iJ_{k,\lambda}(\eta_0)}\lambda\gamma^2\bar{u}_{\vec{k},\lambda}(\eta,\vec{x}), \qquad (3.22)$$

where the integrated time-dependent "frequency" of the diagonal evolution of the annihilationlike variables is

$$\Omega_k(\eta,\eta_0) = 2\int_{\eta_0}^{\eta} d\tilde{\eta}a(\tilde{\eta})h_D^{k,\lambda}(\tilde{\eta}). \qquad (3.23)$$

After using the partial differential equation (2.12) and the relation (2.11), the canonical expression for this frequency is found to be given by

$$2h_D^{k,\lambda} = a^{-1}\omega_k + M\mathrm{Re}(\varphi_{k,\lambda}) - \{F_2^{k,\lambda}, H_{|0}\}. \qquad (3.24)$$

It is worth noticing that this formula would hold as well in the full context of hybrid quantum cosmology, employing the perturbatively corrected variables for the homogeneous cosmological sector, once a solution of equation (2.12) had been constructed (ideally by following the criterion of asymptotic diagonalization).

In the de Sitter cosmology under analysis, we recall that the function $\varphi_{k,\lambda}$ is obtained from the solution $v_{k,\lambda}$ of the confluent equation by means of Eq. (3.10), that involves the logarithmic derivative of this solution with respect to the imaginary time $T_k = -2i\omega_k\eta$. We have proven that the condition of asymptotic diagonalization, inspired by hybrid quantum cosmology, serves to select a unique $v_{k,\lambda}$, given by the Tricomi function $U(-iMH_\Lambda^{-1}, 1-2iMH_\Lambda^{-1}, T_k)$ multiplied by a constant factor v_0. The derivatives of this function have been studied in detail [47], and in our case we have

$$\frac{dv_{k,\lambda}}{dT_k} = iv_0MH_\Lambda^{-1}U(1-iMH_\Lambda^{-1}, 2-2iMH_\Lambda^{-1}, T_k). \qquad (3.25)$$

This is a Tricomi function of the form $U(\bar{\mu}+1/2, 2\bar{\mu}+1, -2iz)$, with $\mu = iMH_\Lambda^{-1}+1/2$ and $z=\omega_k\eta$. Tricomi functions of this special type satisfy the identity [47]

$$U\left(\nu+\frac{1}{2}, 2\nu+1, -2iz\right) = \frac{\sqrt{\pi}}{2}ie^{i(\pi\nu-z)}(2z)^{-\nu}H_\nu^{(1)}(z), \qquad (3.26)$$

that relates them to the Hankel function of the first kind $H_\nu^{(1)}$. Applying this property to our solution, we get

$$\frac{dv_{k,\lambda}}{dT_k} = -iv_0\frac{\sqrt{\pi}}{2}MH_\Lambda^{-1}e^{MH_\Lambda^{-1}}e^{-i\omega_k\eta}(2\omega_k\eta)^{\mu-1}H_{1-\mu}^{(1)}(\omega_k\eta). \qquad (3.27)$$

On the other hand, the Tricomi function that appears as the denominator of the logarithmic derivative of $v_{k,\lambda}$ can also be expressed in terms of Hankel functions by using the recursive relation [47]

$$U(-iMH_\Lambda^{-1}, 1-2iMH_\Lambda^{-1}, T_k) = \frac{1}{2}U(-iMH_\Lambda^{-1}, -2iMH_\Lambda^{-1}, T_k) + \frac{T_k}{2}U(1-iMH_\Lambda^{-1}, 2-2iMH_\Lambda^{-1}, T_k). \qquad (3.28)$$

The two functions on the right-hand side are of the special form (3.26), and hence we can write

$$\frac{v_{k,\lambda}(\eta)}{v_0} = \frac{\sqrt{\pi}}{4}e^{MH_\Lambda^{-1}}e^{-i\omega_k\eta}(2\omega_k\eta)^{\mu}[H_{-\mu}^{(1)}(\omega_k\eta) + iH_{1-\mu}^{(1)}(\omega_k\eta)]. \qquad (3.29)$$

Introducing expressions (3.27) and (3.29) in the relation (3.10) between $v_{k,\lambda}$ and $\varphi_{k,\lambda}$, we find the explicit form of this function selected by the asymptotic diagonalization criterion in de Sitter,

$$\varphi_{k,\lambda}(\eta) = \frac{H_{-\mu}^{(1)}(\omega_k\eta) - iH_{1-\mu}^{(1)}(\omega_k\eta)}{H_{-\mu}^{(1)}(\omega_k\eta) + iH_{1-\mu}^{(1)}(\omega_k\eta)}. \qquad (3.30)$$

Its complex conjugate, that directly appears in the basis decomposition (3.20)–(3.22), is then simply

$$\bar{\varphi}_{k,\lambda}(\eta) = \frac{H_{\mu-1}^{(2)}(\omega_k\eta) + iH_{\mu}^{(2)}(\omega_k\eta)}{H_{\mu-1}^{(2)}(\omega_k\eta) - iH_{\mu}^{(2)}(\omega_k\eta)}, \qquad (3.31)$$

where $H_\nu^{(2)}$ is the Hankel function of the second kind and we have used that $\overline{H_\nu^{(1)}(z)} = H_{\bar{\nu}}^{(2)}(\bar{z})$ [47]. This function $\varphi_{k,\lambda}$, in turn, contains all the information about the norm of $f_2^{k,\lambda}$ as displayed in relation (2.11), that encodes the canonical anticommutation algebra of the annihilation and creationlike variables. Explicitly, we obtain the result

$$|f_2^{k,\lambda}|^2 = \frac{\pi\omega_k\eta}{8}e^{\pi MH_\Lambda^{-1}}|H_{\mu-1}^{(2)}(\omega_k\eta) - iH_{\mu}^{(2)}(\omega_k\eta)|^2, \qquad (3.32)$$

after some algebraic manipulations and using the following identity for the Wronskian of Hankel functions [47]:

$$H_{1-\nu}^{(1)}(z)H_{\nu}^{(2)}(z) + H_{-\nu}^{(1)}(z)H_{\nu-1}^{(2)}(z) = -\frac{4i}{\pi z}e^{i\pi\nu}.$$

The only quantity that remains to be determined in order to reach the final form of the decomposition (3.20)–(3.22) of the Dirac field selected by our criterion is the time dependent frequency $\Omega_k(\eta,\eta_0)$. If we particularize the formula for the coefficients $2h_D^{k,\lambda}$ of the diagonal fermionic Hamiltonian, given in Eq. (3.24), to the considered case of a homogeneous de Sitter background with no backreaction, and the function $\varphi_{k,\lambda}$ is identified as the specific one singled out by our criterion, we get that, up to an additive constant,

$$\Omega_k = \theta_k - F_2^{k,\lambda}, \qquad \theta_k(\eta) = \arg\,[H^{(1)}_{-\mu}(\omega_k\eta) + iH^{(1)}_{1-\mu}(\omega_k\eta)], \tag{3.33}$$

where arg[.] denotes the phase of its complex argument. Combining all our results [cf. Eqs. (3.31), (3.32), and (3.33)], the basis of solutions that describes the particles associated with the Fock representation of the Dirac field in de Sitter, uniquely picked out by the asymptotic diagonalization criterion, reads

$$u_{\vec{k},\lambda}(\eta,\vec{x}) = \frac{e^{i2\pi\vec{k}\vec{x}/l_0}}{\sqrt{l_0^3 a^3}}\left[I - \frac{1-\lambda}{2}(I + i\gamma^0)\right] \times \sqrt{\frac{\pi\omega_k\eta}{8}}e^{i\Theta+\pi M H_\Lambda^{-1}/2} \times \begin{pmatrix} [H^{(2)}_{\mu-1}(\omega_k\eta) + iH^{(2)}_{\mu}(\omega_k\eta)]\xi_\lambda(\vec{k}) \\ [H^{(2)}_{\mu-1}(\omega_k\eta) - iH^{(2)}_{\mu}(\omega_k\eta)]\xi_\lambda(\vec{k}) \end{pmatrix}, \tag{3.34}$$

where Θ is a constant global phase, that is irrelevant for the definition of the vacuum. On the other hand, the solutions that describe antiparticles are given by the charge conjugate of these ones, namely via Eq. (3.22). It is worth noticing that the constant phase Θ includes all possible dependence of the basis of solutions on the choice of initial time η_0 for the definition of the annihilation and creationlike constant coefficients, and thus the vacuum that results from our approach is independent of that choice. We also note that, in the asymptotic regime of large k, the leading time dependence of our basis of solutions determined by $u_{\vec{k},\lambda}$ follows the behavior $\exp(-i\omega_k\eta)$, up to multiplication by $a^{-3/2}$ and a constant, something that is often required as a necessary physical feature of the corresponding Fock representation of fields in conformally flat spacetimes [19,48,49]. In particular, the BD Hadamard vacuum for scalar fields in de Sitter displays such a dominant plane wave behavior [2].

In order to establish more precisely the connection between our result and the statements available in the literature about the choice of vacuum state for Dirac fields in de Sitter, we end this subsection by discussing the relation between the mode decomposition of our solutions and the one assigned in Ref. [19] as corresponding to the BD state. First of all, for such a comparison we need to change from the Weyl representation of the constant Clifford algebra (employed here) to the Dirac representation (used in Ref. [19]). They are related by a unitary change of the spinorial basis for the Dirac field, namely

$$\psi^W = T\psi^D, \qquad T = \frac{1}{\sqrt{2}}\begin{pmatrix} I & -I \\ I & I \end{pmatrix}, \tag{3.35}$$

where the superscripts W and D indicate objects in the Weyl and Dirac representations, respectively. For our mode decomposition, this change leads to a basis in the Dirac representation given (up to a global constant phase) by

$$u^D_{\vec{k},\lambda}(\eta,\vec{x}) = \frac{e^{i2\pi\vec{k}\vec{x}/l_0}}{\sqrt{l_0^3 a^3}}\frac{\sqrt{\pi\omega_k\eta}}{2}e^{\pi M H_\Lambda^{-1}/2}\begin{pmatrix} i\lambda H^{(2)}_{\mu-1}(\omega_k\eta)\xi_\lambda(\vec{k}) \\ H^{(2)}_{\mu}(\omega_k\eta)\xi_\lambda(\vec{k}) \end{pmatrix}, \tag{3.36}$$

together with Eq. (3.22) for the charge conjugate counterpart. The resulting basis of solutions is exactly the same as that corresponding to the BD state in Ref. [19], after one interchanges the two (bidimensional) components of the spinor on the right-hand side. Actually, this difference can be attributed just to a change in the global sign of the tetrads that are employed in the two compared works, as we now briefly explain. With our $(-+++)$ convention for the Minkowski metric, the Dirac equation is

$$e^\nu_b \gamma^b D_\nu \psi - M\psi = 0, \tag{3.37}$$

where γ^b are the generators of the constant Clifford algebra in any representation, and D_ν is the spin covariant derivative [50]. Here, ν denotes a spacetime tensor index, whereas $b = 0, \ldots 3$ is an internal Lorentz index. The spin covariant derivative contains a connection one-form which depends on the tetrads e^ν_b and their derivatives only through quadratic and quartic products. It then follows that interchanging two choices of tetrad that differ only in a global multiplicative sign has exclusively the net effect of an apparent flip of sign in the mass term of the Dirac equation, in what concerns the choice of gauge for the Dirac field as a solution to this equation. According to our comments in Sec. II, in the expanding flat chart of de Sitter (in conformal time) we have selected the tetrad as $e^\nu_b = a^{-1}\delta^\nu_b$, where the scale factor a is given in Eq. (3.1). The choice employed in Ref. [19] is precisely the opposite in sign, i.e., it is given by minus this tetrad. For both choices, if one then works, e.g., in the Dirac representation of the Clifford algebra, the Dirac equation can be recast as a second order Bessel differential equation in $x = \omega_k\eta$ for the time-dependent factor of the first (bidimensional) component of $\eta^{-2}u^D_{\vec{k},\lambda}$. The second component is completely fixed in terms of the first one by means of the Dirac equation. The difference between the two considered conventions in the choice of tetrad (ours and that of Ref. [19]) is reflected in the order of the Bessel equation, that becomes, respectively, $\mu - 1$ and μ. The solutions that have an asymptotic behavior with a dominant time-dependence proportional to $x^{-1/2}\exp(-ix)$ are uniquely given, respectively, by $H^{(2)}_{\mu-1}(x)$ and $H^{(2)}_{\mu}(x)$ [47]. The second component of $\eta^{-2}u^D_{\vec{k},\lambda}$ then results proportional to $H^{(2)}_{\mu}(x)$ and $H^{(2)}_{\mu-1}(x)$, respectively. The remaining factors of the spinor (3.36) are determined by the normalization of the solutions [19]. We recall that the above Hankel functions are precisely the two parts that must be interchanged in Eq. (3.36) in order to identify the bases of solutions constructed in the two considered works, up to a global phase. Therefore, we conclude that the vacuum state for the Dirac field resulting from our analysis corresponds indeed to the BD state defined in Ref. [19], once the same choice of local Lorentz gauge is made.

IV. CONCLUSIONS

In this paper we have shown how the criterion of asymptotic diagonalization, originated in the framework of hybrid quantum cosmology, can serve to single out a privileged Fock representation of the Dirac field in de Sitter spacetime, within the context of QFT in curved spacetimes. The explicit basis of solutions to the Dirac equation associated with that choice of representation has also been computed, in terms of Hankel functions of the first and second kind, and in coordinates associated with the conformal flat slicing of de Sitter. Furthermore, the canonical expression for the resulting diagonal Hamiltonian that dictates the linearized dynamics of the annihilation and creationlike variables selected by our criterion has been found, exclusively in terms of them and functions of the homogeneous variables that describe the cosmological background. In particular, the derived formula (3.24) could be of potential use in hybrid quantum cosmology, if the asymptotic diagonalization problem is solved for more general cosmological backgrounds than de Sitter.

The hybrid approach to quantum FLRW cosmology with perturbations contemplates the natural freedom of making a dynamical splitting between the spatially homogeneous, global, degrees of freedom of the system and the inhomogeneous perturbations. When these perturbations consist of a Dirac field, such freedom can be encoded in choices of annihilation and creationlike variables, given by linear transformations of the field mode coefficients that depend explicitly on the homogeneous background. These transformations can be completed so that they become canonical for the entire cosmological system, truncated at quadratic perturbative order in the action, a procedure that leads to a fermionic contribution to the total Hamiltonian that dictates the linearized dynamics of the annihilation and creationlike variables. The criterion of asymptotic diagonalization consists in restricting almost all the freedom in the selection of these variables, and with it the aforementioned dynamical splitting, together with the Fock quantization of the fermionic degrees of freedom, so that the fermionic Hamiltonian gets diagonalized in a way that is adapted to its local structure. This strategy provides a very precise asymptotic expansion of the functions of the background that define the annihilation and creationlike variables. In turn, this determines the expansion of at least one solution of the partial differential equation (2.12), that arises from the general demand that the Hamiltonian become diagonal.

If one disregards all backreaction effects of the perturbations on the homogeneous background, and considers that this cosmological background is just a solution of the classical FLRW spacetime, the possible definitions of annihilation and creationlike variables compatible with the requirements of hybrid quantum cosmology can directly be understood as different choices of Fock representations of the Dirac field in the context of QFT in curved spacetimes. We have restricted our attention to this situation and, furthermore, we have particularized the FLRW background, identifying it with a de Sitter solution. Then, we have shown that the asymptotic expansion selected by the criterion of asymptotic diagonalization indeed picks out a *unique* function among those that define annihilation and creationlike variables that follow a diagonal evolution for all spatial scales. The basis of solutions to the Dirac equation associated with the resulting Fock representation of the field can be specified completely and in an analytical way.

Our result is potentially relevant within QFT, as well as in the context of quantum cosmology. On the one hand, we have explicitly provided a unique fermionic vacuum in de Sitter spacetime selected by a very well characterized criterion, that has its original motivation in hybrid quantum cosmology. This sheds further light on the question of which is the natural analog of the BD vacuum for a Dirac field. In this context, our analysis precisely leads to the basis of solutions for the field that has been assigned to correspond to such a fermionic BD state in the literature [19]. In particular, it displays the ultraviolet behavior expected to guarantee Hadamard-like properties. This result supports the potential robustness of our criterion to select a privileged fermionic vacuum state in FLRW cosmologies, specially considering that the very same criterion of asymptotic diagonalization has succeeded in predicting the BD vacuum for the well-known cases of scalar and tensor perturbations [42]. On the other hand, our work shows that, at least in certain cases, the criterion employed in hybrid quantum cosmology to (i) determine a dynamical splitting between the homogeneous and inhomogeneous sectors in phase space, and (ii) select a Fock representation for the inhomogeneities, can indeed result into a complete removal of both types of ambiguities, even when this criterion was initially based solely on ultraviolet considerations.

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Non-oscillating power spectra in loop quantum cosmology

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Abstract
We characterize in an analytical way the general conditions that a choice of vacuum state for the cosmological perturbations must satisfy to lead to a power spectrum with no scale-dependent oscillations over time. In particular, we pay special attention to the case of cosmological backgrounds governed by effective loop quantum cosmology and in which the Einsteinian branch after the bounce suffers a pre-inflationary period of decelerated expansion. This is the case more often studied in the literature because of the physical interest of the resulting predictions. In this context, we argue that non-oscillating power spectra are optimal to gain observational access to those regimes near the bounce where loop quantum cosmology effects are non-negligible. In addition, we show that non-oscillatory spectra can indeed be consistently obtained when the evolution of the perturbations is ruled by the hyperbolic equations derived in the hybrid loop quantization approach. Moreover, in the ultraviolet regime of short wavelength scales we prove that there exists a unique asymptotic expansion of the power spectrum that displays no scale-dependent oscillations over time. This expansion would pick out the natural Poincaré and Bunch–Davies vacua in Minkowski and de Sitter spacetimes, respectively, and provides an appealing candidate for the choice of a vacuum for the perturbations in loop quantum cosmology based on physical motivations.

Keywords: loop quantum cosmology, cosmological perturbations, vacuum state, power spectrum

(Some figures may appear in colour only in the online journal)

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1. Introduction

The observational field of high precision cosmology is currently at a full peak of activity, and it is expected to continue growing with feedback from the recent breakthrough of multimessenger astronomy. The success in this field is especially evident when one takes into account the measurements that have been, and are being performed, of the cosmic microwave background (CMB) [1, 2]. These observations, when supplemented with a theoretical model, could shed light on quantum gravity effects of the cosmological geometry that may have had an impact on the evolution of primordial fluctuations of the spacetime content. In fact, these fluctuations are believed to constitute the origin of the spatially inhomogeneous degrees of freedom of the early Universe, and they would have undergone a period of inflation after being originated in epochs of increasingly high energy density and spacetime curvature. In addition, they are believed to be responsible for the measured distribution of temperature anisotropies in the CMB [3, 4]. Under such extreme pre-inflationary conditions, it is reasonable to consider that the quantum nature of the cosmological spacetime may have had an important influence on the physical phenomena that took place before inflation.

Over the last decades, there have been several theoretical attempts to incorporate quantum gravity effects in the study of a primordial cosmology with inhomogeneous perturbations (see, e.g. [5–29] and references therein). Furthermore, many of them have succeeded in deriving first approximations to the type of modifications that one can expect to be relevant in the evolution of the perturbations, coming from the quantum behavior of the cosmological spacetime background. In particular, it is worth pointing out interesting investigations on this topic that, within the context of loop quantum cosmology (LQC) [30–33], lead to modifications that are compatible with the observations of the CMB and, at the same time, are potentially capable of capturing information about the quantum nature of the cosmological background [21, 29, 34].

LQC is known to provide a mathematically robust quantization of homogeneous and isotropic cosmologies of the Friedmann–Lemaître–Robertson–Walker (FLRW) type, with the remarkable result of generally replacing the cosmological big bang singularity with a bounce of quantum origin [35, 36]. The theoretical question of how one should include perturbations in the LQC description of FLRW spacetimes has been widely studied over the last years, starting from a variety of different fundamental hypotheses, and with different strategies motivated by first principles and/or phenomenological issues. Among the proposed approaches, let us mention the effective deformed constraint algebra [10–13], the separate Universe framework [14, 15], quantum reduced loop gravity [16, 17], the dressed metric formalism [18–21], and hybrid LQC [22–29]. All these approaches are limited by the use of a series of assumptions that are specific of each strategy. In this work, we will focus our attention on the two last mentioned strategies. They are two continued lines of research that have led to preliminary predictions that appear to be compatible with cosmological observations at a reasonable level. In hybrid LQC, one considers the cosmological system described in general relativity by an FLRW metric (typically with compact spatial sections) and an inflaton field with inhomogeneous perturbations, truncates the corresponding Einstein–Hilbert action at lowest non-trivial perturbative order, and identifies a complete set of canonical variables for the description of the FLRW cosmology and the perturbative gauge invariants [26]. The total Hamiltonian of this perturbatively truncated system is then a linear combination of constraints, inherited from those of the Arnowitt–Desser–Misner (ADM) canonical formulation of full general relativity. The hybrid strategy to quantize these constraints consists in adopting a polymeric representation for the canonical variables that describe the FLRW background, inspired by the LQC quantization of homogeneous cosmologies, while a more standard Fock representation is employed for the perturbative degrees of freedom. This hybrid approach is affected by the breaking of local

Lorentz symmetry inherent to all of the descriptions in loop quantum gravity that are formulated in terms of $SU(2)$ connections, a fact that is related with the appearance of the Immirzi ambiguity [37], as well as by issues about the quantum preservation of full diffeomorphism covariance that are typical of quantizations that rest on an ADM canonical formalism. Obviously, it also assumes the validity of a perturbative hierarchy and that the genuine loop quantum geometry effects can be neglected except for those arising directly from the canonical degrees of freedom associated with the cosmological scale factor. The combination of representations used in the hybrid strategy should ultimately lead to a consistent and well-defined set of constraint operators. In this process, one frequently studies a rescaled version of the spatial average of the Hamiltonian constraint, in which a power of the scale factor is absorbed by a mathematically well-defined procedure [26, 36]. On the other hand, the dressed metric approach to the LQC treatment of cosmological perturbations does not rely on a canonical framework for the entire system. As a consequence, the resulting formulation is not that of a constrained system, with the subsequent problems for diffeomorphism covariance. Instead, it starts from the LQC solutions of the FLRW background cosmology, and then lifts the main quantum effects on their dynamics to a physical Hamiltonian for the perturbations [19]. The dressed metric approach assumes as well the validity of a perturbative hierarchy (the self-consistency of which may be checked when studying a particular quantum state) and that the genuine loop quantum geometry effects are directly relevant only on the FLRW background. Moreover, it presumes that these quantum effects can be lifted to the dynamics of the perturbations by capturing them in a reduced number of quantities, generally given by some expectation values of the background geometry.

Both of these theoretical frameworks have been able to provide (effective or mean-field) equations for the gauge invariant perturbations that, while possessing the same local and causal structure as the classical ones, display contributions from the background that contain LQC modifications. In particular, these corrections are able to account for the presence of the bounce of quantum origin that replaces the classical singularity. Furthermore, although in principle it is not necessary for the applicability of the two approaches, the state for the homogeneous geometry is often picked out in such a way that those corrections are limited to the vicinity of the bounce, so the evolution of the background cosmology becomes classical very rapidly, and such that the effects of the corrections may be observable today in the CMB [21, 29]. More specifically, as a particularization to cases of particular interest, one usually focuses the attention on certain class of states of the homogeneous geometry for which the cosmological perturbations propagate in practice over a background that is governed by an effective description of LQC. These effective background geometries are characterized by trajectories for the FLRW variables that undergo a bounce when the energy density of the Universe reaches the maximum universal value of (approximately) 41 percent of the Planck density (for the most commonly accepted value of the Immirzi parameter). Away from the vicinity of this bounce, namely when the quotient between the energy density and this maximum can be neglected when compared with the unit, these trajectories behave as if they were solutions to the Friedmann equations. The existence of this type of effective behavior in the loop quantization of massless FLRW cosmologies has been studied in the literature [31–33, 35]. In particular, it is known their relation with certain family of Gaussian states of the FLRW model in LQC, that are globally peaked on values of the homogeneous volume and the homogeneous inflaton that follow these effective trajectories [38]. In this regime of LQC and in the associated quantum description of the cosmological perturbations, the differences between the hybrid and dressed metric approaches can be narrowed precisely to a small region around the bounce, and they affect the effective field equations for the perturbations in that region only through the time-dependent mass that appears in them [39]. In fact, these differences are only due to the respective strategies adopted for the introduction of inhomogeneous perturbations on the quantization of FLRW cosmologies, and they persist even if one considers the same effective LQC trajectories for the background in both approaches.

In general, complete sets of (complex) solutions to the field equations of the gauge invariant perturbations, both for the classical equations and for the quantum corrected ones (whether derived either from hybrid LQC or from the dressed metric approach) give rise to different power spectra that can be eventually confronted with observations. In order to select one of these sets, it suffices to establish initial conditions for the fields at some time of the evolution of the perturbations, thanks to the causal structure of their dynamical equations. Such a choice of initial conditions is usually interpreted as a specification of vacuum state for the perturbations, quantized à la Fock. In particular, in the standard cosmological paradigm this initial time is typically set at the onset of inflation, and the data there are fixed to correspond with the Bunch–Davies state [4, 40]. This choice is physically reasonable because the standard slow-roll inflationary period is well modelled by de Sitter spacetime, and the Bunch–Davies state is the most natural candidate in this context (i.e. it is the unique Hadamard state that is invariant under the de Sitter isometry group). Remarkably, it provides power spectra for the perturbations that lead to predictions which quite accurately match the observations of the CMB, at least for a large sector of angles in the sky [2]. However, when the physics that took place before inflation and all the way back to the cosmological singularity (or its quantum analog) is considered to be relevant, the choice of a natural vacuum state for the perturbations fails to be a settled issue. Indeed, the background spacetime in those pre-inflationary epochs, even in the case it remains semiclassical at least for some stages of the evolution, does no longer resemble de Sitter and its symmetries alone are not enough to fix a unique state. One can restrict this freedom by imposing, on top of invariance of the state under the spatial symmetries, the requirement that the field dynamics is unitarily implementable in the quantum theory (at least in the semiclassical regimes). This criterion actually succeeds in selecting a unique Fock space of states for the perturbations [41, 42]; however additional input is needed to single out a preferred vacuum state there.

The choice of a natural state, or equivalently of initial conditions, for the gauge invariant perturbations is a fundamental question to establish the predictive power of any approach to quantum cosmology that provides equations for the perturbations encoding quantum gravity features of the background geometry. In particular, this question needs to be answered if one wants to have any hope of disentangling the possible modifications on the power spectra resulting from genuine quantum cosmology effects from other features of the spectra caused by alternate choices of vacua, that could also arise in a purely classical pre-inflationary cosmology. Concerning this issue, several proposals have been put forward in the context of hybrid and dressed metric LQC. In these frameworks, a natural choice of initial time to set the data for the perturbations, and thus their vacuum state, is the moment at which the cosmological bounce happened. Certain low order adiabatic states were first considered owing to their nice properties regarding the renormalizability of the energy–momentum tensor [21, 43, 44]. More recently, a somewhat different criterion for the choice of vacuum state has been proposed by Ashtekar and Gupt, based on minimizing the quantum uncertainties of the fields around the bounce and, at the same time, recovering a classical behavior at the onset of inflation [45, 46]. This choice has actually been quite successful in terms of its compatibility with observations in the dressed metric scenario, displaying a slight power suppression for the largest wavelength scales. Nonetheless, all of these vacua lead to power spectra that are highly oscillatory with respect to the scales of observational interest, even in regimes where the pre-inflationary evolution of the background is completely classical, and these oscillations have to be averaged prior to the extraction of predictions. Actually, in the case of adiabatic states, these oscillations are present both in hybrid and dressed metric LQC and they are responsible for an important amplification of the power at medium scales that seems to be in certain tension with the observational data [29, 47]. Even if this possible amplification effect may not be significant in some cases, as it seems to happen with the proposal of Ashtekar and Gupt, one may wonder whether such highly oscillatory behavior of the power spectrum can wash out, or at least obscure, the information about the traces of quantum geometry that the non-Einsteinian evolution of the background cosmology close to the bounce could have imprinted in the dynamics of the perturbations. Motivated by these concerns, Martín de Blas and Olmedo have proposed a different choice of state, based on a selection criterion that is directly tailored to minimize, by numerical methods, the oscillations in the resulting power spectrum [48]. This state has been called the non-oscillating (NO) vacuum state. The resulting power spectrum in hybrid LQC seems to be in very good agreement with observations and, again, predicts power suppression at large scales.

A theoretical drawback of the two mentioned proposals for the choice of a vacuum for the cosmological perturbations in LQC is that their characterization strongly relies on numerical and/or minimization techniques, that are often interrelated. In this context, the purpose of this work is precisely to provide *analytical* insights supporting a specific characterization of vacuum state, gained by studying some of the general properties of power spectra for gauge invariant perturbations in effective descriptions of LQC that include a period of classical (i.e. Einsteinian) pre-inflationary cosmology. In particular, after a study of the solutions to the field equations for the perturbations using explicitly time-dependent transformations, we provide theoretical arguments that put the focus on power spectra that display NO behavior. Then, starting with the Ermakov–Pinney equation [49, 50], we make use of a general formula for the computation of any power spectrum in order to characterize specific conditions that the associated solutions to the field equations must fulfill to minimize the oscillations. After successfully checking that both the Bunch–Davies state in de Sitter spacetime and the Poincaré state in Minkowski spacetime satisfy these conditions, we discuss their application to effective regimes of LQC. Finally, we show that, in the ultraviolet regime of short wavelength scales, there is a unique asymptotic expansion of the power spectrum that displays no oscillations at any asymptotic order. This expansion may potentially serve to fix a unique physically privileged vacuum state for the perturbations, and thus a preferred power spectrum, provided that the NO conditions remain satisfied at all scales.

The paper is structured as follows. In section 2 we formulate the field equation for the perturbations and, analyzing the Hamiltonian that generates this field evolution, we consider time-dependent canonical transformations that render this Hamiltonian diagonal. We use this procedure to construct and conveniently characterize all the normalized solutions. We then provide a qualitative analysis of their power spectra in the context of effective regimes in LQC and argue in favour of the physical importance of finding NO features in it. Section 3 is devoted to the specific characterization of conditions on general power spectra such that they display no scale-dependent oscillations over time, making an auxiliary use of the Ermakov–Pinney equation that is naturally associated with our field equations. We then analyze the feasibility of these conditions in hybrid LQC. In section 4 we focus on the ultraviolet sector of short wavelength scales, and perform a study of the oscillatory behavior of the power spectra there. In particular, we show that there is a unique asymptotic expansion for which one can say that no oscillations appear at any order. We end the section remarking on the physical relevance of such expansion in order to fix a natural vacuum state for the perturbations in effective LQC. Finally, in section 5 we summarize our results. Throughout the paper we work in Planck units, setting $\hbar = c = G = 1$.

2. Solutions from Hamiltonian diagonalization

Consider a real scalar field $\mathcal{V}(\eta, \vec{x})$, where η is a time coordinate and $\vec{x}$ is a triple of spatial coordinates in $\mathbb{R}^3$, with a Fourier expansion in spatial plane waves in which the mode coefficients $v_{\vec{k}}(\eta)$ satisfy the equation

$$v''_{\vec{k}} + (k^2 + s)v_{\vec{k}} = 0, \quad k = |\vec{k}|, \quad \vec{k} \in \mathbb{R}^3 - \{0\}. \tag{2.1}$$

Here, the primes denote derivatives with respect to η, and s is a time-dependent real function that we call mass, owing to the formal similarities between this equation and that of a harmonic oscillator with mass. We notice that, for the field $\mathcal{V}(\eta, \vec{x})$ to be real, these mode coefficients must satisfy the reality condition $\bar{v}_{\vec{k}} = v_{-\vec{k}}$. Here and in the following, the bar indicates complex conjugation. Fields with this type of Fourier expansion and dynamics are precisely the ones that describe the gauge invariant perturbations in effective formalisms and mean-field approximations of LQC, when η is identified with the conformal time. Specifically, these perturbations are the Mukhanov–Sasaki field for scalar degrees of freedom, and the inhomogeneous contributions of tensor nature to the FLRW metric [51–53]. The power spectra associated with these fields are defined in cosmology as [54]

$$\mathcal{P}_{\mathcal{V}}(k, \eta) = \frac{k^3}{2\pi^2}|\mu_k(\eta)|^2, \tag{2.2}$$

where μ_k for all $\vec{k} \neq 0$ is a set of complex solutions to equation (2.1) that is required to be normalized according to

$$\mu_k \bar{\mu}'_k - \mu'_k \bar{\mu}_k = \mathrm{i}. \tag{2.3}$$

This last requirement on the set of solutions guarantees that the resulting spectra can be directly obtained from the two-point function at equal time of a Fock representation of the field $\mathcal{V}(\eta, \vec{x})$ that is invariant under the Euclidean symmetries of the cosmological background.

Power spectra are typically evaluated at the end of the (slow-roll) inflationary period in cosmology. Thus, any effect of the dynamical evolution of the perturbations prior to that period that may be observable in the CMB must be found imprinted in the spectra at that moment. If the spectra have oscillated over time during the previous evolution, and these oscillations depend on the Fourier scale, we expect that they will be captured as oscillations in the scale k at the evaluation time. All our following discussions about oscillatory power spectra will keep in mind this relation between the two possible types of dependence of the oscillations. In fact, this very relation is at the heart of the proposal of vacuum state made by Martín de Blas and Olmedo in reference [48].

For a general time-dependent mass s any dynamical equation of the form (2.1) can be obtained from the Hamiltonian

$$H_{\vec{k}} = \frac{1}{2}\left[\left(k^2 + s\right)|v_{\vec{k}}|^2 + |\pi_{v_{\vec{k}}}|^2\right], \tag{2.4}$$

where $\pi_{v_{\vec{k}}}$ is to be understood as the canonical momentum of $v_{\vec{k}}$ and satisfies analogous reality conditions. Note that this Hamiltonian generates both the evolution of $v_{\vec{k}}$ and $v_{-\vec{k}}$. In order to study some general properties of the solutions to equation (2.1), starting from this Hamiltonian framework it is convenient to perform explicitly time-dependent canonical transformations of $v_{\vec{k}}$, $\pi_{v_{\vec{k}}}$, and their complex conjugates such that the resulting variables obey Hamilton equations that are purely diagonal. With this purpose, we introduce the transformation

$$a_{\vec{k}} = f_k v_{\vec{k}} + g_k \bar{\pi}_{v_{\vec{k}}}, \qquad \bar{a}_{\vec{k}} = \bar{f}_k \bar{v}_{\vec{k}} + \bar{g}_k \pi_{v_{\vec{k}}}, \tag{2.5}$$

where f_k and g_k are unspecified complex functions that depend explicitly on time, and are subject to the constraint

$$f_k\bar{g}_k - g_k\bar{f}_k = -i, \tag{2.6}$$

that in particular imposes that none of these functions can be zero at any instant of time. Condition (2.6) is simply the requirement that the introduced transformation is canonical, up to a constant factor $-\mathrm{i}$. The Hamiltonian for the new variables $a_{\vec{k}}$, $a_{-\vec{k}}$, and their complex conjugates can be obtained by adding to the former one, given in equation (2.4), the explicit time derivative of the generating function of the canonical transformation (2.5). The result is

$$\begin{aligned}\tilde{H}_{\vec{k}} = {} & \left[\left(k^2+s\right)|g_k|^2 + |f_k|^2 + \bar{f}_k g_k' - \bar{g}_k f_k'\right]\left(\bar{a}_{\vec{k}}a_{\vec{k}} + \bar{a}_{-\vec{k}}a_{-\vec{k}}\right) \\ & - \left[\left(k^2+s\right)g_k^2 + f_k^2 - g_k f_k' + f_k g_k'\right]\bar{a}_{\vec{k}}\bar{a}_{-\vec{k}} + \text{c.c.},\end{aligned} \tag{2.7}$$

where c.c. indicates the complex conjugate of the preceeding term. This new Hamiltonian generates diagonal equations for $a_{\vec{k}}$, $a_{-\vec{k}}$, and their complex conjugates if and only if

$$h_k' = k^2 + s + h_k^2, \quad \text{with} \quad h_k = f_k g_k^{-1}. \tag{2.8}$$

This is an ordinary differential equation of the Riccati type for the function h_k, which is equivalent to the set of coupled equations

$$\mathrm{Re}(h_k)' = k^2 + s + \mathrm{Re}(h_k)^2 - \mathrm{Im}\,(h_k)^2, \tag{2.9}$$

$$\mathrm{Im}\,(h_k)' = 2\mathrm{Re}(h_k)\,\mathrm{Im}(h_k), \tag{2.10}$$

for its real and imaginary parts. Furthermore, one can check that the canonical condition (2.6) is equivalent to

$$|g_k|^2 = -\frac{1}{2\,\mathrm{Im}(h_k)}. \tag{2.11}$$

So, consistency requires that any allowed solution h_k of equation (2.8) must have a strictly negative imaginary part. It follows that, given any such complex h_k, the resulting diagonal Hamiltonian acquires the form

$$\tilde{H}_{\vec{k}} = -\Omega_k\left(\bar{a}_{\vec{k}}a_{\vec{k}} + \bar{a}_{-\vec{k}}a_{-\vec{k}}\right), \quad \Omega_k = F_k' + (k^2+s)\frac{\mathrm{Im}(h_k)}{|h_k|^2}, \tag{2.12}$$

where F_k is the phase of f_k. The equations of motion for $a_{\vec{k}}$, $a_{-\vec{k}}$, and their complex conjugates are straightforward to solve in terms of initial data at an arbitrary time η_0. These, in turn, give rise to solutions of our original equation (2.1), obtained by simply taking the inverse of the canonical transformation (2.5). Specifically, these solutions are

$$v_{\vec{k}} = \mathrm{i}\bar{g}_k \mathrm{e}^{-\mathrm{i}\int_{\eta_0}^{\eta}\mathrm{d}\tilde{\eta}\,\Omega_k(\tilde{\eta})}a_{\vec{k}}(\eta_0) - \mathrm{i}g_k\mathrm{e}^{\mathrm{i}\int_{\eta_0}^{\eta}\mathrm{d}\tilde{\eta}\,\Omega_k(\tilde{\eta})}\bar{a}_{-\vec{k}}(\eta_0). \tag{2.13}$$

Let us notice that, since $g_k = f_k h_k^{-1}$, each of the two summands in the above solution depends on F_k only through multiplication by the complex exponential of its constant value at η_0. Furthermore, equation (2.1) is linear with real coefficients, so each of the summands in question (multiplied by any constant) provides a complex solution on its own. It follows that we can freely choose F_k as the phase of h_k, so that g_k becomes real, and then obtain the following solutions to equation (2.1):

$$\mu_k = \frac{1}{\sqrt{-2\,\mathrm{Im}(h_k)}}\mathrm{e}^{\mathrm{i}\int \mathrm{d}\eta\,\mathrm{Im}(h_k)}, \tag{2.14}$$

as well as their complex conjugates. It is straightforward to check that these solutions are normalized according to equation (2.3), which in particular implies that μ_k and its complex conjugate are linearly independent. Actually, one can see that any complex solution to equation (2.1) normalized in this way is of the form (2.14), with the role of $\mathrm{Im}(h_k)$ played by some strictly negative function which satisfies the same second order differential equation as the imaginary part of h_k [equation that can be derived from equations (2.9) and (2.10)] [44]. This function is completely fixed once one supplies its value and its first derivative at the initial time η_0. But we can in fact reproduce any such values by varying the initial data for the real and imaginary parts of h_k, in virtue of equation (2.10). It follows that we can write any normalized solution μ_k of our original equation (2.1) like in formula (2.14), where h_k is any solution of the Riccati equation (2.8) with a strictly negative imaginary part. Finally, linear combinations of μ_k and $\bar{\mu}_k$ provide the general solution to equation (2.1).

The advantages of characterizing the normalized solutions to equation (2.1) by means of formulas (2.8) and (2.14) are many. On the one hand, some general features of these solutions, and of their associated power spectra, can be easily deduced from a direct inspection of the resulting equations for the real and imaginary parts of h_k. On the other hand, we will see in section 4 that it is possible to characterize a very specific solution to equation (2.8) in the asymptotic limit of large k that has an associated spectrum with the most satisfactory properties in this asymptotic regime.

2.1. NO spectra in effective LQC

The analysis performed so far is valid for any real function of time s, playing the role of a mass in equation (2.1). Let us focus now on the case of cosmological perturbations in the hybrid and dressed metric approaches to inflationary LQC, where the mass s becomes a specific function of the quantum FLRW geometry on the state that describes the background [20, 26, 28, 39]. Inflation is accounted for by the presence of a homogeneous scalar field (with inhomogeneous perturbations), that we call the inflaton, subject to a potential that, for concreteness, we choose to be quadratic in the field. In certain regimes of these LQC models, the power spectrum constructed from a solution to equation (2.1) can be understood as the two-point function at equal time of the quantum Heisenberg field operators that describe the Mukhanov–Sasaki perturbations or, as the case may be, the tensor perturbations. Namely, it represents the expectation value on the vacuum state of the product of two field operators, evaluated at different spatial points. This interpretation can be formally justified as follows in the case of hybrid LQC, beginning from the perturbatively truncated system (for specific details and formulas, we refer the reader to references [26, 27, 55, 56]). One starts with a specific ansatz for the quantum states in which the wave function factorizes its dependence on the background FLRW geometry and the gauge invariant perturbations, while both parts are allowed to depend on the inflaton field. Searching for states of physical interest, one usually imposes that the partial wave function that describes the FLRW part is close to a solution of homogeneous and isotropic LQC with an inflaton field. Introducing an approximation that is based on the hypothesis of negligible state transitions on the FLRW geometry, the total Hamiltonian can then be reduced to a constraint operator acting only on the partial wave function that corresponds to the gauge invariant perturbations. This hypothesis mathematically amounts to additional conditions on the partial wave function of the FLRW geometry, namely, that it is peaked with respect to some operators of the homogeneous geometry, that are finite in number (see reference [26] for futher details). Remarkably, the resulting constraint on the perturbations depends on the homogeneous geometry only via expectation values of geometric LQC operators on the partial FLRW wave function of the state. Then, if the Fock representation of the gauge invariant perturbations has been chosen adequately, the Heisenberg evolution of the annihilation and creation operators for the perturbations generated by the aforementioned constraint can be implemented unitarily on Fock space. The construction of the associated unitary operator involves a careful definition of the conformal time to absorb the expectation value of certain geometric operators on the partial state of the FLRW geometry [26, 55]. In fact, this evolution operator can potentially be used to construct solutions to this constraint, namely (approximate) physical states for the perturbations. Furthermore, the Heisenberg equations deduced in this manner turn out to be precisely of the form of equation (2.1). Our quantum states of interest can then be understood within a context of quantum field theory on a quantum FLRW background, in which the computation of the two-point functions for the gauge invariant fields is equivalent to solving equation (2.1) and evaluating the corresponding power spectra. Different solutions to equation (2.1) just correspond to different choices of states for the gauge invariant perturbations. It is worth pointing out that this equivalence is completely independent of the specific details of the wave function that describes the cosmological background, provided that it is close to a solution of homogeneous LQC with negligible geometry transitions, according to our above discussion. Nonetheless, the details of this FLRW state are transcribed into features of s. In what respects the pure computation of the two-point function, in particular, the considered partial FLRW wave function need not obey a semiclassical behavior as long as it fulfills the aforementioned requirements. Moreover, even if the state of the background cosmology does display a prominent semiclassical behavior, the Fock state of the perturbations may still possess genuine quantum features.

Starting from equations of the form (2.1) for the gauge invariant perturbations, where we recall that s contains the most relevant quantum effects of the cosmological background, in this work we will focus only on modifications that are important in what is known as effective LQC. This is a regime obtained by considering a very specific type of state for the background cosmology, motivated as a solution of homogeneous and isotropic LQC, that is peaked on a certain bouncing trajectory. More concretely, this trajectory can be analytically modelled by equations that are of the FLRW type until, towards the past, the energy density ρ reaches a few percentages of Planck density (for the standard value of the Immirzi parameter within homogeneous LQC). For larger densities, the considered equations dictate a departure from general relativity such that the scale factor a reaches a minimum, corresponding to the moment at which the bounce occurs [32]. As it was commented in the Introduction, this bounce happens at a universal value of the energy density that is roughly given by 0.41 times the Planck density (again for the most frequently accepted value of the Immirzi parameter). Furthermore, in order to extract meaningful predictions about the evolution of cosmological perturbations, one typically focuses only on those background trajectories such that the quantum behavior of the Hubble parameter H may only affect the sector of large wavelength scales of the perturbations that are observable nowadays at large angular scales in the CMB. In this way, it is assured that the quantum corrections do not alter the behavior of the shorter scales in the observed spectrum, which is very well explained by general relativity, while some quantum cosmology modifications may survive in the rest of scales.

The commented solutions for the cosmological background in effective LQC, that are of phenomenological interest for the study of perturbations, are characterized by the following type of initial conditions at the bounce. In what concerns the geometry, on the one hand the

Hubble parameter is zero at the bounce, since the scale factor is at a minimum there. On the other hand, with an appropriate use of conformal time, one can make the effective LQC equations (as well as the FLRW ones) only dependent on the relative variation of the scale factor with respect to its value at, e.g. the bounce [57]. We take a as this relative variation; so we have $a = 1$ at the bounce. Concerning the homogeneous matter content, our solutions are characterized by an energy density which is dominated by its kinetic contribution at the bounce, namely the contribution from the time derivative of the inflaton, while the potential there is negligible. In the case of a quadratic inflaton potential, it has been proven that these types of initial data are the only ones that lead to LQC effects that may be observable nowadays in the sector of large angular scales of the CMB, while leaving unaffected the rest of scales which are well described by standard FLRW inflationary cosmology [21, 29, 34, 63]. Explicitly, this feature on the allowed effective LQC solutions requires the contribution of the potential to the energy density of the Universe at the bounce to be approximately of the order 10^{-12}. For further details about the phenomenological viability of the different regions in the parameter space that specifies the initial data of effective LQC (namely, the value of the inflaton at the bounce and its mass), we refer the reader to reference [21]. Let us summarize now the typical evolution of such initial conditions, that is well understood after many studies about effective LQC in the literature (see, e.g. the review [47]). First of all, the second conformal time derivative of the scale factor, a'', is positive at the bounce and, roughly speaking, of a few Planck units in magnitude. This causes that, right after the bounce, a very short superinflationary period occurs. During this period, the rescaled Hubble parameter $aH = a'/a$ grows from zero to a maximum of order one in Planck units, and this happens so fast that the scale factor remains almost constant [18, 47]. Shortly after the end of the superinflationary period when H reaches its maximum, the quantum corrections to the FLRW equations become completely negligible and the primordial Universe starts a classical phase of decelerated expansion, according to the dynamics of general relativity, that is dominated by the kinetic energy of the inflaton. More specifically, the quantum modifications in the evolution become ignorable after the scale factor has increased approximately only 1 or 2 e-folds. This small variation is indeed enough to produce a large decrease in the inflaton energy density, to values as small as 10^{-6} in Planck units, since its dominant kinetic contribution in this regime is proportional to a^{-6}, while the potential contribution varies very little, with values ranging in the interval $[10^{-12}, 10^{-11}]$ (see e.g. [39, 47]). The classical kinetically dominated phase then goes on until the kinetic and potential contributions to the energy density become comparable, moment at which aH reaches a minimum. After a short transition from the kinetically dominated phase to the domination of the potential, a period of short-lived inflation starts, leading finally to a slow-roll inflationary phase. In fact, the variation of the scale factor from the bounce to the subdominance of the kinetic contribution in the inflaton energy density is typically no more than 4 or 5 e-folds. For further details on the semiclassical and classical properties of these background solutions, we refer the reader to references [47, 58–61].

In the evolution equation (2.1) of the Mukhanov–Sasaki and tensor perturbations, the considered effective LQC solutions for the cosmological background are translated into the following features of the mass s in the pre-inflationary period. Since the inflaton potential remains completely negligible from the bounce until almost the end of the kinetically driven classical expansion, in this period we can safely ignore its contribution to s for both types of perturbations. The mass then coincides for the Mukhanov–Sasaki and tensor equations, and is given by [39]

$$s = \frac{8\pi}{3} a^2 \rho, \quad \text{and} \qquad s = -\frac{a''}{a}, \tag{2.15}$$

for hybrid and dressed metric LQC, respectively, where we recall that the energy density varies in time as $\rho \propto a^{-6}$ in the considered period. The difference between the value of the mass s in the two LQC approaches is due to the fact that, in hybrid LQC, the second time derivative of a is expressed canonically before quantization and then evaluated on effective LQC trajectories, while in the dressed metric approach the scale factor is evaluated at effective trajectories prior to taking its explicit derivatives. These discrepancies can, in turn, be traced back to the strategies followed for the quantization of the perturbations. For more details, we refer the reader to reference [39]. In what concerns this work, the fundamental difference between the two considered masses is their positivity and negativity at the bounce, for hybrid and dressed metric LQC respectively, and the subsequent discrepancies in the superinflationary period. Nonetheless, shortly after the end of superinflation any quantum cosmology correction becomes negligible and both masses coincide there on, in particular during the kinetically dominated classical epoch.

In figure 1 we show the relative variation s'/s of the hybrid LQC mass from the bounce to the first epochs of standard slow-roll inflation. Actually, the curve has been computed for the exact expression of the Mukhanov–Sasaki mass, taking into account all contributions from the inflaton potential. However, according to our comments above, this mass must essentially coincide with the one for tensor perturbations approximately until it becomes negative, that is when the potential starts to dominate over the kinetic energy of the inflaton. Indeed, notice that the right-hand side of the first equality in equation (2.15), that only takes into account the kinetic contribution, is strictly positive. Furthermore, we recall that the period with relevant LQC effects stops soon after the very rapid super-inflationary stage following the bounce, so the relative variation of the corresponding Mukhanov–Sasaki mass from the dressed metric approach is also given by figure 1 from a few e-folds on. In particular, even though this mass starts being negative at the bounce in the dressed metric approach, since $a'' > 0$ there, it becomes positive during the decelerated kinetically dominated classical phase, where a'' is negative, until the approximate 4.5 e-folds mark in the figure [39].

With this information at hand, let us turn our attention to normalized solutions to equation (2.1), that we have shown that take the form (2.14), where h_k is a solution of the Riccati equation (2.8) with negative imaginary part, particularized to the case where s is provided by the hybrid or the dressed metric approaches to LQC. The relevant time-dependent quantity for the computation of power spectra from these solutions is $p_k = |\mu_k|^2$. From equation (2.10) we have

$$p'_k = \frac{\mathrm{Re}(h_k)}{\mathrm{Im}(h_k)} = -2|g_k|^2 \mathrm{Re}(h_k). \tag{2.16}$$

It follows that maxima or minima of p_k happen at times when the real part of h_k becomes zero and, taking into account equation (2.9), when

$$k^2 + s - \mathrm{Im}\,(h_k)^2 > 0, \quad \text{or} \quad k^2 + s - \mathrm{Im}\,(h_k)^2 < 0, \tag{2.17}$$

respectively. In particular, let us notice that, within intervals of time and scales k such that $k^2 + s \leqslant 0$, only one minimum may occur for p_k (if any). Therefore, within such intervals, the power spectra cannot oscillate, regardless of the choice of normalized solutions to equation (2.1). For all other scales and intervals of time where $k^2 + s > 0$, the power spectrum obtained from normalized solutions may oscillate in time in a way that depends on the scale k.

Phenomenologically, using Planck units and setting the reference value of the scale factor at the bounce, the wavenumbers k of the perturbations that had physical (wavelength) scales a/k of the order of the Hubble radius H^{-1} around the bounce in LQC and that are

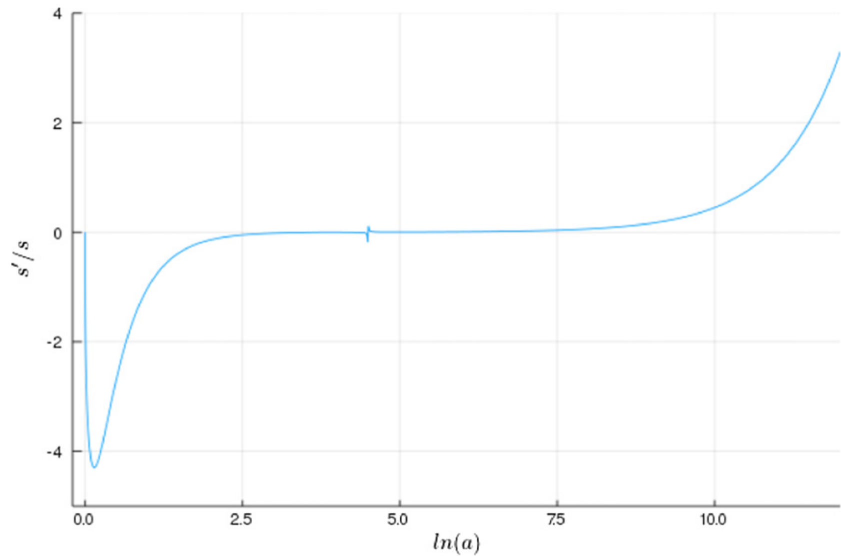

Figure 1. Relative variation of the Mukhanov–Sasaki mass from hybrid LQC in terms of the number of e-folds from the bounce. The plot dispays the Mukhanov–Sasaki mass for the effective FRLW background considered in reference [29], determined by an initial value of the inflaton at the bounce equal to 0.97, and subject to a quadratic potential corresponding to an inflaton mass equal to 1.2×10^{-6}. All quantities are given in Plack units. The (only) apparent discontinuity in the plot shows the moment when this mass becomes negative, close to 4.5 e-folds.

observable today would be in the approximate window $k \in [10^{-1}, 1]$ (for typical cosmological histories and reheating scenarios). This window can be enlarged with some margin to $[10^{-6}, 1]$ in order to include the possible observational effects of non-Gaussian correlations with super-Hubble modes [21, 62]. These are the scales that should have experienced the most significant LQC effects of the homogeneous geometry. On the other hand, if we include scales that certainly were not affected by quantum effects, the total window of wavelengths that we can observe nowadays (directly or by non-Gaussian correlations) would approximately be $[10^{-6}, 10^2]$. Focusing our attention on wavenumbers $k \in [10^{-6}, 1]$ that might have been influenced by LQC phenomena, we see from figure 1, and our discussion about it, that they are such that $k^2 + s > 0$ in the kinetically dominated classical period after superinflation, both for hybrid and dressed metric LQC. Furthermore, the mass s remains almost constant in this period, with values very close to zero (or numbers much smaller than one). If a power spectrum determined by p_k oscillates in this classical period of the evolution of the background then, for modes $k \ll 1$, the maxima of the oscillations display $\mathrm{Im}\,(h_k)^2 \ll 1$, in virtue of the first inequality in equation (2.17). Actually, from equations (2.14) and (2.17), these maxima of $2p_k$ are always greater than $(k^2 + s)^{-1/2}$ evaluated at those critical points, and therefore much larger than one for $k \ll 1$. It follows that at each instant of time the possible maxima of $2p_k$, viewed as a function of k, are bounded from below by the curve $(k^2 + s)^{-1/2}$, which grows as k decreases, and this curve remains approximately the same throughout the whole interval of time that we are considering, where s varies very little. Similarly, this curve sets an upper bound for the minima of an oscillating p_k. In this respect, recall that the bound determined by $(k^2 + s)^{-1/2}$ reaches orders of magnitude much bigger than one for $k \ll 1$. On the other hand, there is no upper bound of this type for the maxima of p_k. These features altogether involve that oscillating power spectra during the kinetically dominated phase, when evaluated later at the onset of inflation, often display a net amplification of the power as k decreases, for those k for which p_k had been oscillating [29, 47, 63]. This statement is also true for power spectra evaluated at the end of inflation in the case of the fields that are often used in cosmology to extract cosmological observations. Indeed, these are not exactly given by the type of field $\mathcal{V}(\eta, \vec{x})$ that we have been considering, but rather by its rescaling with certain functions of the background, that lead to the comoving curvature perturbative field for scalar perturbations, or to its equivalent for tensor ones. The power spectra for these rescaled fields freeze during the period of slow-roll inflation when the wavelength scale a/k gets much larger than H^{-1}, so that the analyzed mode crossed the Hubble horizon sufficiently long ago [4, 54]. For the type of solutions that we are studying for the cosmological background, let us recall that the rescaled Hubble parameter aH reaches a minimum at the end of the kinetically dominated phase, with a typical value in the range $[10^{-4}, 10^{-3}]$ [47]. Therefore, we conclude that the modes corresponding to the sector of largest scales under consideration, let us say approximately $k \in [10^{-6}, 1]$, must have either crossed the horizon well before the onset of inflation or are the first ones to cross after it begins. We then expect that, for such modes, the evaluation of the power spectra of the comoving curvature fields at the end of inflation provides a good picture of the behavior of these fields around the end of the kinetically dominated period and the beginning of the potentially dominated stage, before slow-roll inflation took place.

The presence of oscillations of p_k, and their general net effect of amplification of power for small wavenumbers, can be regarded as a somewhat artificial phenomenon if one takes into account that equation (2.1) in principle admits normalized solutions such that p_k remains approximately constant during the Einsteinian kinetically dominated phase. Indeed, for this to happen, one would naturally require that

$$\left|\frac{p_k'}{p_k}\right| = 2|\mathrm{Re}(h_k)| \ll 1, \tag{2.18}$$

where we have used equation (2.10). We can impose this condition at some time η_i in the beginning of the kinetically dominated phase, and check if it is stable over the whole considered period. For that, it is necessary that we also impose

$$\mathrm{Im}\,(h_k)^2(\eta_i) = k^2 + s(\eta_i) + r_k, \quad |r_k| \ll 1 \tag{2.19}$$

so that $|\mathrm{Re}(h_k)'| \ll 1$ as well in the beginning of the kinetically dominated period. By choosing these initial quantities sufficiently small, the desired condition (2.18) for an approximately constant spectrum can be made consistent throughout the whole period in question, because equations (2.9) and (2.10) imply

$$\mathrm{Re}(h_k)'' = s' + 2(k^2 + s)\mathrm{Re}(h_k) + 2\mathrm{Re}(h_k)^3 - 6\mathrm{Re}(h_k)\,\mathrm{Im}\,(h_k)^2, \tag{2.20}$$

and s' (as well as s) remains much smaller than the unit in the kinetically dominated phase. The existence of very slowly varying power spectra during this phase also means that, for the window $k \in [10^{-6}, 1]$ of modes, the features of the two-point function of the perturbations at the end of the kinetically dominated period can resemble very well those present at the end of the superinflationary period. It is worth recalling that this is the only regime after the bounce where effective LQC corrections are important. One can thus raise doubts as to whether it is physically reasonable to focus the attention on vacuum states for the perturbations that lead to highly oscillating spectra during the times of kinetic domination. Indeed, such oscillatory character can easily erase most of the information coming from the previous epochs near the bounce. Furthermore, these oscillations can result in an enhancement of power that is not due to any quantum cosmology effect nor it is intrinsic to the classical behavior of spacetime after superinflation. Rather, it may correspond to particular features of the specific set of normalized solutions chosen for the perturbations.

In conclusion, we have argued from an analytical perspective that reasonably natural candidates for power spectra which ought to be able to capture most of the genuine LQC corrections on the evolution of the perturbations, without introducing artificial modifications in the part of the pre-inflationary regime that is essentially Einsteinian, are those that present little or no oscillations during such a regime. An argument of continuity of this behavior to the past encourages one to try and characterize NO spectra throughout the entire evolution of the background cosmology, from the bounce to the onset of inflation.

3. General form of the power spectra: NO conditions

We have discussed the physical interest of considering vacua, or equivalently initial conditions, for cosmological perturbations in the framework of effective LQC that lead to power spectra for which the time and k-dependent oscillations are minimal. In order to analytically characterize them, we will now study a general formula for the power spectrum associated with any possible vacuum state, conveniently written in terms of a particular solution to the Ermakov–Pinney equation.

Starting from equation (2.1) and any set of normalized solutions μ_k, let us call again $p_k = |\mu_k|^2$. This is the function that codifies the freedom of choice of vacuum state in the power spectrum (2.2). Using the normalization condition (2.3), we have that any such non-zero function p_k satisfies the following second order differential equation

$$p_k'' + 2(k^2 + s)p_k = \frac{1}{2p_k}\left[(p_k')^2 + 1\right]. \tag{3.1}$$

Since p_k is by construction a positive function, we can write it as $p_k = \rho_k^2/2$, where ρ_k is a real non-zero function that, in virtue of equation (3.1), must satisfy

$$\rho_k'' + (k^2 + s)\rho_k = \frac{1}{\rho_k^3}. \tag{3.2}$$

This is the well-known Ermakov–Pinney equation [49, 50]. It has been widely employed in the context of FLRW cosmology and its perturbations (see e.g. [64–67]). Conversely, given any real and non-zero solution ρ_k of this equation, the function $p_k = \rho_k^2/2$ necessarily satisfies equation (3.1). Therefore, we can completely specify the general solution of this equation if we obtain all possible real solutions ρ_k of the Ermakov–Pinney equation. Actually, this can be done in terms of just one particular solution to equation (3.2), in such a way that the resulting formula manifestly displays the possible oscillatory behavior of p_k. Let us sketch the procedure to do so. For further details, we refer the reader to references [65, 68].

The general solution of any Ermakov–Pinney equation of the form (3.2) can be expressed in terms of two linearly independent solutions to our original equation (2.1), and their Wronskian [50]. These two solutions can, in turn, be chosen as two linearly independent functions, given by one particular real solution ψ_k to equation (3.2), multiplied by a sinusoidal function (a sine or a cosine, respectively, for the two considered solutions) of an arc ϕ_k such that $\phi_k' = \psi_k^{-2}$. Using them, the general real solution of the Ermakov–Pinney equation can be written as

$$\rho_k^2 = \psi_k^2\left[A\cos^2(\phi_k) + B\sin^2(\phi_k) + C\sin(2\phi_k)\right], \quad C^2 = AB - 1, \tag{3.3}$$

where A, B, and C are constants that must be real and such that ρ_k^2 be positive. Therefore, the function p_k that determines the form of any power spectrum associated with any set of normalized solutions to equation (2.1) can be obtained as

$$p_k = \frac{1}{4}\psi_k^2 \left[A + B + (A - B)\cos(2\phi_k) + 2C\sin(2\phi_k)\right], \tag{3.4}$$

where we recall that ψ_k is a real solution to equation (3.2) and $\phi_k' = \psi_k^{-2}$. This last equality guarantees that ϕ_k grows monotonically in time, so that the sine and cosine functions appearing in this formula oscillate in time, generally in a k-dependent way. The overall oscillatory character of their contribution to p_k depends on how fast they oscillate when compared to the relative variation of the global factor ψ_k^2. If they do vary faster, then they generally give rise to an oscillatory p_k unless we have $A = B = 1$ (or at least that these constants take values in a small neighbourhood of 1), case in which the two coefficients of the sinusoidal terms are zero (or negligible). We recall that this can only happen for intervals of time and wavenumbers k such that $k^2 + s > 0$, since we have seen that for $k^2 + s \leqslant 0$ the function p_k cannot oscillate owing to the dynamical equations (2.9) and (2.10). It follows that we can characterize the NO spectra if we can restrict our considerations to real solutions of the Ermakov–Pinney equation such that, for $k^2 + s > 0$,

$$\left|\psi_k' \psi_k\right| < 1 \tag{3.5}$$

(or much smaller than 1, if preferred), and to constants A and B in equation (3.4) that take values in a small neighbourhood of 1. We have taken into account that the frequency of the sinusoidal functions in equation (3.4), and therefore the rate at which they oscillate, is determined by $2\phi_k' = 2\psi_k^{-2}$.

In order to analyze condition (3.5), let us recall that equation (3.1) [equivalent to equation (3.2) for real solutions ρ_k], is satisfied by every $p_k = |\mu_k|^2$, where μ_k is any normalized solution to equation (2.1). Conversely, any real $|\mu_k|$ such that its square satisfies equation (3.1) univocally leads to a normalized solution to equation (2.1) [in virtue of equation (2.3)]. It then follows that, up to a sign, we can specify any particular real solution ψ_k of the Ermakov–Pinney equation (3.2) as $\sqrt{2}|\mu_k|$, where $|\mu_k|$ is completely determined by equation (2.14) and h_k is a solution to equation (2.8) with strictly negative imaginary part. Therefore, we can rewrite the NO condition (3.5) in terms of h_k as

$$\left|\frac{\mathrm{Re}(h_k)}{\mathrm{Im}(h_k)}\right| < 1, \tag{3.6}$$

where we have used equation (2.10).

For illustrative purposes, let us see whether the NO condition (3.6) derived above is satisfied for fields with modes that obey equation (2.1) in two situations where a natural choice of initial conditions is available. The first of these is when the mass s is exactly a constant, namely $s' = 0$, case in which equation (2.1) represents the dynamical equation of a massive Klein–Gordon field in Minkowski spacetime. Natural initial conditions are then given by those corresponding to the Poincaré vacuum state for the field, with associated normalized solutions (2.14) characterized by

$$\mathrm{Im}(h_k) = -\sqrt{k^2 + s}, \tag{3.7}$$

that is a constant. We see that the real part of h_k is identically zero, and the NO condition indeed is satisfied for all k. In fact, from the general formula (3.4), it follows that the Poincaré vacuum is the unique vacuum state for which the power spectrum is a constant, and therefore has the minimal oscillatory character. The second situation that we want to analyze is when the field $\mathcal{V}(\eta, \vec{x})$ describes the Mukhanov–Sasaki or the tensor perturbations of a cosmological background which is the de Sitter solution of general relativity, in flat slicing. In this case, the mass s coincides for both types of perturbations. It is given by $-2\eta^{-2}$, where the conformal time only takes negative values. Standard initial conditions for the normalized solutions to equation (2.1) are in this case those specifying the Bunch–Davies vacuum state. These conditions give rise to solutions with [4]

$$\mathrm{Im}(h_k) = -\frac{k^3\eta^2}{1+\eta^2k^2}. \tag{3.8}$$

Using equation (2.10), it follows that the real part of h_k is given by

$$\mathrm{Re}(h_k) = \frac{1}{\eta+\eta^3k^2}. \tag{3.9}$$

The NO condition is therefore satisfied when $k > |\eta^{-1}|$. It is worth noting that this inequality can always be satisfied for any k by considering sufficiently large negative times, something that is certainly met in the limit $\eta \to -\infty$. Moreover, from equation (3.9) for the real part of h_k, we see that the Bunch–Davies spectrum is completely monotonic in time for any k, so it does not display any oscillations. On the other hand, we know that the possible oscillatory behavior of any other power spectrum in de Sitter, that can be obtained by means of formula (3.4) setting ψ_k as the solution selected by the Bunch–Davies conditions, must stop when $k^2 + s \leqslant 0$. Since $s = -2\eta^{-2}$, this means that there are no oscillatory p_k in de Sitter for $k \leqslant \sqrt{2}|\eta^{-1}|$ (again, when the conformal time tends to minus infinity, the restriction on k disappears). Hence, we conclude that an NO spectrum for the Mukhanov–Sasaki or the tensor perturbations in a de Sitter background is obtained with the choice of a Bunch–Davies vacuum state, and any other NO spectrum must be in a small neighbourhood of it for $k > \sqrt{2}|\eta^{-1}|$, in the sense of setting the constants A and B close to 1 in formula (3.4).

3.1. NO condition in effective hybrid LQC

We have seen that the NO condition (3.6) on the power spectrum is satisfied by the natural Poincaré and Bunch–Davies vacua on their respective Minkowski and de Sitter backgrounds. The main purpose of this section is to analyze if the condition can also be fulfilled in scenarios where the mass s is given by effective hybrid LQC, at least in regimes where $k^2 + s > 0$ for wavenumbers in the phenomenological window $k \in [10^{-6}, 10^2]$ that covers, with some margin, the range corresponding to scales that we can consider observable nowadays, as we have commented [21, 29]. Actually, those regimes include the bounce, which can be understood as a privileged moment to set initial data. In particular, we are going to impose the NO condition at the time η_0 when the bounce occurs, and then study its stability throughout the period elapsed until the onset of inflation. In the case of dressed metric LQC, for a considerable part of the phenomenological window of wavenumbers k that we are investigating, we have that $k^2 + s \leqslant 0$ at the bounce owing to the negativity of the mass, that besides takes an absolute value of approximate order 10 in Planck units [39]. Therefore, it seems unclear whether it is useful to impose NO conditions at the bouncing time in order to restrict the physically viable data in this case, at least as we have posed them; rather, one would have to appeal now to some *additional* criteria to pick out the vacuum state, that then should satisfy the non-trivial requirement of leading to a suppression of the oscillations in the later Einsteinian period of kinetically dominated evolution of the background.

Let us first impose the NO condition (3.6) at the time η_0 of the bounce, chosen as the moment to specify the Cauchy data of the normalized solutions to equation (2.1). This restricts the real part of h_k at that time to be small compared to the imaginary part, so that

$$|\mathrm{Re}(h_k)(\eta_0)| = \epsilon_k |\,\mathrm{Im}(h_k)(\eta_0)|, \tag{3.10}$$

where ϵ_k is a positive real number smaller than one[3]. For this restriction to hold in a small neighbourhood of η_0, it is necessary that the derivative of $\mathrm{Re}(h_k)\,\mathrm{Im}\,(h_k)^{-1}$ is also small initially, namely using equations (2.9) and (2.10),

$$\left|\frac{k^2+s(\eta_0)}{\mathrm{Im}(h_k)(\eta_0)} - (1+\epsilon_k^2)\,\mathrm{Im}(h_k)(\eta_0)\right| < 1. \tag{3.11}$$

We note that, in general, ϵ_k^2 provides a subdominant contribution to the second summand in this inequality. Besides, we recall that the mass s in the kinetically dominated period (that includes the bounce) is given by the first equality in equation (2.15) for hybrid LQC. Taking into account that the energy density at the bounce is a universal quantity, with a fixed value that is approximately a 41 percent of the Planck density, we have that $k^2 + s(\eta_0)$ is always larger than one in Planck units. It then follows that a necessary condition for equation (3.6) to hold is

$$\mathrm{Im}(h_k)(\eta_0) = -\sqrt{k^2+s(\eta_0)} + \delta_k, \qquad \frac{|\delta_k|}{\sqrt{k^2+s(\eta_0)}} < 1 \tag{3.12}$$

(again, see footnote 3) and we have used that the imaginary part of h_k must be negative in order to provide normalized solutions to equation (2.1). Clearly, one can then choose the parameters ϵ_k and δ_k in such a way that the condition (3.11) on the derivative of $\mathrm{Re}(h_k)\,\mathrm{Im}\,(h_k)^{-1}$ is satisfied. Hence, in hybrid LQC, the NO condition can be guaranteed to hold in a small neighbourhood around the bounce if the initial data for the normalized solutions is constrained by equations (3.10) and (3.12), with sufficiently small parameters ϵ_k and δ_k.

Let us now proceed to analyze the stability of the NO condition in the kinetically dominated regime that goes from the bounce to the onset of inflation. We recall that the dynamics experienced by the real and imaginary parts of h_k are governed by a coupled set of real first order differential equations, or equivalently by a decoupled second order equation. Therefore, if the derived conditions (3.10) and (3.12) on those functions are imposed initially, their stability under evolution over the interval of time where one wishes to eliminate oscillations is controlled by the second derivative of $\mathrm{Re}(h_k)\,\mathrm{Im}\,(h_k)^{-1}$, that hence must be small in absolute value. Using equations (2.9) and (2.10) again, we must have, let us say,

$$|s' - 4(k^2+s)\mathrm{Re}(h_k)| < |\,\mathrm{Im}(h_k)|. \tag{3.13}$$

We recall now that the energy density depends on time as $\rho \propto a^{-6}$ in the kinetically dominated region that includes the bounce. Since then $s' \propto a'$, the time derivative of the mass is zero at the bounce and the above stability condition reduces there to

$$\epsilon_k < \left|\frac{1}{4[k^2+s(\eta_0)]}\right|, \tag{3.14}$$

which is perfectly compatible with our previous restrictions to guarantee NO power spectra in a small neighbourhood of the bounce in hybrid LQC.

[3] Or much smaller than one, if preferred.

In order to check the consistency of our conditions deeper into the kinetically dominated regime, we need more details about the behavior of s' there. From the first equality in equation (2.15) and the behavior $\rho \propto a^{-6}$ of the energy density, we straightforwardly see that s' must be negative throughout this whole period (see also figure 1). Furthermore, we recall that in this region $aH = a'/a$ reaches only one maximum of order one, in Planck units, after the superinflationary regime that follows the bounce. Since the scale factor remains almost constant during superinflation, we have that $|s'|$ reaches only one maximum during the kinetically dominated period, that turns out to be approximately four times bigger than $s(\eta_0)$. Afterwards, $|s'|$ rapidly decreases to negligible values after roughly 1 or 2 e-folds (as it is confirmed in figure 1). Therefore, if we want a behavior of the form (3.10) and (3.11) for the real and imaginary parts of h_k that guarantees the NO condition at times after the bounce in the kinetically dominated regime, the only possible tension with stability, governed by equation (3.13), may arise in the region around the end of superinflation. Indeed, elsewhere we have that s' contributes negligibly to this inequality, which is then compatible with the NO condition in a similar way as it was at the bounce. Actually, given that $4(k^2 + s)$ is of the order of $|s'|$ or larger around the end of superinflation, we think it is likely that this tension disappears if one chooses properly the initial parameters ϵ_k and δ_k.

We conclude that, in effective hybrid LQC, conditions for NO power spectra on the gauge invariant perturbations can be consistently set at the bounce via equations (3.10) and (3.12) with appropriately small parameters ϵ_k and δ_k, that in principle can be chosen without obstructions. With such a suitable choice, the associated spectra should display a stable NO behavior throughout the kinetically dominated period after the bounce. Moreover, among the normalized solutions to equation (2.1) of the form (2.14) restricted by these NO considerations, we notice that there consistently exist some that satisfy conditions (2.18) and (2.19) at the beginning of the classical, Einsteinian kinetically dominated regime. These would lead to power spectra that remain approximately constant throughout this classical period so that, even when evaluated around the onset of inflation, they can still provide useful information about the two-point function of the perturbations at those primeval stages right when the effective LQC corrections became negligible.

4. Uniqueness of the NO spectrum in the ultraviolet regime

The procedure of Hamiltonian diagonalization carried out in section 2, using explicitly time-dependent transformations, parallels a similar construction performed in reference [69] for the fully canonical formulation of the classical system formed by a homogeneous FLRW background with perturbations, truncated at lowest non-trivial order in the action. That work addresses the possibility of diagonalizing the resulting (quadratic) perturbative contribution of gauge invariants to the zero mode of the Hamiltonian constraint of the full system, employing transformations of the form (2.5) and (2.6) with coefficients that depend on the canonical variables which describe the homogeneous background cosmology. If one completes these transformations to be canonical in the entire system, the perturbative contributions to the zero mode of the Hamiltonian constraint turn out to be precisely of the form (2.12) (up to a global factor a^{-1} for a standard lapse), where the time derivatives are replaced by conformal Poisson brackets with the Hamiltonian of the unperturbed FLRW cosmology [69]. These perturbative contributions are then diagonal in this context if h_k satisfies equation (2.8), after replacing the time derivative by the mentioned Poisson brackets.

Focusing on the asymptotic regime of unboundedly large wavenumbers k, or ultraviolet regime, it was shown in reference [69] that it is possible to eliminate each contribution to the non-diagonal terms in the perturbative part of the Hamiltonian constraint, order by order in powers of k. The result is an ultraviolet diagonalization characterized by a very specific asymptotic expansion of at least one solution h_k to the analog of our equation (2.8) in that work. Following a completely similar procedure, we can perform the same type of asymptotic diagonalization of our Hamiltonian (2.12), in the regime of large k, yielding the expansion [69]

$$kh_k^{-1} \sim \mathrm{i}\left[1 - \frac{1}{2k^2}\sum_{n=0}^{\infty}\left(\frac{-\mathrm{i}}{2k}\right)^n \gamma_n\right], \tag{4.1}$$

where the coefficients γ_n are real, only depend on time, and are given by the following iterative relation, that is deterministic:

$$\gamma_0 = s, \quad \gamma_{n+1} = -\gamma_n' + 4s\left[\gamma_{n-1} + \sum_{m=0}^{n-3}\gamma_m\gamma_{n-(m+3)}\right] - \sum_{m=0}^{n-1}\gamma_m\gamma_{n-(m+1)}. \tag{4.2}$$

We define $\gamma_{-n} = 0$ for all $n > 0$. This leads to a unique asymptotic expansion of, at least, one solution h_k to equation (2.8), with imaginary part that is strictly negative [69]. Therefore, it provides in turn a very precise asymptotic expansion of, at least, one normalized solution to equation (2.1), via equation (2.14). We call any such solution $\tilde{\mu}_k$. Its associated square norm $\tilde{p}_k = |\tilde{\mu}_k|^2$ is then of the form

$$\tilde{p}_k = \frac{1}{2k}\left(1 - \Gamma_k\right), \tag{4.3}$$

where Γ_k has the following asymptotic expansion:

$$\Gamma_k \sim \frac{1}{2k^2}\left[1 - \frac{1}{2k^2}\sum_{n=0}^{\infty}\left(\frac{\mathrm{i}}{2k}\right)^{2n}\gamma_{2n}\right]^{-1}\sum_{n=0}^{\infty}\left(\frac{\mathrm{i}}{2k}\right)^{2n}\left[\gamma_{2n} - \frac{1}{2k^2}\sum_{m=0}^{2n}(-1)^m\gamma_m\gamma_{2n-m}\right]. \tag{4.4}$$

This is a series where each summand depends on the wavenumber k only through an even inverse power of it. Since we know that any such $\tilde{p}_k$ must be of the form $\tilde{\psi}_k^2/2$, where $\tilde{\psi}_k$ is a real solution to the Ermakov–Pinney equation (3.2), this procedure of ultraviolet diagonalization fixes as well (up to sign) a very specific asymptotic expansion of, at least, one solution $\tilde{\psi}_k$ to that equation, in the regime of unboundedly large k. Let us precisely take it (or one of them, if there were more than one) as the particular solution to insert in the general formula (3.4) for any other power spectrum. Then, any function p_k equal to the square norm of a normalized solution to equation (2.1) is given by

$$p_k = \frac{1}{4k}\left(1 - \Gamma_k\right)\left[A + B + (A - B)\cos(2k\eta + 2\theta_k) + 2C\sin(2k\eta + 2\theta_k)\right], \tag{4.5}$$

where Γ_k has the asymptotic expansion (4.4) and θ_k is a function with dominant contribution in the ultraviolet regime of order k^{-1}. In this asymptotic regime, the dominant term in p_k is

$$\frac{1}{4k}\left[A + B + (A - B)\cos(2k\eta + 2\theta_k) + 2C\sin(2k\eta + 2\theta_k)\right], \tag{4.6}$$

because Γ_k is of order k^{-2}. This is a highly oscillatory function for unboundedly large k unless we strictly impose $A = B = 1$, in which case p_k reduces to $\tilde{p}_k$. Actually, this choice of constants is the only one that succeeds to eliminate, order by order in the expansion of Γ_k in inverse powers of k, all the scale-dependent oscillations in the considered ultraviolet regime.

In this way, we conclude that, in the asymptotic regime of unboundedly large wavenumbers (or short wavelength scales) there exists only one expansion for the power spectrum of the field $\mathcal{V}(\eta, \vec{x})$ for which absolutely no k-dependent oscillations occur over time. Let us notice that this result holds for any mass s that is a smooth function of time. Moreover, any choice of normalized solutions to equation (2.1) that presents a completely NO spectrum for all k, if such a choice exists, must have the asymptotic expansion characterized by equations (4.1) and (4.2). It is reasonable to expect that there exists at least one set of normalized solutions that are, e.g. continuous functions of k and possess such asymptotic expansion. If such continuity in k ensures that the NO condition in the previous section is satisfied for all scales, then we would have a set of preferred choices of power spectrum for the field $\mathcal{V}(\eta, \vec{x})$. There is actual evidence that this should be the case in the context of effective LQC, just by looking at the properties of the asymptotic expansion. Indeed, it has been shown that when s corresponds to a constant or to the mass for cosmological perturbations on a de Sitter background, the series given by equations (4.1) and (4.2) converges for sufficiently large k [69]. The resulting functions are analytically well defined at all other scales, and they correspond to the choices of normalized solutions set by the Poincaré and Bunch–Davies vacuum states, respectively [69]. As we explicitly saw in the previous section, these two states lead to power spectra that display no oscillations at all. Furthermore, the Einsteinian regime reached as part of the effective LQC evolution of the primordial Universe presents two regions where s is very close to either a constant or to the mass for a de Sitter background: these are the classical kinetically dominated period and the slow-roll inflationary phase, respectively. It therefore seems reasonable to expect that there should exist at least one choice of normalized solutions to equation (2.1) that is continuous in k and has an asymptotic expansion fixed by equations (4.1) and (4.2) *at all finite times* such that it gives rise to power spectra that are of NO type in the regime where effective LQC reproduces the classical FLRW evolution. Any such choice would, in turn, correspond to a promising candidate for the vacuum state at the bounce, with a power spectrum capable of capturing the traces left by LQC effects in the dynamics of the primordial perturbations before these effects became ignorable in the background evolution.

5. Conclusions

We have investigated from a theoretical point of view the possibility of obtaining NO power spectra for primordial perturbations in cosmology, putting a special emphasis on cosmological backgrounds that correspond to certain solutions of effective LQC with inflation, such that they display a pre-inflationary regime that is dominated by the kinetic energy density of the inflaton. This type of background is phenomenologically favoured when confronting the expected loop quantum geometry effects on the evolution of the perturbations with CMB observations. Furthermore, we have characterized the general conditions that any power spectrum must satisfy in order to eliminate or minimize its scale-dependent oscillations over time, making use of a well-known equivalence between our hyperbolic field equations with a time-dependent mass and the Ermakov–Pinney equation. Finally, we have discussed the uniqueness of the NO power spectrum in the ultraviolet regime of short wavelength scales, concluding that there is only one asymptotic expansion that displays no scale-dependent oscillations at all. This expansion actually corresponds to the choice of a standard Poincaré or a Bunch–Davies vacuum, respectively, for a Minkowski or a de Sitter background, and constitutes a promising line of attack to completely fix the initial conditions for the primordial perturbations in effective LQC by means of a physically well-motivated criterion.

In more detail, we have first considered the general equation of a harmonic oscillator with a time-dependent mass, and have conveniently characterized its normalized solutions by diagonalizing the associated Hamiltonian employing explicitly time-dependent transformations. This is the type of equation that each mode of the gauge invariant perturbations satisfies, not only in classical perturbation theory around FLRW cosmology, but also in the context of the hybrid and dressed metric approaches to LQC when the unperturbed cosmology can be described effectively. Then, using general features of the effective LQC backgrounds of interest and of the solutions to the considered harmonic oscillator equation, we have discussed the qualitative impact that oscillatory power spectra may have on observations. We have argued that, in order to get rid of any net amplification of power artificially pumped by oscillations in classical regimes where the classical cosmological evolution is recovered, as well as to obtain a neat information about the quantum state of the perturbations in stages where the LQC modifications may not yet be completely negligible in the background evolution, we need to focus our attention on initial conditions that lead to NO spectra.

We have then studied the general conditions that the normalized solutions to our field equation must satisfy in order to avoid the presence of scale-dependent oscillations over time in their associated spectra. For that, we have written any possible power spectrum in terms of one particular solution to the Ermakov–Pinney equation that corresponds to our hyperbolic equations with time-dependent mass, in a way that makes manifest the possible oscillations. Imposing that these oscillations have a minimal contribution in the admissible power spectra results into a very specific condition on the particular solution to the Ermakov–Pinney equation and on the two integration constants that fix each power spectrum in terms of it. We have analyzed if this NO condition can be consistently imposed at the bounce that replaces the classical cosmological singularity, for perturbations in hybrid LQC. The result is in the affirmative. We have also checked that there are no serious obstructions to extend this requirement from the bounce all the way to the onset of inflation. On the other hand, in the case of the dressed metric approach to LQC, we have argued that there is no clear motivation from our analytical considerations to substantiate the imposition of the NO condition at the bounce for the scales of observational interest, owing to the fact that the associated negativity of the time-dependent mass around the bounce implies that, in this case, the oscillations at the considered scales can start only in a later phase of the evolution, which is actually when the main LQC effects are negligible. This fact leads to the need of additional criteria or extra input in order to pick out the initial conditions at the bounce in the dressed metric formalism. Nonetheless, these criteria or input should be non-trivially constrained by requiring the NO condition in the part of the evolution where the background reaches the classical, Einsteinian regime.

To conclude our analysis, we have investigated the asymptotic behavior of the power spectrum in the sector of unboundedly large wavenumbers k. Taking insight from previous results about asymptotic Hamiltonian diagonalization for cosmological perturbations [69], we have determined one specific asymptotic behavior for certain solutions to the Ermakov–Pinney equation, given as a series in inverse powers of k. We have then inserted this asymptotic series in the general formula for power spectra previously derived. The resulting expression manifestly displays rapid oscillations at every order in inverse powers of k, except for a single choice of the otherwise free integration constants. This allows us to conclude that there is only one possible asymptotic NO behavior for the power spectrum, that we have completely characterized. We have finally argued how this asymptotic expansion can reasonably lead, by imposing continuity in the scale k, to a unique (set of) choice(s) of normalized solutions to our field equations with a power spectrum that satisfies the NO condition for all k, in the entire classical pre-inflationary and inflationary phases of effective LQC. The choice suggested by this procedure constitutes a promising candidate as a physically distinguished vacuum state for the cosmological perturbations in effective LQC.

Our work provides an important step towards the analytical characterization of a reasonable set of initial conditions for the cosmological fluctuations in a pre-inflationary Universe with

LQC effects. Completing the specification of these data would not only confer more robustness to the predictions that can be drawn from approaches to LQC such as the hybrid or the dressed metric approaches (as well as to allow one to clearly isolate those predictions from other classical effects, like e.g. the ones arising from a short-lived inflation). Actually, it would be a key ingredient to understand the consequences of these various theoretical models in an analytical way, and discriminate between them. Moreover, it would allow one to falsify them against the CMB observations without the shadow that quantum field theory ambiguities cast on such possible tests nowadays.

Finally, it is worth noticing that the conditions found here for NO power spectra have been obtained for general and unspecified time-dependent (differentiable) mass functions of the perturbations. The same is true for our characterization of a unique asymptotic expansion for such spectra. In this respect, our analysis potentially serves as a first contribution to the study of preferred choices of a vacuum for primordial perturbations in other theoretical approaches to cosmology apart from LQC (e.g. in the context of bouncing cosmologies [70]), that produce modifications to the time-dependent mass of the perturbations with respect to its behavior in the standard inflationary paradigm.

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Review

Uniqueness Criteria for the Fock Quantization of Dirac Fields and Applications in Hybrid Loop Quantum Cosmology

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Abstract: In generic curved spacetimes, the unavailability of a natural choice of vacuum state introduces a serious ambiguity in the Fock quantization of fields. In this review, we study the case of fermions described by a Dirac field in non-stationary spacetimes, and present recent results obtained by us and our collaborators about well-motivated criteria capable to ensure the uniqueness in the selection of a vacuum up to unitary transformations, at least in certain situations of interest in cosmology. These criteria are based on two reasonable requirements. First, the invariance of the vacuum under the symmetries of the Dirac equations in the considered spacetime. These symmetries include the spatial isometries. Second, the unitary implementability of the Heisenberg dynamics of the annihilation and creation operators when the curved spacetime is treated as a fixed background. This last requirement not only permits the uniqueness of the Fock quantization but, remarkably, it also allows us to determine an essentially unique splitting between the phase space variables assigned to the background and the fermionic annihilation and creation variables. We first consider Dirac fields in 2 + 1 dimensions and then discuss the more relevant case of 3 + 1 dimensions, particularizing the analysis to cosmological spacetimes with spatial sections of spherical or toroidal topology. We use this analysis to investigate the combined, hybrid quantization of the Dirac field and a flat homogeneous and isotropic background cosmology when the latter is treated as a quantum entity, and the former as a perturbation. Specifically, we focus our study on a background quantization along the lines of loop quantum cosmology. Among the Fock quantizations for the fermionic perturbations admissible according to our criteria, we discuss the possibility of further restricting the choice of a vacuum by the requisite of a finite fermionic backreaction and, moreover, by the diagonalization of the fermionic contribution to the total Hamiltonian in the asymptotic limit of large wave numbers of the Dirac modes. Finally, we argue in support of the uniqueness of the vacuum state selected by the extension of this diagonalization condition beyond the commented asymptotic region, in particular proving that it picks out the standard Poincaré and Bunch–Davies vacua for fixed flat and de Sitter background spacetimes, respectively.

Keywords: quantum field theory in curved backgrounds; dirac field; loop quantum gravity; cosmology

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1. Introduction

Quantum Field Theory (QFT), namely the description of fields according to quantum rules, is one of the pillars of Modern Physics (see e.g., Refs. [1,2]). In this description, it is common to use a Fock formalism in which the physical processes are formulated in terms of creation and annihilation of field excitations around a vacuum state. Typically, these excitations are interpreted as particles (or antiparticles) of the field. This kind of description has been adopted successfully for all fundamental physical interactions, except for gravity: a fully satisfactory quantum field formulation of General Relativity, or more generally of the gravitational interaction, remains as a defiant challenge.

In standard QFT, the particle excitations develop in flat spacetime. The symmetries of this background spacetime (regarded as classical) are employed in the selection of a natural state for the Fock representation of the field: Poincaré invariance fixes a unique vacuum in Minkowski spacetime [3]. However, it is well known that the generalization of the Fock quantization techniques to field theories in curved spacetimes is by no means straightforward, and in fact involves ambiguities. The most important of these ambiguities concerns the choice of a (quantum) representation of the algebra, obtained under Poisson brackets, of (the complex exponentiation of) the basic variables that describe the field, which are usually chosen to be canonical pairs. In traditional Non-Relativistic Quantum Mechanics, this algebra is known by the name of Weyl algebra (see e.g., Ref. [4]). Fortunately, in such case where the system has a finite number of degrees of freedom, the representation of the algebra in a Hilbert space is unique up to unitary equivalence, provided that certain mild conditions are imposed (including continuity). This uniqueness result is known as the Stone-von Neumann theorem [5]. This means that two different representations of the same Weyl algebra in the same Hilbert space are necessarily related by a unitary operator. This property ensures the robustness of the theoretical predictions of Quantum Mechanics, and in particular of those derived from the evolution of quantum states, something essential for the viability of the probabilistic interpretation of the quantum theory.

In QFT this uniqueness result for the quantum representation of the variables that describe the fields is generally no longer valid. It does not even apply to Fock representations of free field theories, which are typically governed by linear dynamical equations. In fact, it is well known (see e.g., [6]) that for each given vacuum, there is an infinite number of linear canonical transformations, each of which provides a Fock representation of the field that have no unitary correspondence in the Fock space. In short, this means that what in principle ought to be the corresponding unitary transformations just map the vacuum of the given representation to some vector which does not belong to its Hilbert space. Therefore, inequivalent quantum representations do exist in QFT, even in the simplest cases. This issue has been widely studied to be exclusive of systems, such as fields, with an infinite number of degrees of freedom, since a known mathematical criterion for the unitary implementability of a given linear canonical transformation involves a summability condition [7,8], which is trivially satisfied if the number of degrees of freedom is finite. This fundamental obstacle translates into the existence of an infinity of quantum descriptions of the same physical system that in general, are not equivalent. However, one may introduce physically motivated requirements to reduce this ambiguity of the quantum description, and even to eliminate it completely, in certain situations. A remarkable example is given by fields that propagate in stationary spacetimes. This contains the case of fields in flat, Minkowski spacetime that we mentioned above. In these types of scenarios, the possible representations of the analog of the Weyl algebra [commonly known as the field canonical commutation relations (CCRs) for bosons, or canonical anticommutation relations (CARs) for fermionic fields] are restricted to only a single representation if one imposes that the quantum theory incorporate the symmetry displayed by the background under time-like translations and that the evolution be generated by a positive Hamiltonian that plays the role of an energy [6,9]. At the quantum level, this implies that the vacuum state of the field is stationary. There is therefore a natural unitary implementation of the dynamics.

The situation is notably more complicated when one considers fields that propagate in non-stationary spacetimes. Such systems describe scenarios of great physical interest, such as processes of star collapse or the cosmological evolution of the Universe (essentially since its very beginning). In these cases there is no time-like symmetry of the field equations that one can try and impose to restrict the admissible quantizations. The situation gets even worse if one takes into account that the quantum representations of the CCRs or CARs at different times are not necessarily unitarily equivalent. As a consequence, predictions based on the quantum evolution of the states lose robustness. For this reason, it is especially relevant to determine some physical criterion that allows us to remove the ambiguity in the choice of a Fock quantization in non-stationary spacetimes (or at least in a convenient subset of them) and, at the same time, regain a notion of unitary quantum dynamics for the fields.

Actually, this question has been investigated in recent years and the results indicate that the resolutions of the two problems are closely related. Indeed, for scalar fields in a multitude of non-stationary spacetimes of cosmological nature, it has been shown that a requirement of unitarity on the dynamics of the basic field operators in the Heisenberg picture (henceforth referred to as Heisenberg dynamics or evolution) can be used to guarantee the uniqueness of the Fock representation of the CCRs (up to unitary equivalence) if, in addition, one imposes invariance under the symmetries of the field equations [10–29]. These symmetries include the spatial isometries. In many cases, these isometries suffice to reach the desired uniqueness when combined with the demand of a unitary Heisenberg evolution. Recent discussions on the topic of unitary dynamics in QFT in curved spacetimes from the canonical perspective can be found in Ref. [10] (see also Ref. [30] for related investigations on this issue). On the other hand, the nature of the vacuum state for fields in curved spacetimes and the Fock quantization of such fields from a covariant perspective have been widely investigated over recent decades, see e.g., Refs. [31–34].

In this review, instead, we focus our attention on fermionic fields. Many of the most abundant elementary particles in standard matter are fermions, and in this respect one can say that fermionic fields describe more realistic matter contents than scalar fields. In addition, although there exist well-founded results about the selection of Fock representations of fermionic fields in cosmology, the literature on this topic is not as prolific as in the case of scalar fields. In this sense, a review of the recent results obtained by us and our collaborators about uniqueness criteria for the Fock representation of fermionic fields, based on a unitary Heisenberg dynamics or other related properties, appears especially useful. For the sake of concreteness, most of our discussion is devoted to the particular case of a Dirac fermion field, to which we will henceforth refer simply as *Dirac field*.

The issue of determining Heisenberg dynamics that can be realized as a unitary quantum transformation in fact involves a freedom in the splitting of the time dependence of the (fermionic) field. This time dependence can be separated in two parts: one that can be assigned to the quantum evolution of the creation and annihilation operators of the Fock representation and another that is due to the evolution of the background in which the field propagates. This second part can be treated as an explicit time dependence, via the background, when this is considered to be a classical entity. Strictly speaking, this part of the evolution is not contained in the Heisenberg dynamics of the fermionic degrees of freedom. A fundamental idea in the search for a criterion to select a Fock quantization by imposing a notion of unitary dynamics is that the freedom in the splitting of the time dependence of the field can be employed to restrict the quantization in such a way that one ends up with a single family of equivalent representations while keeping nontrivial information about the fermionic evolution.

The idea of using the aforementioned freedom to arrive at a preferred class of Fock representations has proven to be very fruitful in frameworks that surpass the scheme of QFT in a curved classical spacetime. This is the case of fields with a dynamics that can be viewed as a propagation in an auxiliary background, or even quantum geometries that present regimes in which they can be treated effectively. For instance, this idea has been applied in the framework of hybrid loop quantum cosmology (hLQC), in which the spacetime is no longer a classical entity, but a quantum object [23–25,28]. For cosmological systems of notable physical interest, hLQC combines a loop quantization of the zero modes that (classically) describe the Friedmann–Lemaître–Robertson–Walker (FLRW) spacetime that would correspond to a cosmological universe, with a Fock quantization of the field degrees of freedom that propagate in such a cosmological spacetime, typically viewed as perturbations [35,36]. The action of the gravitational system and its matter content is truncated at second order in these perturbations (generally assuming compact spatial sections). The combination of the loop and Fock techniques must give rise to a consistent quantization of the total system, composed by the background cosmology and the perturbations. This consistency involves the imposition à la Dirac of a global Hamiltonian constraint that interrelates the two types of representations as well as the evolution of the homogeneous universe and of its perturbations. For most of the relevant dynamical aspects of these perturbations, the information about the quantum geometry can be encapsulated in an effective geometry that in many respects can be considered to be emerging from a mean-field approximation of the geometric degrees of freedom contained in the cosmological background. In this approximation, the fields that correspond to the (gauge invariant part of the) perturbations admit a QFT description where the background is the aforementioned effective geometry [35,36]. In this context, it is even clearer that building a formalism capable to maintain the unitarity of the Heisenberg dynamics in non-stationary spacetimes transcends the need to guarantee the robustness of the physical predictions of the theory. In hLQC, in particular, the additional advantage to pick out a unique family of equivalent Fock representations of the gauge invariant perturbations is that one can construct a Heisenberg evolution (with respect to some parameter of the complete quantum system) that behaves as a unitary quantum transformation in regimes where an effective background emerges.

Despite the attention that scalar (and tensor) perturbations deserve in cosmology, it is clear that a realistic matter content must include other types of fields, such as those that describe fermions, as we have already pointed out. Actually, in hLQC, recent works have introduced Dirac fermions and treated them as part of the perturbations [37]. The interest of contemplating the presence of these fields in the very early Universe goes beyond a formal question about the completeness of the description, because it is necessary to confirm that these fermionic fields do not affect substantially the otherwise well-established evolution of the primordial scalar perturbations, nor of the tensor ones. The results obtained in Refs. [37,38] support the expectation that the possible effects are ignorable.

It is worth remarking that there exists an inherent freedom to choose the splitting between the (fermionic) field variables and the degrees of freedom that describe the background, allowing one to change between different families of annihilation and creation variables. This can be done by means of transformations that mix all these degrees of freedom while preserving the canonical symplectic structure of the combined system, including the field canonical (anti-)commutation relations. If the fields are treated as perturbations, it suffices that the canonical symplectic structure is preserved at the level of the perturbative truncation adopted in the system. Instead of considering this freedom a nuisance, one can try and exploit it to define variables for which the Hamiltonian of the selected fermionic degrees of freedom has certain nice quantum properties, desirable from the viewpoint of a good physical and mathematical behavior [38].

In fact, when fermions were studied for the first time within the hybrid approach to loop quantum cosmology in Ref. [37], considering them as perturbations around a homogeneous and isotropic cosmological spacetime, the selection of fermionic variables for the corresponding Dirac field was restricted only by the requirements of invariance of the resulting Fock vacuum under the spatial isometries, a unitarily implementable Heisenberg evolution in the regime of QFT in a curved background, and a standard convention for particles and antiparticles. Nonetheless, with a rather reasonable choice made among the family restricted by these conditions, it was realized that the resulting Schrödinger equation for the fermionic degrees of freedom (after a sort of mean-field approximation) involved ultraviolet divergences. To solve these divergences, one either must appeal to a regularization scheme with *subtraction of infinities* or, alternatively, employ the remaining freedom in the choice of fermionic variables and restrict it even further by introducing additional requirements. Specifically, in Ref. [38] it was required that the fermionic backreaction be finite. In practice, this new restriction lowers the asymptotic order of the interaction part of the fermionic Hamiltonian at large wave numbers (defined for the Dirac field as the eigenvalues of the Dirac operator on the spatial sections of the background, in absolute value). Consequently, the production of pairs of particles and antiparticles decreases for large wave numbers, becoming negligible asymptotically.

Actually, it is possible to go one step beyond in the same direction and, by taking advantage again of the freedom to split the degrees of freedom, demonstrate that one can absorb all the interaction terms of the fermionic Hamiltonian to make them identically zero order by order in the asymptotic regime of large wave numbers [39]. In this way, one clearly improves the quantum behavior of the (fermionic) field contribution to the Hamiltonian of the gravitational system. Moreover, one also greatly reduces the surviving ambiguity in the choice of Fock representation and vacuum for the field. Moreover, since the resulting (fermionic) field Hamiltonian contribution is diagonal by construction on states with a definite number of particle (and antiparticle) excitations, at least asymptotically, the dynamics ruled by it is very simple. The vacuum of the naturally associated Fock representation changes only by a rotating phase. In this sense, one can interpret that this vacuum and the corresponding splitting of degrees of freedom in the hybrid quantization approach are those that get best adapted to the cosmological evolution. Finally, it is remarkable that this criterion of asymptotic diagonalization reproduces the standard choices of vacuum state in well-understood situations, within the scheme of QFT in a curved classical background [39,40]. This happens e.g., in the case of a flat spacetime, as well as for a de Sitter cosmology, scenario where the Bunch–Davies state is a natural vacuum [41].

The rest of this review is organized as follows. In Section 2 we provide the basics for the construction of a Fock representation of the CARs for a Dirac field, within the framework of QFT in a curved spacetime. We also summarize the results about the use of symmetries and of the unitarity of the Heisenberg evolution as criteria to select a preferred family of equivalent Fock representations. We then explicitly apply these criteria in Section 3 that deals with the case of a Dirac field in a non-stationary spacetime in 2 + 1 dimensions. The more interesting case of Dirac fields in a cosmological spacetime in 3 + 1 dimensions is reviewed in Section 4. After reviewing these aspects and results of QFT in curved spacetimes, in Section 5 we consider the use of canonical transformations to introduce a suitable splitting between the degrees of freedom of the cosmological background and of the Dirac field, treated in principle as a perturbation. In that section, we show how to use this freedom in the splitting to improve the quantum properties of the fermionic contribution to the Hamiltonian of the system, and in particular to make finite the backreaction that appears in it. The possibility of further employing this freedom to diagonalize the fermionic contribution to the Hamiltonian in the asymptotic limit of large wave numbers is reviewed in Section 6. There, we also explain that this diagonalization requirement can pick out a unique vacuum state under reasonable conditions, and that this state coincides with the natural one in situations of interest in QFT, like for Minkowski and de Sitter backgrounds. In addition, we also comment on the relation of adiabatic states with the vacuum selected by our criterion. Finally, we present the conclusions and some additional remarks in Section 7. We set the speed of light in vacuo, the Newton gravitational constant, and the reduced Planck constant equal to the unit.

2. Fock Quantization of the Dirac field

This section contains some background material about the Fock quantization of a Dirac field in a curved spacetime. Special emphasis is put on the inherent ambiguity in the representation of the CARs associated with the infinitely many inequivalent complex structures available to construct the quantum theory, as well as on the combined criteria of symmetry invariance and of unitary implementability of the dynamics that have been successfully employed to remove this ambiguity (and, even more, the ambiguity in the choice of basic field variables) in diverse, physically interesting fermionic (and bosonic) systems.

For the sake of clarity, let us begin our discussion by introducing the classical setting.

2.1. Background Spacetime and Dirac Equation

As backgrounds for the propagation of the field, we consider globally hyperbolic spacetimes, or just globally hyperbolic regions, $(\mathcal{M} \approx \mathbb{I} \times \Sigma, g_{\mu\nu})$, in either three or four dimensions. Here, $\mathbb{I}$ denotes an interval of the real line, and Σ is a Riemannian, Cauchy (hyper-)surface of dimension d, with $d = 2, 3$. For mathematical convenience, we restrict this surface to be topologically compact. In order to ensure that the spacetime (or region) admits a spin structure [42], we additionally require that $\mathcal{M}$ admit a global orthonormal frame [43]. Therefore, the spacetime metric can be globally written as

$$g_{\mu\nu} = e^a_\mu e^b_\nu \eta_{ab}, \tag{1}$$

where η_{ab} is the Minkowski metric in $(d+1)$-dimensions, with signature $\{-, +, \ldots, +\}$, and e^a_μ is a(n orthonormal) coframe field, with dual frame e^μ_a. Throughout this work, Greek indices from the middle of the alphabet denote spacetime indices $(\mu, \nu, \ldots = 0, \ldots, d)$, whereas Latin indices from the beginning of the alphabet account for the internal Lorentz gauge introduced by the frame $(a, b, \ldots = 0, \ldots, d)$. Moreover, Greek indices from the beginning of the alphabet denote spatial indices $(\alpha, \beta, \ldots = 1, \ldots, d)$.

By employing an Arnowitt–Deser–Misner (ADM) decomposition of the considered spacetime (region) [44], we introduce a coordinate system in $\mathcal{M}$, say $\{x^\mu\} = \{x^0, x^\alpha\}$, with $x^0 = t \in \mathbb{I}$ being the time parameter and $\{x^\alpha\}$ coordinatizing Σ. The line element in coordinates $\{x^\mu\}$ reads

$$\mathrm{d}s^2 = g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu = -(N^2 - N_\alpha N^\alpha)\mathrm{d}t^2 + 2N_\alpha \mathrm{d}x^\alpha \mathrm{d}t + h_{\alpha\beta}\mathrm{d}x^\alpha \mathrm{d}x^\beta, \tag{2}$$

where N and N^α are, respectively, the lapse function and the shift vector, and $h_{\alpha\beta}$ is the induced metric on the Cauchy surface Σ.

Let then Ψ be a free, complex, and anticommuting Dirac spinor with mass m, propagating in $(\mathcal{M}, g_{\mu\nu})$. The dynamics of Ψ is governed by the first-order linear equation

$$e^\mu_a \gamma^a \nabla^S_\mu \Psi - m\Psi = 0. \tag{3}$$

Here, the operator ∇^S_μ stands for the spin lifting of the Levi–Cività covariant derivative [42], and γ^a are the constant Dirac matrices that generate the Clifford algebra of a flat spacetime in $(d+1)$ dimensions:

$$\gamma^a \gamma^b + \gamma^b \gamma^a = 2\eta^{ab} I, \tag{4}$$

where I is the identity matrix and η^{ab} is the (inverse of the) Minkowski metric.

On account of the global hyperbolicity of $(\mathcal{M}, g_{\mu\nu})$, the Dirac Equation (3) has a well-posed Cauchy formulation [45]. Therefore, given any smooth initial value $\Psi(\vec{x})$ of the spinor field on a certain (compact) Cauchy surface Σ_0, say at $t = t_0$ (where $t_0 \in \mathbb{I}$ is a fixed, but arbitrary, reference time), there exists a unique smooth solution $\Psi(t, \vec{x})$ to Equation (3) which is defined on all of $\mathcal{M}$ and such that $\Psi(t, \vec{x})|_{\Sigma_0} = \Psi(\vec{x})$. The solution $\Psi(t, \vec{x})$, restricted to the domain of dependence of an arbitrary closed subset S of Σ_0, depends only upon $\Psi(\vec{x})|_S$. Henceforth, we fix Σ_0 (i.e., the section at $t = t_0$) as the Cauchy reference surface. Let $\mathcal{S}$ be the complex linear space of (smooth) solutions to the Dirac Equation (3) which arises from the complex vector space $\mathcal{P} = \{\Psi(\vec{x})\}$ of (smooth) initial conditions at time t_0. Please note that by construction, the map $\mathcal{S} \ni \Psi \mapsto I_{t_0}(\Psi) = \Psi|_{\Sigma_0}$ is an isomorphism between the linear spaces $\mathcal{S}$ and $\mathcal{P}$.

The space of Cauchy data $\mathcal{P}$ is naturally equipped with the product [45]

$$(\Psi_1, \Psi_2)_D = \int_{\Sigma_0} \mathrm{d}^d\vec{x}\, \sqrt{\mathrm{h}}\, \Psi_1^\dagger \gamma^0 n^\mu e^a_\mu \gamma_a \Psi_2, \tag{5}$$

where $\gamma_a = \eta_{ab}\gamma^b$, h is the determinant of $h_{\alpha\beta}$, the dagger denotes the Hermitian adjoint, and n^μ are the spacetime components of the future-directed unit normal to the Cauchy surface Σ_0. The space of solutions $\mathcal{S}$ is endowed with an inner product of the form (5), though now at an arbitrary Cauchy surface $\Sigma_{t'}$; this is so because of the independence of the mapping $(\,\cdot\,,\,\cdot\,)_D : \mathcal{S} \times \mathcal{S} \to \mathbb{C}$ upon the spatial section on which it is evaluated.

The exact meaning of what we understand by classical dynamical evolution in the space $\mathcal{P}$ is as follows. Given any solution $\Psi(t,\vec{x})$ in $\mathcal{S}$, the evaluation $\Psi(t,\vec{x})|_{\Sigma_{t'}}$ at a fixed time t' defines the spinor $\Psi'(\vec{x}) = \Psi(t',\vec{x})$ on Σ_0. Namely we can take the induced spinor field on $\Sigma_{t'}$ as initial condition on Σ_0. Clearly, the mapping $I_{t'} : \mathcal{S} \to \mathcal{P}$ defined by $\Psi(t,\vec{x}) \mapsto I_{t'}\big(\Psi(t,\vec{x})\big) = \Psi(t',\vec{x}) = \Psi'(\vec{x})$ is an isomorphism. Then, by considering the entire interval $\mathbb{I}$, we get a one-parameter family of isomorphisms $I_t : \mathcal{S} \to \mathcal{P}$. The action of this family of mappings on a solution $\Psi \in \mathcal{S}$ gives the dynamical orbit of the Cauchy initial datum $\Psi(t,\vec{x})|_{\Sigma_0} = \Psi(\vec{x})$ in $\mathcal{P}$; that is, time evolution in the space of Cauchy data $\mathcal{P}$ is given by the one-parameter family of linear transformations $T_{(t,t_0)} = I_t \circ I_{t_0}^{-1}$.

2.2. Fock Quantization, Unitarity, and Uniqueness

Let us next discuss the Fock quantization of Dirac fields using an approach based on the space of Cauchy data. It is worth remarking that an analogous approach constructed from the space of solutions is readily available, given the isomorphism I_{t_0} between both spaces.

We start by equipping the space of Cauchy data $\mathcal{P}$ with a complex structure, namely a real linear automorphism $J : \mathcal{P} \to \mathcal{P}$ with the property $J^2 = -I$, and such that it leaves the inner product (5) invariant. The complex structure allows for a natural splitting of $\mathcal{P}$ into two mutually complementary orthogonal subspaces (with respect to the considered inner product) $\mathcal{P}_J^{\pm} = (\mathcal{P} \mp iJ\mathcal{P})/2$ that are eigenspaces of J with eigenvalue $\pm i$. Let $\bar{\mathcal{P}}$ be the complex conjugate of $\mathcal{P}$, endowed with the complex conjugate of Equation (5) as its inner product. The complex structure J is naturally defined by linearity on $\bar{\mathcal{P}}$, and we similarly have that the corresponding $\pm i-$eigenspaces, $\bar{\mathcal{P}}_J^{\pm} = (\bar{\mathcal{P}} \mp iJ\bar{\mathcal{P}})/2$, provide a decomposition of $\bar{\mathcal{P}}$ into mutually orthogonal subspaces. Please note that $\bar{\mathcal{P}}_J^{\pm}$ and $\mathcal{P}_J^{\pm}$ are related by $\bar{\mathcal{P}}_J^{\pm} = \overline{\mathcal{P}_J^{\mp}}$.

By performing the Cauchy completion of $\mathcal{P}_J^{+}$ and $\bar{\mathcal{P}}_J^{+}$ in their inner products, we get the one-particle Hilbert spaces $\mathcal{H}_J^{p}$ and $\mathcal{H}_J^{ap}$ of, respectively, *particles* and *antiparticles*. The Hilbert space of the quantum theory is taken to be the antisymmetric Fock space

$$\mathcal{F}_J = \oplus_{n=0}^{\infty}(\otimes_n^a \mathcal{H}_J), \tag{6}$$

where $\mathcal{H}_J = \mathcal{H}_J^{p} \oplus \mathcal{H}_J^{ap}$ is the one-particle Hilbert space associated with the complex structure J, and $\otimes_n^a \mathcal{H}_J$ denotes the n-fold antisymmetric tensor product of $\mathcal{H}_J$, with $\otimes_0^a \mathcal{H}_J = \mathbb{C}$ [3,46].

Let $\{\psi_n^p(\vec{x})\}$ and $\{\psi_n^{ap}(\vec{x})\}$ be complete orthonormal bases for, respectively, $\mathcal{H}_J^{p}$ and $\mathcal{H}_J^{ap}$. Then, the quantum field is (formally) represented in $\mathcal{F}_J$ by

$$\hat{\Psi}(\vec{x}) = \sum_n [\hat{a}_n \psi_n^p(\vec{x}) + \hat{b}_n^{\dagger} \bar{\psi}_n^{ap}(\vec{x})], \tag{7}$$

where $\hat{a}_n$ is the annihilation operator associated with the spinor $\bar{\psi}_n^{p}$, whereas $\hat{b}_n^{\dagger}$ is the creation operator associated with the spinor ψ_n^{ap}. The adjoint operators $\hat{a}_n^{\dagger}$ and $\hat{b}_n$ correspond to the creation and annihilation operators of, respectively, particles and antiparticles. For a detailed discussion about the definition of fermionic annihilation and creation operators, see for instance Ref. [46]. For now, let us stress that the annihilation and creation operators here displayed correspond to the mode expansion projections of the (smeared) annihilation and creation operators specified in Ref. [46]. The basic operators $\{\hat{a}_n, \hat{a}_n^{\dagger}, \hat{b}_n, \hat{b}_n^{\dagger}\}$ satisfy the anticommutation relations,

$$[\hat{a}_n, \hat{a}_m^{\dagger}]_+ = \delta_{nm}, \qquad [\hat{b}_n, \hat{b}_m^{\dagger}]_+ = \delta_{nm}, \tag{8}$$

with the remaining anticommutators being null. The vacuum state of the theory corresponds to the unique (up to a phase) normalized cyclic vector in $\mathcal{F}_J$ which vanishes under the action of all the annihilation operators, $\hat{a}_n$ and $\hat{b}_n$.

Let us emphasize that the choice of a complex structure for the Fock quantization determines the annihilation and creation operators of the theory. Thus, in general, different complex structures define different representations of the CARs. Furthermore, there exist infinitely many of these representations that fail to be unitarily equivalent [3]. This is where the ambiguity in the Fock representation of the Dirac field resides. Let us be more specific. Let $\mathcal{F}_J$ and $\mathcal{F}_{J'}$ be two distinct Fock spaces, constructed from the different complex structures J and J'. It can then be shown that on the Fock space $\mathcal{F}_J$, the annihilation and creation operators defined by J' (and which are naturally associated with the basis of $\mathcal{F}_{J'}$) are given by expressions of the form

$$\hat{a}'_n = \sum_m (\alpha^f_{nm}\hat{a}_m + \beta^f_{nm}\hat{b}^\dagger_m), \qquad \hat{a}'^\dagger_n = \sum_m (\bar{\alpha}^f_{nm}\hat{a}^\dagger_m + \bar{\beta}^f_{nm}\hat{b}_m), \tag{9}$$

$$\hat{b}'_n = \sum_m (\bar{\alpha}^g_{nm}\hat{b}_m + \bar{\beta}^g_{nm}\hat{a}^\dagger_m), \qquad \hat{b}'^\dagger_n = \sum_m (\alpha^g_{nm}\hat{b}^\dagger_m + \beta^g_{nm}\hat{a}_m). \tag{10}$$

Here, $\alpha^f_{nm}, \beta^f_{nm}, \alpha^g_{nm}$, and β^g_{nm} are (complex) coefficients satisfying the relationships

$$\sum_l (\alpha^h_{nl}\bar{\alpha}^h_{ml} + \beta^h_{nl}\bar{\beta}^h_{ml}) = \delta_{nm}, \qquad \sum_l (\alpha^f_{nl}\bar{\beta}^g_{ml} + \beta^f_{nl}\bar{\alpha}^g_{ml}) = 0, \qquad h = f, g. \tag{11}$$

That is, the annihilation and creation operators defined by the two distinct complex structures J and J' are related by a Bogoliubov transformation.

By definition, unitary equivalence between the representations defined by J and J' means that there exists a unitary operator $\hat{U} : \mathcal{F}_J \to \mathcal{F}_J$ intertwining the two representations, i.e., such that $\hat{a}'_n = \hat{U}^{-1}\hat{a}_n\hat{U}$ and $\hat{b}'_n = \hat{U}^{-1}\hat{b}_n\hat{U}$. The transformation defined in Equations (9) and (10) is unitarily implementable then, in the sense that the transformation defined by the coefficients α^f_{nm}, β^f_{nm}, α^g_{nm}, and β^g_{nm} is a *bona fide* canonical transformation between the classical annihilation and creation variables corresponding to the considered operators.

A well-known result [8] states that unitary equivalence is achieved if and only if

$$\sum_{n,m} (|\beta^f_{nm}|^2 + |\beta^g_{nm}|^2) < \infty. \tag{12}$$

In general, given any two arbitrary complex structures, this condition is not satisfied. In fact, infinitely many inequivalent Fock representations of the CARs are possible, just as it happens with bosonic fields and their corresponding CCRs. The usual strategy to remove these types of ambiguities and to arrive at a (hopefully) unique Fock representation is to exploit the symmetries of the system. One typically requires that the complex structure (or the vacuum, in more physical terms) be invariant under some natural existing symmetries. As already mentioned in the Introduction, a crucial role is played here by time-translation invariance, and therefore that strict strategy fails to produce a unique representation in non-stationary scenarios, including very familiar and cosmologically relevant spacetimes.

Notice that a complex structure that remains invariant under time evolution immediately gives rise to a unitary implementation of (the canonical transformations generated by) the dynamics, therefore allowing the standard probabilistic interpretation of the quantum theory. It is, therefore, natural that in non-stationary settings, one should try to preserve the unitary implementation of dynamical transformations, though giving up on (non-available) fully time-translation invariant complex structures, taking into account that this invariance is a sufficient, but by no means necessary, condition for such a unitary implementation. Let us make this more explicit. Suppose we are given a complex structure J on $\mathcal{P}$, and construct the corresponding Fock representation, with associated operators $\hat{a}_n$ and $\hat{b}_n$ as above. Since the field equations are linear, the transformations that correspond to time evolution from initial time t_0 to arbitrary time t are linear, and we obtain, for each t, new operators of the general form

$$\hat{a}_n(t) = \sum_m \left(\alpha^f_{nm}(t,t_0)\hat{a}_m + \beta^f_{nm}(t,t_0)\hat{b}^\dagger_m \right), \tag{13}$$

$$\hat{b}^\dagger_n(t) = \sum_m \left(\alpha^g_{nm}(t,t_0)\hat{b}^\dagger_m + \beta^g_{nm}(t,t_0)\hat{a}_m \right), \tag{14}$$

with $\hat{a}^\dagger_n(t)$ and $\hat{b}_n(t)$ being supplied by the adjoint expressions of, respectively, Equations (13) and (14). It should be clear that since the field evolution is a canonical transformation, the new operators satisfy the CARs, and we therefore have a family of new Fock representations. In fact, the new operators are simply those associated with the transformed complex structures $T_{(t,t_0)} J T^{-1}_{(t,t_0)}$ [10], where $T_{(t,t_0)}$ is the evolution map introduced at the end of Section 2.1. Then, a unitary implementation of the dynamical transformations implies the unitary equivalence between all the new representations, for all t, and the original one defined by J. Of course, for a complex structure J that remains invariant under time evolution, the fulfillment of the unitary equivalence condition (12) is trivial, since all the nondiagonal beta coefficients of the associated Bogoliubov transformations are null.

On the other hand, there seems to be no compelling reason to relax the requirement of invariance under other natural remaining symmetries, such as isometries of the spatial manifold Σ, since invariant complex structures under these types of symmetries typically exist. Therefore, the strategy that we adopt to deal with the ambiguity of the Fock quantization in non-stationary settings is the following. We require that the complex structure be invariant under the spatial isometries (and possibly other remaining symmetries of the system) and that it allows a unitary implementability of the dynamics. These combined criteria have been shown to be viable and effective in addressing the issue of the uniqueness of the quantization for a large class of field systems. The criteria were introduced for the first time in the context of midisuperspace models[1], concretely to specify a unique preferred quantization of the inhomogeneous fields in Gowdy cosmological models [12–16,49], and since then they have been profusely and successfully employed to address the uniqueness of the quantization of (test) scalar fields in various, physically relevant cosmological backgrounds [17–22,24,25,27,29,50] (for a review, see Ref. [51]). Concerning fermionic fields and CARs, the same criteria have been successfully applied to single out a unique preferred quantum description for (test) Dirac fields in $2+1$ dimensions [52] and in FLRW spacetimes [53–56], as we discuss in the next two sections.

It is worth pointing out that as discussed in the Introduction, to achieve unitarily implementable dynamics in the type of non-stationary scenarios here considered, it is inevitable to explore the freedom in the splitting of the time dependence of the field between a genuine quantum Heisenberg evolution and an explicit dependence on the spacetime background. Typically, superimposed on the intrinsic dynamical evolution of the field variables, there is an explicitly time-dependent part coming from the non-stationary background spacetime itself. This last contribution to the total time dependence may be viewed as classical in nature, and effectively obstructs the possibility of a unitary quantum evolution. The solution is to extract the latter part by means of a time-dependent canonical transformation (performed at the classical level). This type of modification of the quantum notion of the field evolution is unavoidable in all the cosmological systems analyzed so far, in order to recover a unitary implementability of the dynamics. Crucial in this approach is to pinpoint exactly the correct splitting between the intrinsic time dependence of the field and the time dependence coming from external factors, such as a non-stationary background. It is of the utmost importance to stress that this

1 The term *midisuperspace*, originally introduced by K. Kuchař [47,48], refers to models that even though possessing some symmetry, retain an infinite number of degrees of freedom, e.g., certain inhomogeneous models.

splitting is far from being arbitrary. It is guided, and to a great extent determined, by the requirement of a unitarily implementable dynamics.

3. Dirac Fields in 2 + 1 Dimensions

This section is devoted to discussing the applicability of the criteria of symmetry invariance and of unitary implementability of the dynamics in the Fock quantization of a concrete class of field systems, namely the case of a free Dirac field in $2+1$-dimensional spacetimes which are conformally ultrastatic, with a time-dependent conformal factor. We show that under rather non-stringent conditions on the time dependence of the cosmological background, and once a convention on the notions of particle and antiparticle has been established, a unique family of equivalent Fock representations is singled out by imposing (i) invariance under the unitary transformations that implement the symmetries of the equations of motion, and (ii) a nontrivial and unitarily implementable dynamics [52].

3.1. Dirac Spinor in Conformally Ultrastatic Spacetimes

Let us consider a fermionic field coupled to a globally hyperbolic, smooth manifold (or region) $\mathcal{M}$, with the topology of $\mathbb{I} \times \Sigma$, where (as before) $\mathbb{I} \subseteq \mathbb{R}$ is an interval of the real line, and Σ is a connected, compact, and orientable two-dimensional Riemannian manifold. Since, in particular, $\mathcal{M}$ is an orientable three-dimensional manifold, it is stably parallelizable [57]. We consider here conformally ultrastatic background geometries, so that the metric can be written as

$$\mathrm{d}s^2 = a^2(\eta)\left(-\mathrm{d}\eta^2 + {}^0h_{\alpha\beta}(\vec{x})\mathrm{d}x^\alpha \mathrm{d}x^\beta\right). \tag{15}$$

Up to the scale factor $a(\eta)$, which contains the non-stationary information of the metric, ${}^0h_{\alpha\beta}$ is the metric induced on the spatial surfaces Σ_η defined at each fixed value of the conformal time η.

The Dirac field couples to the geometry by means of the global (co)frame (1) defined, up to $SO(2,1)$ (orthochronous) gauge transformations, by the metric (15). Since in three dimensions any of the two irreducible complex representations of the Clifford algebra (4) are generated by 2×2 Dirac matrices, complex fermionic fields are locally represented by two-component spinors Ψ. In turn, we describe the components of these spinors by Grassmann variables, to encode the anticommuting nature of the fermionic field. We represent the Dirac matrices by

$$\gamma^0 = i\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \gamma^1 = i\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{16}$$

The action for a fermionic field of mass m is given by

$$I_f = -i\int \mathrm{d}\eta\, \mathrm{d}^2\vec{x}\sqrt{-\mathrm{g}}\left[\frac{1}{2}(\Psi^\dagger\gamma^0 e^\mu_a\gamma^a\nabla^S_\mu\Psi - \mathrm{h.c.}) - m\Psi^\dagger\gamma^0\Psi\right], \tag{17}$$

where g is the determinant of the spacetime metric $g_{\mu\nu}$ and h.c. stands for Hermitian conjugate. Moreover, using the spin connection one-form

$$\omega^{ab}_\mu = \frac{1}{2}\left(e^{\nu a}\partial_\mu e^b_\nu + e^{\nu a}e^{\lambda b}\partial_\lambda g_{\mu\nu} - e^{\nu b}\partial_\mu e^a_\nu - e^{\nu b}e^{\lambda a}\partial_\lambda g_{\mu\nu}\right), \tag{18}$$

the spin lifting of the Levi–Cività covariant derivative is locally defined on the spinors as [42]

$$\nabla^S_\mu\Psi = \partial_\mu\Psi - \frac{1}{4}\omega^{ab}_\mu\gamma_b\gamma_a\Psi. \tag{19}$$

It is convenient to partially fix the internal Lorentz gauge by choosing $n^\mu e^a_\mu = \delta^a_0$, where n^μ is the future-directed unit vector field normal to the spatial surfaces Σ_η. This leads to a reduction of the structure group of the bundle of oriented frames from $SO(2,1)$ (orthochronous) to $SO(2)$ [58], restricting the spin structure to the double cover of the reduced frame bundle. For each of the considered spacetime manifolds and choice of spin structure on them, this restriction is well defined and provides an identical spin structure on each of all the two-dimensional leaves that foliate the spacetime manifold [42]. Thus, for each value of the time parameter, the field behaves as a spinor geometrically defined on each of the two-dimensional spatial manifolds Σ_η that foliate the background. Equivalently, within the Cauchy data approach, the field can be described by one-parameter families of spinors, parametrized by the conformal time η, defined on an *initial* Cauchy reference surface Σ_0, specified by $\eta = \eta_0$. Let us denote by $\mathcal{P}$ the space of Cauchy data, namely the space of spinors at Σ_0. The aforementioned one-parameter families on $\mathcal{P}$ are nothing but the result of evolving the Cauchy data in time (see Section 2). Thanks to the adopted gauge fixing, we can make a direct use of the spectral analysis of the Dirac operator defined on the two-dimensional Cauchy surface Σ_0, instead of the Dirac operator on the whole Lorentzian geometry. In fact, in this gauge, the covariant derivative on spinors becomes simply

$$\nabla^S_0 \Psi = \partial_0 \Psi, \quad \nabla^S_\alpha \Psi = {}^{(2)}\nabla^S_\alpha \Psi - \frac{1}{4}\tilde{\omega}^{ab}_\alpha \gamma_b \gamma_a \Psi, \tag{20}$$

$$\tilde{\omega}^{ab}_\alpha = \frac{1}{2}\left(e^{\beta a} e^{0b} \partial_0 g_{\alpha\beta} - e^{\beta b} e^{0a} \partial_0 g_{\alpha\beta}\right), \tag{21}$$

where ${}^{(2)}\nabla^S_\alpha$ is the spin covariant derivative on the spatial leaf with metric ${}^0h_{\alpha\beta}$. It can then be checked that

$$e^\mu_a \gamma^a \nabla^S_\mu \Psi = \frac{\gamma^0}{a}\left(\partial_0 + \frac{a'}{a}\right)\Psi - \frac{i}{a}\not{D}\Psi, \tag{22}$$

where the prime stands for the derivative with respect to the conformal time η, and $\not{D}$ denotes the Dirac operator on Σ_0.

Once the partial gauge fixing is performed, the inner product (5) on the space of Cauchy data $\mathcal{P}$ simplifies to

$$(\Psi_1, \Psi_2)_D = a_0^2 \int_{\Sigma_0} \mathrm{d}^2\vec{x}\sqrt{{}^0\mathrm{h}}\,\Psi_1^\dagger(\vec{x})\Psi_2(\vec{x}), \tag{23}$$

where $a_0 = a(\eta_0)$ and ${}^0\mathrm{h}$ is the determinant of ${}^0h_{\alpha\beta}$.

The Dirac operator $\not{D}$ is essentially self-adjoint with respect to the inner product (5) and, since Σ_0 is compact, it necessarily has a discrete spectrum, with eigenvalues $\pm\omega_n$, labeled by natural numbers n, with ω_n (≥ 0) growing with n [42]. Then, the space of Cauchy data $\mathcal{P}$ can be endowed with a basis formed by a set of eigenspinors of the Dirac operator. Let $a_0^{-1}\rho^{np}(\vec{x})$ be the eigenspinors with positive eigenvalue ω_n and orthonormal with respect to the inner product (5), where the index p accounts for the degeneracy. Since $\not{D}$ anticommutes with $\gamma^1\gamma^2 = \gamma^0$, we can choose as eigenspinors with negative eigenvalue $-\omega_n$ those defined as $\bar{\sigma}^{np}(\vec{x}) = -\gamma^0\rho^{np}(\vec{x})$. Like $\rho^{np}(\vec{x})$, these eigenspinors form an orthonormal set when the product is rescaled by the factor a_0^{-2}. With this rescaling, the set $\{\rho^{np}(\vec{x}), \bar{\sigma}^{np}(\vec{x})\}$ provides a complete, orthonormal basis for $\mathcal{P}$.

Let g_n be the degeneracy of the eigenspace labeled by n, so that $p = 1, \ldots, g_n$. The explicit form of g_n depends on the spectral details of the Dirac operator $\not{D}$ and, consequently, on the particular 2-manifold considered. Nevertheless, for our purposes, we do not need the actual value of g_n, but only to know its behavior in the ultraviolet regime of large eigenvalues ω_n. Therefore, let us introduce the counting function $\chi_{\not{D}}(\omega)$ of the Dirac operator on a d-dimensional compact Riemannian manifold; that is, $\chi_{\not{D}}(\omega)$ is the function that counts the number of positive eigenvalues of $\not{D}$ that are not greater than ω (including degeneracy). From the Weyl asymptotic formula [59], it follows that $\chi_{\not{D}}(\omega)$ grows at most as ω^d when ω goes to infinity. Using this result with $d = 2$, we conclude that the degeneracy behaves in the large n limit as $g_n = o(\omega_n^2)$, where the symbol $o(\omega_n^2)$ means negligible with respect to ω_n^2.

In terms of the basis $\{\rho^{np}(\vec{x}), \bar{\sigma}^{np}(\vec{x})\}$, the *dynamical* families of spinors in $\mathcal{P}$ (each one of them parametrized by the conformal time η) are given by

$$\Psi(\eta,\vec{x}) = \frac{1}{a(\eta)}\psi(\eta,\vec{x}), \quad \psi(\eta,\vec{x}) = \sum_{n=0}^{\infty}\sum_{p=1}^{g_n}\left[s_{np}(\eta)\rho^{np}(\vec{x}) + \bar{r}_{np}(\eta)\bar{\sigma}^{np}(\vec{x})\right]. \tag{24}$$

Here, we use overlined symbols to indicate complex conjugation. Apart from the global factor $a^{-1}(\eta)$, the time dependence (equivalently, the η-parameterization) is captured by the time-dependent coefficients s_{np} and $\bar{r}_{np}$ of ψ, which take care of the Grassmannian nature of the fermionic field. The auxiliary field ψ shows symmetric canonical Dirac brackets with its corresponding adjoint field that do not depend on the background [60,61]. We represent the algebra generated by these brackets in a Fock space, with the brackets being replaced with anticommutators , thus obtaining a Fock representation of the CARs and therefore a quantization of both the auxiliary and the original field, ψ and Ψ.

By writing the field anticommutation relations in terms of the modes s_{np}, $\bar{r}_{np}$, and their complex conjugates, one finds that the only nonvanishing Dirac brackets are $\{s_{np}, \bar{s}_{np}\} = -i$ and $\{r_{np}, \bar{r}_{np}\} = -i$, which are symmetric due to the anticommutativity of our Grassmann variables. In the quantum theory, they become anticommutators of the corresponding operators [60].

From Equations (17) and (24), the equations of motion for the fermionic modes are given by [52]

$$s'_{np} = i(\omega_n + ima)\bar{r}_{np}, \qquad r'_{np} = -i(\omega_n + ima)\bar{s}_{np}, \tag{25}$$

and their complex conjugates. These equations only couple the modes s_{np} and $\bar{r}_{np}$ (respectively $\bar{s}_{np}$ and r_{np}) with the same labels n and p, and do not depend on the degeneracy label p. They can be combined into the second-order differential equation

$$z''_{np} = -(\omega_n^2 + m^2a^2)z_{np} + i\frac{ma'}{\omega_n + ima}z'_{np}, \tag{26}$$

where z_{np} denotes either s_{np} or r_{np}. The general solution to this equation does not depend on the label p, except through the initial conditions, and is a linear combination of two complex independent solutions that we write in the form $\exp[(-1)^{l+1}i\Theta_n^l(\eta)]$ with $l = 1,2$. Let $\Theta_n^l(\eta_0) = \Theta_{n,0}^l$ and $(\Theta_n^l)'(\eta_0) = \Theta_{n,1}^l$ be the initial conditions at the initial reference time η_0, and let us call $\Omega_{n,0}^l = \exp[(-1)^{l+1}i\Theta_{n,0}^l]$. A simple inspection shows that the integration constants of the general solution relate the initial conditions on Θ_n^l and their derivatives to the initial conditions s_{np}^0 and r_{np}^0 for the modes (and their complex conjugates), via Equation (25). One can then deduce that time evolution in the complex linear space of spinors ψ is dictated by the linear transformation [52]

$$\begin{pmatrix} s_{np} \\ \bar{r}_{np} \end{pmatrix}_{\eta} = \mathcal{V}_n(\eta,\eta_0)\begin{pmatrix} s_{np} \\ \bar{r}_{np} \end{pmatrix}_{\eta_0}, \tag{27}$$

$$\mathcal{V}_n(\eta,\eta_0) = \begin{pmatrix} \Delta_n^2 e^{i\Theta_n^1(\eta)} + \Delta_n^1 e^{-i\Theta_n^2(\eta)} & \zeta_n^1 e^{i\Theta_n^1(\eta)} - \zeta_n^2 e^{-i\Theta_n^2(\eta)} \\ \bar{\zeta}_n^2 e^{i\bar{\Theta}_n^2(\eta)} - \bar{\zeta}_n^1 e^{-i\bar{\Theta}_n^1(\eta)} & \bar{\Delta}_n^2 e^{-i\bar{\Theta}_n^1(\eta)} + \bar{\Delta}_n^1 e^{i\bar{\Theta}_n^2(\eta)} \end{pmatrix}, \tag{28}$$

where the subindex η in column-vectors denotes evaluation at the given value of the conformal time, and the constants Δ_n^l and ζ_n^l are

$$\Delta_n^l = \frac{\Theta_{n,1}^l}{\Omega_{n,0}^{\tilde{l}}(\Theta_{n,1}^1 + \Theta_{n,1}^2)}, \qquad \zeta_n^l = \frac{\omega_n + ima_0}{\Omega_{n,0}^l(\Theta_{n,1}^1 + \Theta_{n,1}^2)}, \tag{29}$$

where $\tilde{l}$ is the complementary of l in $\{1,2\}$, namely $\{l,\tilde{l}\} = \{1,2\}$.

To analyze whether the quantum theory admits a unitarily implementable dynamics, we do not really need to obtain the solution for $\mathcal{V}_n(\eta, \eta_0)$. It is sufficient to know its behavior in the ultraviolet regime of large ω_n. Under the mild condition that the scale factor be twice differentiable and with a second derivative that is integrable over each compact subinterval of the time domain $\mathbb{I}$, a careful asymptotic analysis of the dynamics of the modes $\{z_{np}\} = \{s_{np}, r_{np}\}$ shows that two independent solutions to Equation (26) can be specified as follows [52]:

$$\Theta_n^l = \omega_n \Delta\eta + \int_{\eta_0}^{\eta} d\tilde{\eta} \Sigma_n^l(\tilde{\eta}), \qquad \Sigma_n^l(\tilde{\eta}) = \Lambda_n^l(\tilde{\eta}) - (-1)^l \frac{m a'(\tilde{\eta})}{2[\omega_n + i m a(\tilde{\eta})]}, \tag{30}$$

for $l = 1, 2$, where $\Delta\eta = \eta - \eta_0$, and $\Lambda_n^l(\eta)$ is a function with $\Lambda_n^l(\eta_0) = 0$ that in the ultraviolet regime, is at most of order ω_n^{-1}. With this choice, the constants (29) turn out to be

$$\Delta_n^l = \frac{1}{2} - (-1)^l \frac{m a_0'}{4\omega_n(\omega_n + i m a_0)}, \qquad \zeta_n^l = \frac{1}{2} + i \frac{m a_0}{2\omega_n}. \tag{31}$$

3.2. Fock Quantization and Unitary Evolution

Let us now discuss the quantization of our fermionic system. Concretely, in this section we present the unique, preferred Fock quantization singled out by the criteria of symmetry invariance and of unitary implementability of the dynamics introduced in Section 2. The construction is performed in three steps. (1) We first focus on determining the family of invariant complex structures; namely those that commute with the action of the group of symmetries of the equations of motion for the modes. By construction, these complex structures lead to Fock vacuum states that are invariant under the unitary transformations generated by the symmetry group. We then consider time-dependent families of annihilation and creation variables associated with the invariant complex structures. By interpreting these families as dynamical trajectories, a specific redistribution of the implicit and explicit time dependence of the field is made. The dynamics that we wish to implement quantum mechanically is that of the implicitly time-dependent part, corresponding to the evolution of the annihilation and creation variables. (2) Each of the families of annihilation and creation variables defines an invariant Fock representation and a specific quantum evolution in the corresponding Fock space. We impose the criterion of unitary implementability of the dynamics, together with the requirement that the evolution be not trivialized. This leads us to set (or better said, characterize) all invariant Fock quantizations with a nontrivial and unitarily implementable dynamics. (3) Finally, we show that all such Fock quantizations turn out to be, in fact, unitarily equivalent, up to conventions in the notions of particles and antiparticles.

On account of Equation (25), it is clear that the field equations are invariant under the set of transformations that interchange eigenmodes of the Dirac operator with the same value of ω_n. Since the Dirac operator is built from the spatial metric ${}^0h_{\alpha\beta}$, these symmetries include the isometries (if any) of the Cauchy surface Σ_0. It should be clear that linear transformations commuting with the action of the symmetry group of the Dirac equation are composed of 2×2 blocks which at most, can mix the modes s_{np} and $\bar{r}_{np}$ with the same value of p. In addition, using all the available symmetries one can reason that the blocks are necessarily the same for all the modes corresponding to the same eigenvalue of the Dirac operator (in norm) [52]. Therefore, in particular, invariant complex structures are completely determined by a series of 2×2 matrices labeled by $n \in \mathbb{N}$.

Let us remark that given a complex structure, their associated annihilation and creation variables, namely the classical counterparts of the corresponding operators in an expansion of the type (7), diagonalize its action. Since invariant complex structures can mix only modes s_{np} and $\bar{r}_{np}$ with the same labels, the corresponding annihilation and creation variables must be linear combinations of these modes. The annihilation variables of particles and antiparticles are denoted by a_{np} and b_{np}, respectively, while the creation variables are their complex conjugates $\bar{a}_{np}$ and $\bar{b}_{np}$. These variables must satisfy the usual Dirac brackets for annihilation and creation sets, $\{a_{np}, \bar{a}_{np}\} = \{b_{np}, \bar{b}_{np}\} = -i$ and $\{a_{np}, b_{np}\} = 0$, which lead to the CARs (8) in the quantum theory.

Now, let us consider time-dependent families of annihilation and creation variables associated with invariant complex structures. Specifically,

$$\begin{pmatrix} a_{np} \\ \bar{b}_{np} \end{pmatrix}_\eta = \mathcal{F}_n(\eta) \begin{pmatrix} s_{np} \\ \bar{r}_{np} \end{pmatrix}_\eta, \qquad \mathcal{F}_n(\eta) = \begin{pmatrix} f_1^n(\eta) & f_2^n(\eta) \\ g_1^n(\eta) & g_2^n(\eta) \end{pmatrix}. \tag{32}$$

In order that we get the required Dirac brackets for a_{np}, b_{np}, and their complex conjugates, the time-dependent functions f_l^n and g_l^n $(l = 1, 2)$ must satisfy

$$|f_1^n|^2 + |f_2^n|^2 = 1, \qquad |g_1^n|^2 + |g_2^n|^2 = 1, \qquad f_1^n \bar{g}_1^n + f_2^n \bar{g}_2^n = 0. \tag{33}$$

Combining these conditions, we can write

$$g_1^n = \bar{f}_2^n e^{iG^n}, \qquad g_2^n = -\bar{f}_1^n e^{iG^n}, \qquad f_1^n g_2^n - g_1^n f_2^n = -e^{iG^n}, \tag{34}$$

where G^n is a certain phase. Thus, it suffices just one complex function and two (real) phases for each n to characterize one family of annihilation and creation variables of the form (32).

If we interpret the variables in each of these families as conforming to dynamical trajectories, their evolution differs (from each other, in general, and) from that of the modes s_{np} and $\bar{r}_{np}$ that dictate the evolution of the auxiliary spinor field ψ, because of the explicit dependence on η of the matrices $\mathcal{F}_n$. By substituting the inverse of Equation (32) in Equation (24), we obtain the expression of Ψ in terms of the introduced variables $a_{np}(\eta)$ and $\bar{b}_{np}(\eta)$. The result makes it clear that the dynamics of Ψ is determined by the evolution of the annihilation and creation variables, and by the explicitly time-dependent contributions coming from $\mathcal{F}_n$ and the scale factor. It is only the implicitly time-dependent part, i.e., the part corresponding to the evolution of the annihilation and creation variables, the one that we want to implement as a quantum Heisenberg evolution. In the following, we restrict our attention to quantizations that are not only invariant, but also admit a unitary implementability of these dynamics.

For any of the allowed families of variables given in Equation (32), the dynamical evolution is a Bogoliubov transformation relating those variables at two different times, say the arbitrary time η and the initial time η_0. By using Equations (27) and (32), we get

$$\begin{pmatrix} a_{np} \\ \bar{b}_{np} \end{pmatrix}_\eta = \mathcal{B}_n(\eta,\eta_0) \begin{pmatrix} a_{np} \\ \bar{b}_{np} \end{pmatrix}_{\eta_0}, \qquad \mathcal{B}_n(\eta,\eta_0) = \begin{pmatrix} \alpha_n^f(\eta,\eta_0) & \beta_n^f(\eta,\eta_0) \\ \beta_n^g(\eta,\eta_0) & \alpha_n^g(\eta,\eta_0) \end{pmatrix}, \tag{35}$$

where $\mathcal{B}_n(\eta,\eta_0) = \mathcal{F}_n(\eta)\mathcal{V}_n(\eta,\eta_0)\mathcal{F}_n^{-1}(\eta_0)$. This Bogoliubov transformation introduces the family of evolved complex structures $J_\eta = \mathcal{B}_n(\eta,\eta_0) J_{\eta_0} \mathcal{B}_n^{-1}(\eta,\eta_0)$ on the space of initial Cauchy data, where J_η is the invariant complex structure associated with (i.e., has a diagonal action on) the annihilation and creation variables at time η. As we have seen in Section 2, the transformations (35) are implementable as unitary operators on the Fock space defined by J_{η_0} if and only if

$$\sum_n g_n |\beta_n^f(\eta,\eta_0)|^2 < \infty \qquad \text{and} \qquad \sum_n g_n |\beta_n^g(\eta,\eta_0)|^2 < \infty, \quad \forall \eta \in \mathbb{I}. \tag{36}$$

Let us recall that the number of eigenstates of the Dirac operator with positive eigenvalue not greater than ω grows as ω^2 in the ultraviolet regime. Using this asymptotic behavior, it is possible to show [52] that for large N_1 and arbitrary $N_2 > N_1$, and with $N_1 \geq \omega_{n_1} > N_1 - 1$ and $N_2 \geq \omega_{n_2} > N_2 - 1$,

$$\sum_{n=n_1}^{n_2} \frac{g_n}{\omega_n^4} \leq \sum_{N=N_1}^{N_2} \frac{K}{N^3}, \tag{37}$$

where K is some positive constant. This identity is important for the subsequent analysis because it implies that the sequence $\{\sqrt{g_n}\omega_n^{-2}\}_{n\in\mathbb{N}}$ is square summable.

Employing Equations (30) and (31), as well as relations (33) and (34), one can check that in the asymptotic regime of large ω_n,

$$\begin{aligned}|\beta_n^h| = \frac{1}{2}\Bigg|&(h_2^{n,0} - h_1^{n,0})\left[h_1^n\left(1+i\int\Sigma_n^1\right) + h_2^n\left(1+i\int\bar{\Sigma}_n^2\right)\right]e^{i\omega_n\Delta\eta}\\ &+(h_2^{n,0} + h_1^{n,0})\left[h_1^n\left(1-i\int\Sigma_n^2\right) - h_2^n\left(1-i\int\bar{\Sigma}_n^1\right)\right]e^{-i\omega_n\Delta\eta}\\ &+\frac{2ma_0}{\omega_n}\left(h_1^{n,0}h_1^n + h_2^{n,0}h_2^n\right)\sin(\omega_n\Delta\eta)\Bigg| + \mathcal{O}(\omega_n^{-2}),\end{aligned} \tag{38}$$

where the integrals are over conformal time from η_0 to η, the symbol $\mathcal{O}$ stands for asymptotic order, and h can be set equal to either f or g. To lighten the notation, we have omitted the dependence of these functions on η and denoted the evaluation at η_0 with the superscript 0, preceded by a comma. It is worth noticing that Relations (33) and (34) guarantee that $|\beta_n^f| = |\beta_n^g|$. Therefore, for the purpose of unitarity, it suffices to analyze just one of these types of coefficients.

It is convenient to employ again the notation $\{l,\tilde{l}\} = \{1,2\}$. Then, given that $|h_{\tilde{l}}^n|^2 + |h_l^n|^2 = 1$, we get $h_{\tilde{l}}^n = e^{iH_{\tilde{l}}^n}\sqrt{1-|h_l^n|^2}$, where $H_{\tilde{l}}^n$ denotes some phase that may depend on time.

It is worth remarking that in addition to conditions (36) which severely restrict the behavior of the coefficients h_l^n, both in their mode and time dependence, one should naturally demand that h_l^n be such that the dynamics of the annihilation and creation variables is not trivialized when compared with the original Dirac evolution. Otherwise, the criterion of a unitary implementation of the dynamics would be useless, since it would pose no restriction on the Fock representation. Indeed, one may always extract all the asymptotically dominant time dependence of the fermionic field by means of explicitly time-dependent canonical transformations, and trivialize in this way the requirement of a unitarily implementable evolution. More specifically, by examining Equation (38), it can be seen that the dominant contribution of the Dirac dynamics dictated by $\mathcal{V}_n(\eta,\eta_0)$ is given by imaginary exponentials of the phases $\pm\omega_n\Delta\eta$. Thus, to avoid a trivial evolution, we rule out the possibility that these dynamical contributions are counterbalanced with a specific choice of (time and mode-dependent) phases in the linear combinations that determine the annihilation and creation variables.

Altogether, taking h as either f or g, the requirements of a nontrivial and unitarily implementable dynamics impose, as a necessary condition that asymptotically [52]

$$h_l^n = \frac{e^{iH_l^n}}{\sqrt{2}} + \vartheta_{h,l}^n, \qquad h_{\tilde{l}}^n = \pm e^{iH_{\tilde{l}}^n}\sqrt{1-|h_l^n|^2} = \pm e^{iH_{\tilde{l}}^n}\left[\frac{1}{\sqrt{2}} - \mathrm{Re}(e^{-iH_l^n}\vartheta_{h,l}^n)\right] + \mathcal{O}(|\vartheta_{h,l}^n|^2), \tag{39}$$

for a subset of the natural numbers, $n \in \mathbb{N}_l^{\pm}$, and with $\vartheta_{h,l}^n$ being some mode-dependent and time-dependent complex function that goes to zero in the limit of large ω_n. Here, the union of the four subsets $\mathbb{N}_l^{\pm}$ gives (up to a finite number of elements) the natural numbers, allowing for the possibility that up to three of these subsets be empty, and with identified h_l^n with h_1^n for $n \in \mathbb{N}_1^{\pm}$ and with h_2^n for $n \in \mathbb{N}_2^{\pm}$, with the $\pm$ superscripts indicating the relative sign for $h_{\tilde{l}}^n$ in the second and third identities of Equation (39). By substituting this equation into Relation (38), as well as using that the integral of $(\bar{\Sigma}_n^1 - \Sigma_n^2)$ behaves as $m\,(a-a_0)\,/\omega_n + \mathcal{O}(\omega_n^{-2})$ in the ultraviolet regime [52], one gets that the asymptotic behavior of the complex norm of the beta coefficients, for all $n \in \mathbb{N}_l^{\pm}$, is

$$|\beta_n^h| = \frac{1}{\sqrt{2}}\Bigg| \left[\vartheta_{h,l}^{n,0} e^{-iH_l^{n,0}} + \mathrm{Re}(e^{-iH_l^{n,0}}\vartheta_{h,l}^{n,0}) - i(-1)^l \frac{ma_0}{\sqrt{2}\omega_n}\right] e^{\pm i\omega_n \Delta\eta} \\ - \left[\vartheta_{h,l}^{n} e^{-iH_l^{n}} + \mathrm{Re}(e^{-iH_l^{n}}\vartheta_{h,l}^{n}) - i(-1)^l \frac{ma}{\sqrt{2}\omega_n}\right] e^{\mp i\omega_n \Delta\eta}\Bigg|, \quad (40)$$

up to certain terms that are negligible compared with the largest order between ω_n^{-1} and $\vartheta_{h,l}^n$.

So far, no condition has been set on $\vartheta_{h,l}^n$ other than it must go to zero in the ultraviolet limit. However, by adding the requirement that the sequence $\{g_n|\beta_n^h|^2\}_{n\in\mathbb{N}_l^\pm}$ be summable, one gets a restriction on how fast $\vartheta_{h,l}^n$ must tend to zero. The line of reasoning is the following. One assumes that the beta coefficients are square summable in the subsets $\mathbb{N}_l^\pm$, including degeneracy, and then one looks for the functions $\vartheta_{h,l}^n$ (if any) that solve the resulting conditions. From Equation (40), one finds that there are two different situations that lead to distinct conditions on $\vartheta_{h,l}^n$, namely either the sequence $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^\pm}$ is square summable, or not. In the first situation, it is not difficult to check that $\{\sqrt{g_n}\vartheta_{h,l}^n\}_{n\in\mathbb{N}_l^\pm}$ must be square summable. For the alternative situation (that is when $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^\pm}$ is not a square summable sequence), by using the implications of Equation (37) and recalling that any trivialization of the fermionic dynamics is excluded, one can see that the functions [52]

$$\tilde{\vartheta}_{h,l}^n = \vartheta_{h,l}^n + e^{iH_l^n}\mathrm{Re}(e^{-iH_l^n}\vartheta_{h,l}^n) - i(-1)^l \frac{ma}{\sqrt{2}\omega_n} e^{iH_l^n} \quad (41)$$

must form a sequence that is square summable, including degeneracy, in the subsets $\mathbb{N}_l^\pm$ where $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^\pm}$ fails to satisfy such square summability.

In total, given an invariant family of complex structures J_η characterized by the annihilation and creation variables (32), the necessary and sufficient conditions for the corresponding Fock representations of the CARs to be unitarily equivalent, and therefore to support a unitarily implementable nontrivial dynamics, are the following. (1) The functions h_l^n and $h_{\bar{l}}^n$ must be asymptotically of the form (39) for $n \in \mathbb{N}_l^\pm$. (2) The terms $\vartheta_{h,l}^n$ must be such that either (2a) if $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^\pm}$ is square summable, they form a sequence that is square summable (including over the degeneracy), or otherwise, (2b) the sequence $\{\sqrt{g_n}\tilde{\vartheta}_{h,l}^n\}_{n\in\mathbb{N}_l^\pm}$ is square summable, with $\tilde{\vartheta}_{h,l}^n$ given in Equation (41).

Up to now, we have characterized all families of annihilation and creation variables that (i) share the symmetries of the equations of motion, and (ii) evolve according to nontrivial dynamics that are unitarily implementable at the quantum level. Each of these families determines an invariant Fock representation (e.g., that associated with the choice of an invariant complex structure at the initial time η_0) with a nontrivial, unitary quantum evolution in the corresponding Hilbert space. By referring to the combination of a Fock representation and a specific quantum dynamics as a *Fock quantization* of the system, the question now is whether the invariant Fock quantizations with unitarily implementable nontrivial dynamics are equivalent quantum theories or not. Before we address this issue of uniqueness, let us make some remarks about the preceding results.

Please note that the criterion of unitary implementability, together with the requirement of a nontrivial dynamics, fix (up to phases) the leading order behavior of the coefficients h_l^n in the asymptotic regime of large ω_n, as it is shown in Equation (39). In addition, for all those cases where $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^\pm}$ fails to be a square summable sequence, the imaginary part of $e^{-iH_l^n}\vartheta_{h,l}^n$ must have its dominant asymptotic contribution of order ω_n^{-1}, and equal to the function $ma/(\sqrt{2}\omega_n)$ in absolute value. This follows simply by realizing that the square summability of the sequence $\{\sqrt{g_n}\tilde{\vartheta}_{h,l}^n\}_{n\in\mathbb{N}_l^\pm}$ implies that $\tilde{\vartheta}_{h,l}^n = o(\omega_n^{-1})$ in Equation (41). Hence, for a nonzero fermionic mass m, the coefficients h_l^n asymptotically depend in a very specific way on the eigenvalue of the Dirac operator and on the mass of the field. Most importantly, there is also a specific dependence on time, by means of a dependence on the background where the field propagates. Finally, let us emphasize that the analysis about unitarity holds not only for a positive value of the mass m, but also when this mass is zero, i.e., the families of annihilation and creation variables for the massless Dirac field, selected by the criteria of symmetry invariance and of unitarity, are fully characterized by coefficients (h_l^n, h_l^n) with an asymptotic form given by Equation (39), and such that the sequences $\{\sqrt{g_n}\vartheta^n_{h,l}\}_{n\in\mathbb{N}_l^\pm}$ are square summable. It is worth noticing that within this family, the choice $f_1^n = f_2^n = g_1^n = -g_2^n = 1/\sqrt{2}$ provides a representation which corresponds to the Fock quantization constructed from the (celebrated) conformal vacuum, i.e., the natural vacuum specified by imposing the conformal symmetry of the massless Dirac equation in the quantum theory.

3.3. Uniqueness of the Quantization

Let us now address the issue of uniqueness. With this aim, we proceed as follows. First, as a reference, we adopt a certain Fock quantization that is invariant and possesses a nontrivial and unitarily implementable dynamics. Next, we consider any other invariant Fock quantization that admits a nontrivial, unitarily implementable dynamics, and we examine whether it is unitarily related with the reference Fock quantization or not. If the answer is in the affirmative, then the uniqueness is proven.

A simple choice of reference quantization is the Fock quantization characterized by annihilation and creation variables with $f_1^n = 1/\sqrt{2} - iam/(\sqrt{2}\omega_n)$, $f_2^n = \sqrt{1-|f_1^n|^2}$, $g_1^n = f_2^n$, and $g_2^n = -\bar{f}_1^n$. Please note that in the case of the massless field, this choice defines the natural quantization with conformal vacuum. Let $\{\tilde{\bar{a}}_{np}, \tilde{\bar{b}}_{np}, \tilde{a}_{np}, \tilde{b}_{np}\}$ be *any* other choice of annihilation and creation variables that defines a Fock quantization with a nontrivial, unitarily implementable dynamics. The coefficients $\tilde{f}_l^n$ and $\tilde{g}_l^n$ that characterize these variables then satisfy all the conditions stipulated in the previous subsection.

Given our reference Fock quantization and this other arbitrary one allowed by our criteria, it follows from Equation (32) that the annihilation and creation variables associated with them are related via the time-dependent Bogoliubov transformation $\mathcal{K}_n(\eta) = \tilde{\mathcal{F}}_n(\eta)\mathcal{F}_n^{-1}(\eta)$, so that

$$\begin{pmatrix} \tilde{a}_{np} \\ \tilde{\bar{b}}_{np} \end{pmatrix}_\eta = \mathcal{K}_n(\eta) \begin{pmatrix} a_{np} \\ \bar{b}_{np} \end{pmatrix}_\eta, \qquad \text{with} \quad \mathcal{K}_n = \begin{pmatrix} \kappa_n^f & \lambda_n^f \\ \lambda_n^g & \kappa_n^g \end{pmatrix}. \tag{42}$$

It is not difficult to check that the norm of the off-diagonal coefficients is $|\lambda_n^h| = |\tilde{h}_1^n h_2^n - \tilde{h}_2^n h_1^n|$. Moreover, using Equation (34), one gets that $|\lambda_n^f| = |\lambda_n^g|$. Thus, the square summability conditions on λ_n^f and λ_n^g that must be satisfied for the Bogoliuvov transformation to be unitarily implementable, turn out to be just one (and the same) condition. Then, the transformation determined by the sequence of matrices $\mathcal{K}_n$ is implementable on the reference Fock space as a unitary operator if and only if

$$\sum_n g_n |\lambda_n^f(\eta)|^2 < \infty, \quad \forall \eta \in \mathbb{I}, \tag{43}$$

where $|\lambda_n^f| = \left|\tilde{f}_1^n \sqrt{1-|f_1^n|^2} - \tilde{f}_2^n f_1^n\right|$. In case this condition is satisfied, we can consider the two analyzed quantizations as physically equivalent. Please note that the above condition ensures that the Fock representations defined for every value of the conformal time η are unitarily equivalent.

Taking e.g., $h = f$ in the formulas of the preceding subsection, we have that the coefficients $\tilde{f}_l^n$ and $\tilde{f}_l^n$ are, respectively, of the asymptotic form (39). Then, one gets that for $n \in \mathbb{N}_l^+$ [52],

$$|\lambda_n^f| = \frac{1}{\sqrt{2}} \left| \vartheta^n_{\tilde{f},l} + e^{i\tilde{F}_l^n} \mathrm{Re}(e^{-i\tilde{F}_l^n} \vartheta^n_{\tilde{f},l}) \right|, \tag{44}$$

up to terms $\mathcal{O}(|\vartheta^n_{h,l}|^2)$ in the asymptotic limit of large ω_n if the field is massless, or up to terms $\mathcal{O}(\omega_n^{-1})$ if the mass does not vanish and $\{\sqrt{g_n}\omega_n^{-1}\}_{n\in\mathbb{N}_l^+}$ happens to be square summable. Alternatively, if this sequence is not square summable and the field is massive, one must have

$$|\lambda_n^f| = \frac{1}{\sqrt{2}}|\tilde{\vartheta}^n_{\tilde{f},l}| + \mathcal{O}(\omega_n^{-2}), \tag{45}$$

for $n \in \mathbb{N}_l^+$. Since the sequences formed by $\vartheta^n_{\tilde{f},1}$ and $\vartheta^n_{\tilde{f},2}$ in the two first cases above, and by $\tilde{\vartheta}^n_{\tilde{f},1}$ and $\tilde{\vartheta}^n_{\tilde{f},2}$ in the last case, are square summable by hypothesis in their respective subsets, including degeneracy, it follows that the unitary equivalence condition (43) is immediately satisfied for all $n \in \mathbb{N}_l^+$.

On the other hand, it can be shown that Equation (43) fails to be satisfied if any of the considered subsets of integers $\mathbb{N}_l^-$ has infinite cardinality. The reason for this failure is rooted at the difference in the relative sign of the coefficients in the pair $(\tilde{f}_1^n, \tilde{f}_2^n)$ with respect to that in (f_1^n, f_2^n) [52]. Therefore, if one then insists and interchanges the roles of $\tilde{f}_l^n$ and $\tilde{g}_l^n$ in the definition of the annihilation and creation variables for the subsets $\mathbb{N}_l^-$, something that in practice amounts to an interchange between the relative signs of the pair $(\tilde{f}_1^n, \tilde{f}_2^n)$ and the signs for the pair $(\tilde{g}_1^n, \tilde{g}_2^n)$ [see Equation (34)], one gets that both pairs would display the same relative signs as the coefficients of the reference quantization, and then condition (43) would be satisfied for $n \in \mathbb{N}_l^-$. According to Equation (32), the exchange of $\tilde{f}_l^n$ and $\tilde{g}_l^n$ can be interpreted as a change in the convention of what are particles and what are antiparticles. In this sense, the inequivalence between quantizations before one performs the explained interchange can be understood as a spurious result coming from the fact that we are just considering two Fock quantizations with the opposite convention for the concept of particle and antiparticle in an infinite number of modes.

In summary, the criterion of invariance under the symmetries of the equations of motion and the unitary implementability of a nontrivial quantum dynamics removes the ambiguities in the representation of the CARs, both for the massive and for the massless Dirac fields in $2+1$ dimensions, selecting a unique family of unitarily equivalent Fock representations, together with a notion of quantum evolution, up to conventions about the concept of particles and antiparticles.

4. Fock Quantization of Dirac Fields in FLRW Cosmologies

We now discuss the Fock quantization of Dirac fields in cosmological spacetimes of the FLRW type. In particular, in this section we show that one can achieve results about the uniqueness of the quantization very much like in the previous section. More precisely, we consider minimally coupled massive Dirac fields, propagating in homogeneous and isotropic FLRW spacetimes, with 3-dimensional spatial hypersurfaces that can be either spherical or toroidal. The spherical case was notably analyzed in great depth by D'Eath and Halliwell [62], within the context of the Wheeler-DeWitt approach to quantum cosmology. In that seminal treatment, a special time-dependent family of Fock representations was chosen for the Dirac field, by means of an instantaneous diagonalization of the Dirac Hamiltonian. In particular, such family is associated with vacua which are invariant under the symmetries of the Dirac equation. Moreover, it was shown in Ref. [62] that particle production over time remains finite for those vacua, a fact that is an exclusive characteristic of quantizations that admit a unitary implementation of the dynamics. We now show that this family of Fock representations is in fact uniquely selected, up to unitary equivalence, by the criteria of invariance under spatial symmetries and unitary implementability of the dynamics. Also, we present a similar result concerning the Dirac field in flat (compact) FLRW spacetime. In this case, moreover spatial translations, the symmetry group includes helicity-generated spin rotations as well.

4.1. Dirac Spinors in FLRW Cosmologies

As before, we consider spacetime manifolds with topology of the type $\mathbb{I} \times \Sigma$, where $\mathbb{I}$ is a connected interval of the real line and Σ is certain spatial Cauchy surface. In the case of a spherical universe,

Σ is isomorphic to the 3-sphere, S^3, whereas for universes with (compact) flat spatial sections Σ is isomorphic to the 3-torus, T^3. In the following, we often refer to the above two situations as the spherical case and the flat case, for S^3 and T^3 respectively. The metrics associated with such universes can be written as

$$ds^2 = a^2(\eta)(-d\eta^2 + {}^0h_{\alpha\beta}dx^\alpha dx^\beta), \tag{46}$$

where ${}^0h_{\alpha\beta}$ is either the 3-dimensional spherical metric or the flat metric, and $a(\eta)$ is the scale factor.

It follows from previous comments in Section 2 that spin structures can always be defined in the above types of cosmological spacetimes [42,43]. Dirac fields Ψ, of mass m, correspond therefore to sections of the associated spinor bundle. Explicitly, we adopt the Weyl representation of the Dirac matrices

$$\gamma^a = i\begin{pmatrix} 0 & \sigma^a \\ \tilde{\sigma}^a & 0 \end{pmatrix}, \tag{47}$$

where $\sigma^0 = \tilde{\sigma}^0$ is the identity 2×2 matrix and $\sigma^i = -\tilde{\sigma}^i$ (with $i = 1,2,3$) are the Pauli matrices. Such representation of the generators of the Clifford algebra allows us to describe Dirac fields by means of a pair of two-component spinors ϕ^A and $\bar{\chi}_{A'}$ possessing well-defined and opposite chirality. We take ϕ^A to be the left-handed projection of Ψ, while $\bar{\chi}_{A'}$ is the right-handed one. Moreover, we adopt the same conventions as in Ref. [62] concerning the treatment of spinor indices.

In these cosmological spacetimes, the action for the Dirac field of mass m is

$$I_f = -i\int d\eta\, d^3\vec{x}\, a^4\sqrt{{}^0\mathrm{h}}\left[\frac{1}{2}(\Psi^\dagger\gamma^0 e^\mu_a\gamma^a\nabla^S_\mu\Psi - \mathrm{h.c.}) - m\Psi^\dagger\gamma^0\Psi\right], \tag{48}$$

where the spin covariant derivative ∇^S_μ is given by relations (18) and (19), adapted to the models in question.

Let us perform again a partial fixing of the internal Lorentz gauge, with the purpose of providing a rigorous treatment of the spatial dependence of spinors, as well as to analyze their properties under the symmetry groups associated with the considered FLRW cosmologies. To be specific, the gauge group of the orthonormal and oriented frame bundle can be reduced from $SO(3,1)$ to $SO(3)$ [58]. In the considered spacetime models, this procedure gives rise to a well-defined restriction of the spin structures to the double cover of the reduced bundles, with $SU(2)$ as gauge group. Finally, this restriction provides one (and the same) spin structure on each of the spatial hypersurfaces that constitute the foliation of the considered cosmologies. In the case of S^3, the spin structure turns out to be unique [63,64]. In the flat case, on the other hand, there are eight possible spin structures associated with distinct periodic conditions for the spinors in T^3 [65,66]. In practice, this partial gauge fixing is obtained again by imposing the conditions $n^\mu e^a_\mu = \delta^a_0$ which, moreover, greatly simplify the Hamiltonian analysis of the system [61]. In particular, one can check that the Dirac operator (defined over left and right-handed spinors) on the reference spatial hypersurface Σ_0 takes the form

$$ia\sqrt{2}\, e^{\alpha AA'}\, {}^{(3)}D_\alpha, \tag{49}$$

where $e^{\alpha AA'}$ is the spinor version of the triad and ${}^{(3)}D_\alpha$ is the spin lifting of the Levi–Cività covariant derivative with respect to the metric ${}^0h_{\alpha\beta}$ [62].

Once the gauge fixing has been performed, we introduce the following inner product on the space of left-handed spinors defined on the spatial hypersurface Σ_0 (as well as the corresponding definition for right-handed spinors):

$$\int_{\Sigma_0} d^3\vec{x}\, \sqrt{{}^0\mathrm{h}}\, \bar{\chi}_{A'} I^{AA'} \phi_A, \tag{50}$$

where summation over repeated indices is assumed, $I^{AA'}$ denotes the components of the identity matrix, and ϕ_A and χ_A are arbitrary spinors. Since both the spherical and the toroidal hypersurfaces are geodesically complete [67], it follows that the Dirac operator (49) is essentially self-adjoint with respect to the inner product (50), with discrete spectrum in both cases.

The spectrum of the Dirac operator on S^3 consists of the following sequence of eigenvalues [62,64]:

$$\pm\omega_n = \pm\left(n + \frac{3}{2}\right), \qquad n \in \mathbb{N}, \tag{51}$$

each of which has a corresponding degeneracy $g_n = (n+1)(n+2)$. Using a notation similar to that employed in the previous section, the left-handed eigenspinors with eigenvalues ω_n and $-\omega_n$ are denoted by ρ_A^{np} and $\bar{\sigma}_A^{np}$, respectively, where the label $p = 1, \ldots, g_n$ accounts for the degeneracy. Once normalized, the set of all such elements forms an orthonormal basis—with respect to the inner product (50)—for the space of left-handed spinors in S^3. An analogous basis for right-handed spinors is readily obtained by complex conjugation.

In the spherical case, the chiral projections of the Dirac field can then be written as

$$\phi_A(\eta, \vec{x}) = a^{-3/2}(\eta) \sum_{npp'} \breve{\alpha}_n^{pp'} [m_{np}(\eta)\rho_A^{np'}(\vec{x}) + \bar{r}_{np}(\eta)\bar{\sigma}_A^{np'}(\vec{x})], \tag{52}$$

$$\bar{\chi}_{A'}(\eta, \vec{x}) = a^{-3/2}(\eta) \sum_{npp'} \breve{\beta}_n^{pp'} [\bar{s}_{np}(\eta)\bar{\rho}_{A'}^{np'}(\vec{x}) + t_{np}(\eta)\sigma_{A'}^{np'}(\vec{x})], \tag{53}$$

with analogous expressions for the complex conjugate versions, and with

$$\sum_{npp'} = \sum_{n=0}^{\infty} \sum_{p=1}^{g_n} \sum_{p'=1}^{g_n}.$$

The anticommutative nature of the fermionic field Ψ is encoded in the Grassmann variables m_{np}, r_{np}, t_{np}, and s_{np} (and their complex conjugate versions) that moreover carry the time dependence of the Dirac field. Finally, the constant coefficients $\breve{\alpha}_n^{pp'}$ and $\breve{\beta}_n^{pp'}$ are included for convenience, to avoid the dynamical coupling of modes with different values of the label p.

Concerning now the flat FLRW model, the spectrum of the corresponding Dirac operator – with compactification period l_0 – consists of the following sequence of eigenvalues [65,66]:

$$\pm\omega_k = \pm\frac{2\pi}{l_0}\left|\vec{k} + \vec{\tau}\right|, \qquad \vec{\tau} = \frac{1}{2}\sum_{j=1}^{3} \epsilon^j \vec{v}_j, \qquad \vec{k} \in \mathbb{Z}^3, \tag{54}$$

where the three $\vec{v}_j$'s form the standard orthonormal basis for the lattice $\mathbb{Z}^3$, and the three numbers $\epsilon^j \in \{0, 1\}$ characterize each of the possible choices of spin structure[2]. Given any such spin structure, we identify the label k in ω_k (or equivalently in $-\omega_k$) with the norm of any of the wave vectors $\vec{k} \in \mathbb{Z}^3$ corresponding to ω_k. The degeneracy g_k associated with each eigenvalue ω_k (or $-\omega_k$) does not possess in this case a closed expression. However, well-known results in Riemannian geometry allow us to conclude that g_k grows asymptotically as $\mathcal{O}(\omega_k^2)$, for unboundedly large ω_k [24,68]. Let us then fix a spin structure on T^3 and choose a set of triads associated with the flat metric. The eigenspinors of the Dirac operator then form a basis of the space of spinors in T^3, basis that can be made orthonormal with respect to the inner product (50). In particular, if one chooses a diagonal triad such that the spin

[2] These spin structures determine the periodicity or antiperiodicity of the Dirac field in each of the orthogonal directions that define T^3. If, in harmony with spatial isotropy, one imposes the same global behavior for the field in all these directions, the choice of spin structure is restricted to either $\epsilon_j = 0$ or $\epsilon_j = 1$ for all j.

connection 1-form becomes null, the Dirac operator turns out to be the standard one for flat Euclidean space. Its (left-handed) eigenspinors corresponding to eigenvalues $\pm\omega_k$ are

$$w^{(\pm)}_{\vec{k}\,A}(\vec{x}) = u^{(\pm)}_{\vec{k}\,A} \exp\left[i\frac{2\pi}{l_0}(\vec{k}+\vec{\tau})\cdot\vec{x}\right], \tag{55}$$

where $u^{(\pm)}_{\vec{k}\,A}$ are some $\vec{x}$-independent two-component spinors, subject to the condition that the eigenvalue equation must hold. They can be chosen so that the spinors $w^{(\pm)}_{\vec{k}\,A}$ are normalized in the inner product (50) and such that

$$\int_{\Sigma_0} d^3\vec{x}\, w^{(+)}_{\vec{k}'A}\epsilon^{AB}w^{(-)}_{\vec{k}B} = 0, \qquad \int_{\Sigma_0} d^3\vec{x}\, w^{(\pm)}_{\vec{k}'A}\epsilon^{AB}w^{(\pm)}_{\vec{k}B} = e^{iC^{(\pm)}_{\vec{k}}}\delta_{\vec{k}',-\vec{k}-2\vec{\tau}}, \tag{56}$$

for all $\vec{k},\vec{k}' \neq -\epsilon^j\vec{v}_j/2$. Summation over repeated indices is assumed[3]. Finally, the constants $C^{(\pm)}_{\vec{k}}$ are some phases that can be chosen conveniently by modifying those of $u^{(\pm)}_{\vec{k}\,A}$. Just like in the case of S^3, the chiral projections ϕ_A and $\bar{\chi}_{A'}$ in the current flat case can be expanded in Dirac modes in an analogous fashion as in Equations (52) and (53), with corresponding Grassmann variables $m_{\vec{k}}$, $r_{\vec{k}}$, $t_{\vec{k}}$, and $s_{\vec{k}}$.

Returning to the spherical FLRW case, notice that upon introduction of the mode Expansions (52) and (53) in the Dirac action, and once the second-class constraints of the fermionic system are solved [69], one ends up with the following symmetric Dirac brackets for the mode variables [60,61]:

$$\{x_{np}, \bar{x}_{np}\} = -i, \qquad \{y_{np}, \bar{y}_{np}\} = -i, \tag{57}$$

where the ordered pair (x_{np}, y_{np}) stands for (m_{np}, s_{np}) or (t_{np}, r_{np}). Using Grassmann variational derivatives and requiring stationarity of the action, one obtains Dirac equations for the modes:

$$x'_{np} = i\omega_n x_{np} - ima\bar{y}_{np}, \qquad y'_{np} = i\omega_n y_{np} + ima\bar{x}_{np}, \tag{58}$$

as well as the complex conjugate versions. One can combine these dynamical equations to obtain decoupled second-order equations that are actually the same for all modes $\{x_{np}, y_{np}\}$ with the same label n. Denoting the mode variables generically by $\{z_{np}\}$, the resulting equation for given ω_n and (nonzero[4]) mass m is the following:

$$z''_{np} = \frac{a'}{a}z'_{np} - \left(\omega_n^2 + m^2a^2 + i\omega_n\frac{a'}{a}\right)z_{np}. \tag{59}$$

The general solution to this equation is a linear combination of two independent complex solutions, which we write again in the form $\exp[i\Theta^1_n(\eta)]$ and $\exp[-i\Theta^2_n(\eta)]$. The general expression of the fermionic modes at arbitrary time η can then be written as a linear transformation of the corresponding initial values that assigns a different weight to the two independent solutions of Equation (59):

$$\begin{aligned} x_{np}(\eta) &= \left[\Delta^2_n e^{i\Theta^1_n(\eta)} + \Delta^1_n e^{-i\Theta^2_n(\eta)}\right]x^0_{np} - \left[\zeta^1_n e^{i\Theta^1_n(\eta)} - \zeta^2_n e^{-i\Theta^2_n(\eta)}\right]\bar{y}^0_{np}, \\ y_{np}(\eta) &= \left[\Delta^2_n e^{i\Theta^1_n(\eta)} + \Delta^1_n e^{-i\Theta^2_n(\eta)}\right]y^0_{np} + \left[\zeta^1_n e^{i\Theta^1_n(\eta)} - \zeta^2_n e^{-i\Theta^2_n(\eta)}\right]\bar{x}^0_{np}, \end{aligned} \tag{60}$$

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[3] Except for the index $\vec{k}$ on the right-hand side of the second relation in Equation (56).

[4] The case $m = 0$ is slightly different, although straightforward to handle.

where Δ_n^l and ζ_n^l, $l = 1, 2$, are constants that depend on the initial conditions of the independent solutions $\exp[i\Theta_n^1(\eta)]$ and $\exp[-i\Theta_n^2(\eta)]$, and of their derivatives, at the reference time η_0 (see Ref. [53] for explicit expressions and details).

Just as in the previous section, one can obtain the asymptotic behavior of the linear transformations (60) in the ultraviolet regime of large ω_n, and subsequently study the unitary implementability of such transformations at the quantum level. For that matter, let us impose the initial conditions $\Theta_n^l(\eta_0) = 0$. One obtains the following expressions for the (exponents of the) solutions to Equation (59) [53]:

$$\Theta_n^l(\eta) = \omega_n \Delta\eta + \frac{i}{2}[1 + (-1)^l] \ln\left(\frac{a}{a_0}\right) + \int_{\eta_0}^{\eta} d\tilde{\eta}\, \Lambda_n^l(\tilde{\eta}), \tag{61}$$

where $a_0 = a(\eta_0)$, $\Delta\eta = \eta - \eta_0$, and the functions Λ_n^l are solutions of an equation of Riccati type which become negligible in the limit of unboundedly large ω_n. In particular, the functions Λ_n^l have a behavior of the type $\mathcal{O}(\omega_n^{-1})$. The asymptotic values obtained for the constants Δ_n^l and ζ_n^l are the following [53]:

$$\Delta_n^1 = 0, \qquad \Delta_n^2 = 1, \tag{62}$$

$$\zeta_n^1 = \zeta_n^2 = \zeta_n = \frac{m a_0^2}{2\omega_n a_0 + i a_0'} = \frac{m a_0}{2\omega_n} + \mathcal{O}(\omega_n^{-2}). \tag{63}$$

The analysis concerning the fermionic dynamics in the flat case is quite similar, leading to mode solutions that are the analogs of Equation (60):

$$\begin{aligned} x_{\vec{k}}(\eta) &= e^{i\Theta_k^1(\eta)} x_{\vec{k}}^0 - \zeta_k \left[e^{i\Theta_k^1(\eta)} - e^{-i\Theta_k^2(\eta)}\right] \bar{y}^0_{-\vec{k}-2\vec{\tau}}, \\ y_{\vec{k}}(\eta) &= e^{i\Theta_k^1(\eta)} y_{\vec{k}}^0 + \zeta_k \left[e^{i\Theta_k^1(\eta)} - e^{-i\Theta_k^2(\eta)}\right] \bar{x}^0_{-\vec{k}-2\vec{\tau}}. \end{aligned} \tag{64}$$

The corresponding asymptotic expressions, in the limit of large ω_k, are

$$\zeta_k = \frac{m a_0^2}{2\omega_k a_0 + i a_0'} = \frac{m a_0}{2\omega_k} + \mathcal{O}(\omega_k^{-2}) \tag{65}$$

and

$$\Theta_k^l(\eta) = \omega_k \Delta\eta + \frac{i}{2}[1 + (-1)^l] \ln\left(\frac{a}{a_0}\right) + \int_{\eta_0}^{\eta} d\tilde{\eta}\, \Lambda_k^l(\tilde{\eta}), \tag{66}$$

where the functions Λ_k^l are solutions of a Riccati equation with an asymptotic behavior of the type $\mathcal{O}(\omega_k^{-1})$.

4.2. Fock Quantization and Unitary Evolution

Considering both the spherical and the flat FLRW cosmologies, we proceed now to characterize all Fock representations for the Dirac field which satisfy the following requirements. First, the associated vacua must be invariant under the action of the natural symmetries of the system, among them the spatial isometries (and helicity-generated spin rotations, in the flat case). Secondly, the Fock quantizations are required to admit a (nontrivial) unitary implementation of the dynamics at the quantum level.

Let us start by analyzing the behavior of Dirac spinors in the spherical case, when the isometry transformations of S^3 are applied. The transformation group is then $SO(4)$, or equivalently the double cover $\text{Spin}(4) = SU(2) \times SU(2)$, with action in S^3 defined by means of a Clifford multiplication. Consequently, Spin(4) acts on the cross-sections of the spinor bundle on S^3 [64]. Notice that this action, when viewed on the four-component Dirac spinor, is reducible to two blocks: the action of Spin(4) over spinors ϕ^A, and the complex conjugate action over spinors $\bar{\chi}_{A'}$. Both such representations of

Spin(4) are unitary with respect to the inner product (50), and it follows that each block is further decomposable in a direct sum of irreducible representations.

Invariant vacua are associated with invariant complex structures, and we therefore seek complex structures which commute with the action of Spin(4) over spinors. To begin with, given the decompositions (52) and (53), any complex structure can be seen as an infinite-dimensional matrix in the basis formed by the modes $\{m_{np}, \bar{r}_{np}, t_{np}, \bar{s}_{np}\}$. From this point on, we follow the analysis carried out in Ref. [64], concerning the eigenspaces of the Dirac operator on S^3. Consider the action of Spin(4) on spinors of the type ϕ^A. Using Frobenius theorem [70], it is shown in Ref. [64] that each eigenspace corresponds exactly to a representation space of one of the irreducible representations of Spin(4) on spinors. Moreover, each such irreducible component shows up in the direct sum with multiplicity equal to one. This means that the representation spaces generated for each n by the sets

$$\{\rho_A^{np}\}_{p=1,\dots,g_n} \qquad \text{and} \qquad \{\bar{\sigma}_A^{np}\}_{p=1,\dots,g_n} \tag{67}$$

provide two irreducible representations which are necessarily inequivalent. Likewise, the representations associated with the sets

$$\{\bar{\rho}_{A'}^{np}\}_{p=1,\dots,g_n} \qquad \text{and} \qquad \{\sigma_{A'}^{np}\}_{p=1,\dots,g_n} \tag{68}$$

simply reproduce those generated by the sets (67), and therefore each irreducible representation associated, for each n, with one of the sets (68) is unitarily equivalent to a corresponding one coming from the sets (67). All this information (combined with an inspection of the dynamical mode equations [54]) allows us to apply Schur's lemmas [71] to conclude that a complex structure that commutes with the action of the group of isometries of S^3 over the space of Dirac spinors cannot mix modes m_{np}, $\bar{r}_{np}$, t_{np}, and $\bar{s}_{np}$ with different values of n. Moreover, within the subspace associated with a fixed value of n, such complex structures cannot mix the modes $\{m_{np}, \bar{s}_{np}\}$ with $\{t_{np}, \bar{r}_{np}\}$, since the two sets provide inequivalent irreducible representations of Spin(4). Let us consider first, for each given n, the subspace generated by the modes $\{m_{np}, \bar{s}_{np}\}$. The restriction of an invariant complex structure to any such subspace can then be characterized by means of four linear maps, relating in all possible pairings the two subspaces generated by $\{m_{np}\}$ and by $\{\bar{s}_{np}\}$. Each of these four maps must be proportional to the identity, as ensured by Schur's lemma. Finally, similar considerations can be applied to the subspace generated by the modes $\{t_{np}, \bar{r}_{np}\}$ [54].

We now turn to the flat FLRW model, and consider the action of isometries of T^3 on the Dirac field. Restricting our attention to continuous transformations, the isometry group is generated by constant translations along each of the orthogonal directions of the 3-torus. A general translation on the torus is thus $\vec{x} \to \vec{x} + \vec{\theta}$, where for each component we have $2\pi\theta_\alpha/l_0 \in S^1$. For any given choice of spin structure on T^3, one can easily check that a general translation simply results into the following transformation:

$$w_{\vec{k}A}^{(\pm)}(\vec{x}) \longrightarrow e^{i2\pi\vec{k}\cdot\vec{\theta}/l_0} e^{i2\pi\vec{\tau}\cdot\vec{\theta}/l_0} w_{\vec{k}A}^{(\pm)}(\vec{x}) \tag{69}$$

in each of the elements (55) of the basis of (left-handed) eigenspinors. For each $\vec{k} \in \mathbb{Z}^3$ there are therefore two copies of the same 1-dimensional complex irreducible representation, with different $\vec{k}$'s giving rise to inequivalent representations [55]. Again, one can perform the same analysis for the spinors of opposite chirality. Then, taking into account the mode decomposition of the Dirac field Ψ, and using again Schur's lemma, one concludes the following. A complex structure that commutes with the action of translations on T^3 can at most mix the modes $(m_{\vec{k}}, \bar{s}_{-\vec{k}-2\vec{\tau}}, t_{-\vec{k}-2\vec{\tau}}, \bar{r}_{\vec{k}})$ among themselves, for each fixed $\vec{k} \in \mathbb{Z}^3$, and is trivial otherwise.

In the flat case there is an additional symmetry of the Dirac system, following from the conservation of helicity in the evolution of the Dirac field in conformal time η. In fact, one can consider the projection of the spin angular momentum in the direction of the linear momentum of the particle, a projection that (except for the subspace generated by the modes with $\omega_k = 0$) defines the helicity operator $\mathfrak{h}$ [72]:

$$\mathfrak{h} = [-\vec{\nabla}^2]^{-1/2} \begin{pmatrix} -i\vec{\sigma}\cdot\vec{\nabla} & 0 \\ 0 & -i\vec{\sigma}\cdot\vec{\nabla} \end{pmatrix}. \tag{70}$$

Here, $\vec{\nabla}$ is the standard 3-dimensional Euclidean gradient and $\vec{\sigma}$ denotes a vector with components given by the Pauli matrices. Eigenspinors of $\mathfrak{h}$ with eigenvalues $+1$ or -1 are said to have positive or negative helicity, respectively. With the choice of gauge such that the spin connection vanishes, it turns out that the matrix blocks of $\mathfrak{h}$ (apart from the factor $[-\vec{\nabla}^2]^{-1/2}$) correspond exactly to the Dirac operator on T^3. One can then check that the positive helicity part of the Dirac field Ψ is generated by the coefficients $m_{\vec{k}}$ and $\bar{s}_{\vec{k}}$, for all $\vec{k} \in \mathbb{Z}^3$ different from $\vec{\tau}$. On the other hand, the negative helicity contribution is generated by the modes $t_{\vec{k}}$ and $\bar{r}_{\vec{k}}$, for all $\vec{k} \in \mathbb{Z}^3$ different from $\vec{\tau}$. A simple inspection of the equations of motion (58) shows that helicity is indeed a conserved quantity. Therefore, one can include, as an additional symmetry of the fermionic system, the 1-parameter group of spin rotations generated by helicity, by means of the complex exponentiation of $\mathfrak{h}/2$ multiplied by the angle of rotation. Such group is immediately unitary with respect to the inner product (5), since the operator $\mathfrak{h}$ is essentially self-adjoint. It follows that the unitary implementation of this symmetry at the quantum level is ensured whenever the complex structure that defines the quantization does not mix positive helicity modes with negative helicity ones.

The complex structures characterized above define the sets of creation and annihilation operators that provide invariant Fock representations of the CARs for the Dirac field in the considered homogeneous and isotropic scenarios. In the spherical case, let us denote the classical counterparts of the annihilation operators for particles and antiparticles by $a_{np}^{(x,y)}$ and $b_{np}^{(x,y)}$, respectively. The corresponding creation variables are the complex conjugate ones, $\bar{a}_{np}^{(x,y)}$ and $\bar{b}_{np}^{(x,y)}$. In the case of T^3, we denote the annihilation variables by $a_{\vec{k}}^{(x,y)}$ and $b_{\vec{k}}^{(x,y)}$, respectively for particles and antiparticles. We recall that the pairs (x, y) (with the appropriate labels) denote any of the ordered pairs of mode coefficients (m, s) or (t, r). In the following, we consider all the possible (time-dependent) families of fermionic creation and annihilation variables selected by invariant complex structures.

In the case of S^3, the creation and annihilation variables in question can then be written as

$$\begin{pmatrix} a_{np}^{(x,y)} \\ \bar{b}_{np}^{(x,y)} \end{pmatrix}_\eta = \begin{pmatrix} f_1^n(\eta) & f_2^n(\eta) \\ g_1^n(\eta) & g_2^n(\eta) \end{pmatrix} \begin{pmatrix} x_{np} \\ \bar{y}_{np} \end{pmatrix}_\eta. \tag{71}$$

Once more, the label η denotes dependence on conformal time. Notice that the time-dependent functions f_l^n and g_l^n (with $l = 1,2$) may differ for the pairs of modes $(m_{np}, \bar{s}_{np})$ and $(t_{np}, \bar{r}_{np})$, although this is not explicit in the notation. The following relations must again be satisfied:

$$|f_1^n|^2 + |f_2^n|^2 = 1, \qquad |g_1^n|^2 + |g_2^n|^2 = 1, \qquad f_1^n \bar{g}_1^n + f_2^n \bar{g}_2^n = 0, \tag{72}$$

such that anticommutators of the type (8) are obtained at the quantum level.

Turning to the flat case, the relations (71) are replaced with

$$\begin{pmatrix} a_{\vec{k}}^{(x,y)} \\ \bar{b}_{\vec{k}}^{(x,y)} \end{pmatrix}_\eta = \begin{pmatrix} f_1^{\vec{k}}(\eta) & f_2^{\vec{k}}(\eta) \\ g_1^{\vec{k}}(\eta) & g_2^{\vec{k}}(\eta) \end{pmatrix} \begin{pmatrix} x_{\vec{k}} \\ \bar{y}_{-\vec{k}-2\vec{\tau}} \end{pmatrix}_\eta, \tag{73}$$

where conditions analogous to Equation (72) again apply.

When evaluated at different times, the sets of variables (71) are related to each other by means of dynamical Bogoliubov transformations. The general form of such linear transformations can be obtained taking into account Equation (60) for the evolution of the fermionic modes in the spherical case. In general, terms, the Bogoliubov transformation relating the annihilation and creation variables at the initial time η_0 with those at any time η is given by a sequence of blocks $\mathcal{B}_n$ such that

$$\begin{pmatrix} a_{np}^{(x,y)} \\ \bar{b}_{np}^{(x,y)} \end{pmatrix}_{\eta} = \mathcal{B}_n(\eta,\eta_0) \begin{pmatrix} a_{np}^{(x,y)} \\ \bar{b}_{np}^{(x,y)} \end{pmatrix}_{\eta_0}, \qquad \mathcal{B}_n = \begin{pmatrix} \alpha_n^f & \beta_n^f \\ \beta_n^g & \alpha_n^g \end{pmatrix}. \tag{74}$$

The absolute values of the coefficients β_n^f and β_n^g have the following expression [53,54]:

$$|\beta_n^h(\eta,\eta_0)| = \Bigg| \left[-h_1^n \left(h_2^{n,0} + \zeta_n h_1^{n,0} \right) e^{i\int \Lambda_n^1} + \bar{\zeta}_n h_2^n h_2^{n,0} \frac{a}{a_0} e^{i\int \bar{\Lambda}_n^2} \right] e^{i\omega_n \Delta\eta} + \left[h_2^n \left(h_1^{n,0} - \bar{\zeta}_n h_2^{n,0} \right) e^{-i\int \bar{\Lambda}_n^1} + \zeta_n h_1^n h_1^{n,0} \frac{a}{a_0} e^{-i\int \Lambda_n^2} \right] e^{-i\omega_n \Delta\eta} \Bigg|, \tag{75}$$

where the integrals are over conformal time from η_0 to η, h denotes either f or g, and the superscript 0 stands for evaluation at the initial time.

Analogous considerations, of course, apply to the flat case, with dynamical Bogoliubov transformations between variables of the type (73) that are characterized by matrices $\mathcal{B}_{\vec{k}}$, with corresponding coefficients $\beta_{\vec{k}}^f$ and $\beta_{\vec{k}}^g$, for which the explicit expressions can be found in Ref. [55].

Considering for instance the Fock representation defined by the annihilation and creation variables at the initial time η_0 (or equivalently by the associated complex structure), the dynamical Bogoliubov transformations (74) can be implemented on the corresponding Fock space by means of unitary quantum operators if and only if [7,8]

$$\sum_n g_n |\beta_n^h(\eta,\eta_0)|^2 < \infty \qquad \text{for} \qquad h = f, g. \tag{76}$$

Actually, it is sufficient to ensure the above condition for either $h = f$ or $h = g$, since it follows again from relations (72) that $|\beta_n^g(\eta,\eta_0)| = |\beta_n^f(\eta,\eta_0)|$ [53]. Let us then fix h to be either f or g. The unitary implementability of the dynamics therefore depends on the asymptotic behavior of the beta coefficients in the limit of large ω_n that in turn depends on the behavior of the sequences h_l^n. A detailed analysis, carried out in Ref. [54], shows that apart from an uninteresting alternative which would effectively trivialize the quantum dynamics in a similar way as it was discussed in the previous section, the fulfillment of the unitarity condition (76) requires that the functions h_l^n behave asymptotically as

$$h_l^n = (-1)^{l+1} \frac{ma}{2\omega_n} e^{iH_{\tilde{l}}^n} + \vartheta_{h,l}^n, \qquad h_{\tilde{l}}^n = e^{iH_{\tilde{l}}^n} + \mathcal{O}(\omega_k^{-2}), \tag{77}$$

where $\{l,\tilde{l}\}$ is the set $\{1,2\}$. Moreover, the sequences $\vartheta_{h,l}^n$ must be square summable, including degeneracy.

Before continuing with our discussion, a comment is in order. Since we have not put any restriction on the global asymptotic behavior of the sequences h_l^n for fixed l, it is possible that neither h_1^n nor h_2^n actually converges over $\mathbb{N}$. In fact, the sum (76) can be made finite with h_1^n taking the role of h_l^n in Equation (77) for n in a subset of $\mathbb{N}$ and h_2^n taking that role over a complementary subset (modulo finite subsets of $\mathbb{N}$). Hence, the above behavior of h_l^n is required only for $n \in \mathbb{N}_l \subset \mathbb{N}$, with $\mathbb{N}_1 \cup \mathbb{N}_2 = \mathbb{N}$ modulo finite subsets (including the possibility of one of the subsets $\mathbb{N}_l$ being empty).

The analysis concerning the flat case follows similar lines, apart from a careful handling of the already mentioned issue of the accidental degeneracy of the Dirac eigenspaces (for full details, see Ref. [55]). The conclusion is that the requirement of (nontrivial) unitary implementation of the dynamics completely fixes the explicit dependence on time in the dominant part of the Dirac field, in a very similar way as in the spherical case [see Equation (77)], for an infinite number of modes in the asymptotic sector of large ω_k. Hence, the time-dependent scaling that must be introduced in the mode dynamics of the Dirac field, such that the remaining part of the evolution can be unitarily implemented, is completely fixed (in absolute value) at dominant order. In particular, the scaling factor for each mode is similarly determined in terms of $ma/(2\omega_k)$, and includes the global term $a^{-3/2}$, introduced in the mode expansions (52) and (53) adapted to the case of T^3.

4.3. Uniqueness of the Quantization

In the previous subsection we have characterized the Fock quantizations of the Dirac field which allow a unitary implementation of the dynamics and which possess vacua that are invariant under the natural symmetries of the considered cosmological models. We now show that for each of these models, all such quantizations are unitarily equivalent. Direct consequences are the removal of quantization ambiguities typically present in QFT and the selection of a very specific, well-defined notion of quantum evolution.

Let us start with the case of spherical sections. One of the simplest choices of functions that satisfy the conditions derived above for a unitarily implementable quantum dynamics is

$$f_1^n = \frac{ma}{2\omega_n}, \qquad f_2^n = \sqrt{1-(f_1^n)^2}, \qquad g_1^n = f_2^n, \qquad g_2^n = -f_1^n, \tag{78}$$

for all $n \in \mathbb{N}$ and for both pairs $(m_{np}, \bar{s}_{np})$ and $(t_{np}, \bar{r}_{np})$. We take this choice as defining our *reference* family of complex structures. Let us then consider any other family of invariant complex structures allowing a unitary implementation of the dynamics. Such family is defined by certain annihilation and creation variables, $\tilde{a}_{np}^{(x,y)}$ and $\tilde{\bar{b}}_{np}^{(x,y)}$, with coefficients $\tilde{h}_l^n$ (for h identified with f or g and for $l = 1,2$) that have the asymptotic behavior described at the end of the preceding subsection. In particular, the subdominant sequences $\vartheta_{\tilde{h},l}^n$ appearing in Equation (77) are square summable (degeneracy included) over subsequences $\mathbb{N}_l$. The relation between this family and the reference one is given by a Bogoliubov transformation determined by a sequence of matrices $\mathcal{K}_n$ such that

$$\begin{pmatrix} \tilde{a}_{np}^{(x,y)} \\ \tilde{\bar{b}}_{np}^{(x,y)} \end{pmatrix}_\eta = \mathcal{K}_n(\eta) \begin{pmatrix} a_{np}^{(x,y)} \\ \bar{b}_{np}^{(x,y)} \end{pmatrix}_\eta, \qquad \mathcal{K}_n = \begin{pmatrix} \kappa_n^f & \lambda_n^f \\ \lambda_n^g & \kappa_n^g \end{pmatrix}. \tag{79}$$

One can check that the absolute values of the nondiagonal elements of these matrices have the following expression [53,54]:

$$|\lambda_n^h| = |\tilde{h}_1^n h_2^n - \tilde{h}_2^n h_1^n|, \tag{80}$$

where h stands again for both types of functions f and g. The two Fock quantizations, namely the reference one associated with the family (78) and the one defined by the coefficients $\tilde{h}_l^n$, are unitarily equivalent if and only if the Bogoliubov transformation (79) is itself unitarily implementable, a demand that is equivalent to the fulfillment of the conditions

$$\sum_n g_n |\lambda_n^f(\eta)|^2 < \infty \qquad \text{and} \qquad \sum_n g_n |\lambda_n^g(\eta)|^2 < \infty, \tag{81}$$

for all η of interest. Once more, one of the above conditions is redundant, since the equality $|\lambda_n^g| = |\lambda_n^f|$ is again ensured by relations (72).

Let us then focus on the first condition in Equation (81) and consider the situation such that the asymptotic behavior (77) applies to the functions $\tilde{f}_l^n$. The alternative, with Equation (77) applying to the functions $\tilde{g}_l^n$, can be treated in a completely analogous way. One can show from Equation (80) that in the limit of unboundedly large ω_n, the coefficients λ_n^f have the following behavior on the subsequence $\mathbb{N}_1$:

$$|\lambda_n^f| = |\vartheta_{\tilde{f},1}^n| + \mathcal{O}(\omega_n^{-2}). \tag{82}$$

Since by hypothesis $\vartheta_{\tilde{f},1}^n$ is square summable (including the degeneracy g_n) over $\mathbb{N}_1$, it follows immediately that the condition for unitary equivalence is satisfied if the set $\mathbb{N}_2$ is finite (or empty). Suppose now that $\mathbb{N}_2$ is an infinite set. It is clear that λ_n^f behaves asymptotically like $\mathcal{O}(1)$ for $n \in \mathbb{N}_2$, and therefore the summability required in Equation (81) cannot be attained, leading to apparently inequivalent quantizations. However, this inequivalence stems, as it happened in the previous section, from the fact that the quantization associated with the coefficients $\tilde{h}_l^n$ defines a convention for the concept of particles and antiparticles which is completely the opposite, for an infinite number of modes, of the convention corresponding to the reference quantization. Once both conventions are reconciled, the quantizations are seen to be physically equivalent. In fact, suppose that in our reference quantization (78), we switch the convention concerning particles and antiparticles for all modes corresponding to $\mathbb{N}_2$. This redefinition is effectively attained with the interchange $f_l^n \leftrightarrow g_l^n$ ($n \in \mathbb{N}_2$), as follows from the definition (71). Then, the behavior of the new coefficients λ_n^f would no longer be $\mathcal{O}(1)$ on $\mathbb{N}_2$, but they would behave (in norm) as $|\vartheta_{\tilde{f},2}^n| + \mathcal{O}(\omega_n^{-2})$ instead. Since, also by the hypothesis of a unitarily implementable evolution, $\vartheta_{\tilde{f},2}^n$ is square summable (degeneracy included) over $\mathbb{N}_2$, one concludes that conditions (81) are now satisfied, confirming therefore the unitary equivalence between the two Fock quantizations, after the two conventions concerning particles and antiparticles have been harmonized.

The analysis of the uniqueness of the Fock quantization of the Dirac field in the flat FLRW case proceeds in a similar fashion. One can again choose a reference complex structure allowing a unitary implementation of the dynamics, namely the one characterized by the following matrix elements in Equation (73), for all $\omega_k \neq 0$:

$$f_1^k = \frac{ma}{2\omega_k}, \qquad f_2^k = \sqrt{1 - (f_1^k)^2}, \qquad g_1^k = f_2^k, \qquad g_2^k = -f_1^k. \tag{83}$$

Applying the same type of arguments as above, one can prove [55] that as it happened in the case of S^3, once a convention concerning particles and antiparticles is fixed, the condition that there exists a nontrivial unitary implementation of the dynamics is sufficient to ensure the unitary equivalence of all Fock quantizations associated with invariant vacua.

Let us conclude with a brief comment on a key difference between the current study and previous analogous works on quantum scalar fields in FLRW cosmologies [17,19,20,24,25,50]. Like in the scalar field case, our criteria uniquely fix not only the Fock representation once a suitable set of variables for the field has been chosen, but actually they greatly reduce the ambiguity in this choice of variables that arises from time-dependent linear redefinitions as well. Considering, for instance, a spherical spatial topology, this affects the global scaling introduced in the decompositions (52) and (53), as it does for the scalar field, but now it affects also the scaling in the particle and antiparticle contributions that are induced by the time dependence of the functions f_l^n and g_l^n subject to the unitarity conditions (77). As such, the Dirac field presents specific and different time-dependent scaling in its particle and antiparticle parts that are also different for each of the two chiralities, introducing an aspect which is absent in the scalar field analysis. For the scalar field, the requirement of unitary dynamics imposes a global scaling of the original field variable, such that the scaled field in practice behaves like a conformally coupled field, and one might wrongly believe that the possibility of attaining a unitarily implementable dynamics is somehow constrained by the availability of a conformal symmetry in the scaled theory (at least in the ultraviolet regime). The work on Dirac fields definitely puts aside such type of misconceptions.

5. Hamiltonian Backreaction of Dirac Perturbations in hLQC

The previous uniqueness results about the Fock quantization of Dirac fields in FLRW cosmologies are of special importance beyond the context of QFT. Actually, they can be used (and further developed) to confer great robustness to the full quantization of a homogeneous and isotropic cosmological spacetime perturbed with small matter inhomogeneities described by a Dirac field, in the context of hybrid quantum cosmology. As mentioned in the Introduction, this framework for the quantum description of cosmological systems employs techniques from a theory of quantum cosmology (here we focus our attention on the case of loop quantum cosmology) for quantizing the spatially homogeneous zero modes of the geometry, while the inhomogeneous fields are quantized using standard Fock representations. In this setting, the features of the resulting quantum theory and its predictions are strongly affected by the precise knowledge obtained not only about a unique preferred Fock space for the fields, but also about which part of their degrees of freedom displays a genuine unitary quantum evolution when one reaches regimes where the cosmological background behaves classically. This knowledge serves in hLQC to separate in a specific way this homogeneous background from the variables that describe the fermionic perturbations, and such splitting can be refined by further imposing some physically sound properties on the full quantum system, such as a proper definition of the fermionic part of the Hamiltonian operator. Along these lines, in this section we are going to revisit the main results in the hybrid loop quantization of a flat homogeneous and isotropic cosmology with fermionic perturbations, in particular in what concerns the study of the Hamiltonian operator and the consequences on the quantum backreaction of the fermionic matter on the cosmological background.

5.1. Fermionic Perturbations in flat FLRW: Splitting of the Phase Space

Let us start by considering the Einstein-Hilbert action restricted to symmetry-reduced universes with a metric given in Equation (46), taking ${}^0h_{\alpha\beta}$ as the Euclidean metric in coordinates adapted to the spatial homogeneity, and letting the lapse function that we call N_0, be arbitrary. We particularize again the discussion to a topology of the flat spatial sections equal to the compact T^3-topology. In order to include standard inflationary scenarios in our system, we minimally couple a homogeneous scalar field ϕ with potential $V(\phi)$ that plays the role of an inflaton. In the canonical ADM framework, the degrees of freedom of this cosmological model can be described with the scale factor a, the inflaton ϕ, and their canonical momenta, respectively denoted by π_a and π_ϕ. On classical FLRW solutions, these variables are subject only to one constraint, arising from the zero mode of the Hamiltonian constraint that generates global time reparameterizations:

$$H_{|0} = \frac{1}{2l_0^3a^3}\left[\pi_\phi^2 - \frac{4\pi}{3}a^2\pi_a^2 + 2l_0^6a^6V(\phi)\right], \tag{84}$$

where we recall that l_0 is the compactification length of T^3.

To include inhomogeneous fermionic content in this cosmological model, we minimally couple a Dirac field Ψ of mass m and treat it entirely as a perturbation (including its purely homogeneous part, if it had any). For physical completeness, one may also introduce purely inhomogeneous and anisotropic perturbations of the metric and the inflaton field[5]. Within this perturbative hierarchy, we conduct the analysis at the lowest nontrivial order and thus we truncate the whole action of the system (and its associated symplectic structure) at quadratic order in all the perturbations. Since the Dirac action is precisely quadratic in the fermionic field, at this order it only couples with the homogeneous sector of the cosmology[6]. Therefore, in practice, we can treat its associated spinor

[5] The zero modes of the metric and scalar field can be conveniently isolated and accounted for in the scale factor and homogeneous inflaton, owing to the compactness of the spatial sections.

[6] Henceforth, to simplify the terminology and shorten the notation we will refer to the variables that describe this homogeneous and isotropic background as FLRW variables, even when they are not evaluated on classical solutions.

bundle as if it were defined on a pure (spatially flat) FLRW universe. Furthermore, this coupling implies that the Dirac field is a perturbative gauge invariant at our order of truncation, namely it is independent of perturbatively linear coordinate redefinitions that respect the manifest homogeneity of the background.

To take advantage of the previous results about the uniqueness of the Fock quantization of the Dirac field, and to allow for a convenient spatial mode expansion of the fermionic fields, we partially fix again the local Lorentz gauge imposing the condition $n^\mu e^a_\mu = \delta^a_0$ on the tetrad of our background. This allows us to generically perform a decomposition of the two chiral components of the fermionic perturbations as that given in Equations (52) and (53) (after replacing the eigenspinors of the Dirac operator on S^3 by their analogs for T^3). Recall that these behave under local gauge transformations as $SU(2)$ spinors defined in T^3, with a spin structure that is given by the choice of the vector $\vec{\tau}$ [c.f. Equation (54). Of equal importance is the fact that this partial gauge fixing eliminates all the nontrivial canonical brackets between the homogeneous FLRW geometry and the (rescaled) Dirac field [61]. Then, the only nonvanishing brackets between the fermionic mode coefficients $m_{\vec{k}}$, $\bar{r}_{\vec{k}}$, $t_{\vec{k}}$, and $\bar{s}_{\vec{k}}$ (and their complex conjugates) are

$$\{x_{\vec{k}}, \bar{x}_{\vec{k}}\} = -i, \qquad \{y_{\vec{k}}, \bar{y}_{\vec{k}}\} = -i, \tag{85}$$

where (x, y) again denotes any of the two possible ordered pairs of mode coefficients (m, s) or (t, r) (omitting their associated wave vector labels). The introduction of this fermionic mode expansion in the Dirac Hamiltonian coupled to our considered background gives rise to the following contribution to the total Hamiltonian of the system:

$$N_0 H_D = N_0 \left[\delta^{\vec{\tau}}_{\vec{0}} H_{\vec{0}} + \sum_{\vec{k}\neq\vec{\tau}} \sum_{(x,y)} H^{(x,y)}_{\vec{k}} \right], \tag{86}$$

$$H_{\vec{0}} = m\left(s_{\vec{0}}\bar{r}_{\vec{0}} + r_{\vec{0}}\bar{s}_{\vec{0}} + m_{\vec{0}}\bar{t}_{\vec{0}} + t_{\vec{0}}\bar{m}_{\vec{0}}\right), \tag{87}$$

$$H^{(x,y)}_{\vec{k}} = m\left(y_{-\vec{k}-2\vec{\tau}}x_{\vec{k}} + \bar{x}_{\vec{k}}\bar{y}_{-\vec{k}-2\vec{\tau}}\right) - \frac{\omega_k}{a}\left(\bar{x}_{\vec{k}}x_{\vec{k}} - y_{\vec{k}}\bar{y}_{\vec{k}}\right). \tag{88}$$

As we have explained above, N_0 is the homogeneous lapse function of the FLRW background. It follows that the Dirac perturbations, at our considered order of quadratic truncation in the action, contribute only to the global zero mode of the Hamiltonian constraint of the entire system. Explicitly, if one ignores the rest of perturbative fields in our model (which do not couple to the fermionic field at quadratic order), the zero mode of the Hamiltonian constraint is given by the sum of $H_{|0}$ and H_D.

At this point in the discussion, it is worth remarking that there exists an inherent freedom in the description of the cosmological model at hand. Treating the system formed by the FLRW universe and its perturbations as a whole entity, one can always mix the different sectors of the phase space by means of canonical transformations. Even if this mixing does not affect the physical behavior of the system at the classical level at the end of the day, the freedom in identifying the sets of basic variables that describe each sector can strongly affect the properties of the hybrid quantization, given that the perturbative fields are quantized with a different type of representation (à la Fock) than the homogeneous background (with loop techniques). Focusing the attention on the choice of splitting between the FLRW sector and the fermionic one, one can understand this as the specific assignment of how each of these two types of degrees of freedom contributes to the dynamics of the entire system. To take into account this panorama, and with the aim put on characterizing the Fock representation for the fermionic perturbations, we introduce general families of annihilation and creation variables of the

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In fact, in this section they are rather generic canonical variables, subject to being represented as quantum operators in a Hilbert space.

form (73) where the coefficients $f_1^{\vec{k}}, f_2^{\vec{k}}, g_1^{\vec{k}}$, and $g_2^{\vec{k}}$ are now taken as functions of the canonical variables that describe the geometric sector of the cosmological background, understood hereafter as the sector that corresponds to the scale factor and its momentum[7]. Furthermore, these functions are subject to the conditions

$$g_1^{\vec{k}} = e^{iG^{\vec{k}}} \bar{f}_2^{\vec{k}}, \qquad g_2^{\vec{k}} = -e^{iG^{\vec{k}}} \bar{f}_1^{\vec{k}}, \qquad f_2^{\vec{k}} = e^{iF_2^{\vec{k}}} \sqrt{1 - |f_1^{\vec{k}}|^2}, \tag{89}$$

where $G^{\vec{k}}$ and $F_2^{\vec{k}}$ are phases given by generic real functions of the FLRW geometry. These conditions are nothing but the equivalent of Equation (72) (adapted to the case of T^3). Therefore, they guarantee that the definition of the fermionic annihilation and creation variables is a canonical transformation in the fermionic sector of the phase space (namely if one freezes the FLRW background variables and ignores their Poisson brackets).

Each of these new families of fermionic variables can codify in different ways the possible splitting in the dynamical behavior, between the homogeneous cosmological geometry and the fermionic perturbations that preserve the linearity in the perturbative sector. However, when the cosmological system is viewed as a whole dynamical entity, and unless the coefficients $f_1^{\vec{k}}$, $f_2^{\vec{k}}$, $g_1^{\vec{k}}$, and $g_2^{\vec{k}}$ are constant, the new fermionic variables do not form a canonical set with the scale factor and its canonical momentum. These variables must be modified if one wishes to restore the canonical algebra fulfilled by the original basic set for the description of the system. In other words, the canonical transformation that started with the above definition of families of fermionic annihilation and creation variables must be completed. This can be readily done, at our order of quadratic perturbative truncation, by demanding that the symplectic potential of the FLRW and fermionic sectors remain unchanged after the transformation, up to contributions that are of higher perturbative order than quadratic. This procedure leads to the new corrected variables for the scale factor and its momentum:

$$\tilde{a} = a + \frac{i}{2} \sum_{\vec{k},(x,y)} [(\partial_{\pi_a} x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_{\pi_a} \bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_{\pi_a} y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_{\pi_a} \bar{y}_{\vec{k}})y_{\vec{k}}], \tag{90}$$

$$\tilde{\pi}_a = \pi_a - \frac{i}{2} \sum_{\vec{k},(x,y)} [(\partial_a x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_a \bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_a y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_a \bar{y}_{\vec{k}})y_{\vec{k}}]. \tag{91}$$

Here, the partial derivatives affect only the explicit dependence of the fermionic modes on the cosmological background geometry, via the functions $f_1^{\vec{k}}$, $f_2^{\vec{k}}$, $g_1^{\vec{k}}$, and $g_2^{\vec{k}}$. Thus, the new FLRW variables $\tilde{a}$, $\tilde{\pi}_a$, ϕ, and π_ϕ form a canonical set with the fermionic annihilation and creation variables defined by means of Equations (73) and (89).

In the following, for convenience, we restrict our attention to families of annihilation and creation variables defined by coefficients f_1^k, f_2^k, g_1^k, and g_2^k that depend on the wave vector $\vec{k}$ only through the corresponding Dirac eigenvalue ω_k. Actually, this restriction comes from the symmetry of the fermionic equations of motion that ultimately can be related to the isotropy of the background spacetime in the limit where the spatial sections become noncompact. We refer the reader to Ref. [38] for an extended version of the subsequent analysis, including the possibility of a general dependence of the functions $f_1^{\vec{k}}$, $f_2^{\vec{k}}$, $g_1^{\vec{k}}$, and $g_2^{\vec{k}}$ on $\vec{k}$.

5.2. Fermionic Hamiltonian: Restrictions on the Quantization

Every new set of canonical variables for the FLRW background and the fermionic perturbations, namely every new choice of phase space splitting, naturally contributes to the total Hamiltonian of

[7] One can generalize the analysis to coefficients that are functions also of the inflaton and its momentum, thus allowing for a dependence on all the degrees of freedom of the FLRW background. However, this generalization is not necessary for our discussion, except at some point in Section 6, where we comment on it explicitly.

the system in a different way. In particular, if one writes the original zero mode of the Hamiltonian constraint (that we recall is the sum of $H_{|0}$ and H_D) in terms of an arbitrary new canonical set of variables as defined above, and truncates it at quadratic order in the perturbations, one obtains [38,39]

$$H_{|0}(\tilde{a}, \tilde{\pi}_a, \phi, \pi_\phi) + \tilde{H}_D(\tilde{a}, \tilde{\pi}_a, \phi), \tag{92}$$

where the round brackets indicate functional evaluation of the corresponding, preceding function on the new set of FLRW variables, namely the direct replacement of its dependence on the old untilded set by the new one. The term $\tilde{H}_D$ is the contribution of the new fermionic variables to the zero mode of the Hamiltonian constraint. As our notation indicates, it can be made independent of the canonical momentum of the inflaton. This is always possible by means of a suitable redefinition of the homogeneous lapse function at our perturbative truncation order [37]. It is given by

$$\tilde{H}_D = \sum_{\vec{k}\neq\vec{\tau},(x,y)} \Bigg[h_D^k \left(\bar{a}_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)} - a_{\vec{k}}^{(x,y)} \bar{a}_{\vec{k}}^{(x,y)} + \bar{b}_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)} \right) \\ + h_G^k \left(\bar{b}_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)} \right) + \bar{h}_I^k \left(a_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} \right) - h_I^k \left(\bar{a}_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)} \right) \Bigg], \tag{93}$$

where we have ignored the contribution from the fermionic zero modes, since they can be isolated and quantized separately without obstructions, and

$$h_D^k = \frac{\omega_k}{2a} \left(|f_2^k|^2 - |f_1^k|^2 \right) + m\mathrm{Re} \left(f_1^k \bar{f}_2^k \right) + \frac{i}{2} \left(\bar{f}_1^k \{f_1^k, H_{|0}\} + \bar{f}_2^k \{f_2^k, H_{|0}\} \right), \tag{94}$$

$$h_G^k = \frac{1}{2}\{G^k, H_{|0}\}, \tag{95}$$

$$h_I^k = e^{-iG^k} \left[i f_1^k \{f_2^k, H_{|0}\} - i f_2^k \{f_1^k, H_{|0}\} + \frac{2\omega_k}{a} f_1^k f_2^k + m (f_1^k)^2 - m (f_2^k)^2 \right], \tag{96}$$

modulo changes that can be absorbed by the aforementioned redefinition of the homogeneous lapse. At the considered perturbative level, this redefinition amounts to eliminate π_ϕ^2 in the above equations by identifying $H_{|0}$ with the zero function [37]. It is worth noticing that in the context of QFT in curved spacetimes, the product of this lapse function and $\tilde{H}_D$ is the Hamiltonian that generates the evolution of the chosen family of fermionic annihilation and creation variables, evolution that generally differs from the original Dirac dynamics generated by $N_0 H_D$.

There are infinitely many possible families of fermionic annihilation and creation variables defined by means of Equations (73) and (89), even when restricting to coefficients that depend on $\vec{k}$ only through ω_k. This freedom not only reflects the infinitely many inequivalent Fock representations of the fermionic degrees of freedom, but also the different possible splitting of the phase space between the fermionic sector and the homogeneous FLRW geometry. Before proceeding to the hybrid quantization of the entire system, it is, therefore, of the utmost importance to adhere to physical criteria and restrict the allowed families of fermionic annihilation and creation variables. In view of the results presented in the previous sections, a first reasonable condition to impose is that when a QFT regime in a classical background spacetime is recovered, the quantum Heisenberg evolution of the fermionic annihilation and creation operators can be implemented unitarily. As we have seen, once we set a convention for particles and antiparticles, this criterion on the considered families of variables completely fixes the (symmetry invariant) quantum representation of the field, up to unitary equivalence. In other words, it allows us to determine the Fock space for the representation of the fermionic field. For concreteness, let us set the particle/antiparticle convention to be such that it corresponds to the standard one in Minkowski spacetime as the mass of the fermions goes to zero (situation in which the rescaled Dirac field propagates as if it were in flat spacetime, in conformal time) [55]. Then, the families of annihilation and creation variables restricted by the criterion of a unitarily implementable dynamics are those such that in the asymptotic limit of large ω_k:

$$f_1^k = \frac{ma}{2\omega_k} e^{iF_2^k} + \vartheta^k \quad \text{with} \quad \sum_{\vec{k}} |\vartheta^k|^2 < \infty. \tag{97}$$

The above condition greatly restricts the asymptotic behavior of the allowed families of annihilation and creation variables. Furthermore, all such choices lead to unitarily equivalent representations. However, there is still much freedom left, even in the asymptotic regime of large ω_k, as the function ϑ^k is only constrained to be square summable (including degeneracy). Actually, this freedom can be used to refine the phase space splitting in such a way that the part of the hybrid quantization that concerns the fermionic degrees of freedom displays several desirable properties. In particular, it appears physically sound to demand that the Fock quantization of the contribution $\tilde{H}_D$ to the Hamiltonian constraint result into a well-defined operator on the fermionic vacuum state (and thus on the dense Fock subspace of its associated n-particle states). Such an operator can be simply obtained by promoting the variables $a_{\vec{k}}^{(x,y)}$ and $b_{\vec{k}}^{(x,y)}$, on the one hand, and $\bar{a}_{\vec{k}}^{(x,y)}$ and $\bar{b}_{\vec{k}}^{(x,y)}$, on the other hand, respectively to annihilation and creation operators in the fermionic Hamiltonian given in Equation (93). As these variables commute with the (perturbatively corrected) ones that describe the homogeneous FLRW background, the well-definiteness of $\tilde{H}_D$ on the fermionic vacuum is insensitive to whether these FLRW variables are fixed as classical or promoted to quantum operators as well (within the hybrid loop scheme). In turn, if one imposes normal ordering on the products of annihilation and creation operators, it is easy to see that this property on the Fock quantization of $\tilde{H}_D$ depends exclusively on the asymptotic dependence on ω_k of the terms h_I^k defined in Equation (96). These provide the interactive part of the fermionic Hamiltonian that is responsible for the annihilation and creation of pairs of particles and antiparticles, and the resulting operator is well defined (with normal ordering) on the vacuum state if and only if they form a square summable sequence, including the degeneracy of the Dirac eigenvalues. Specifically, if one introduces condition (97), together with Relation (89), in h_I^k, the dominant contribution to this function in the asymptotic regime of large ω_k is canceled out. From a Hamiltonian perspective, this cancelation is the ultimate responsible for the unitarity of the Heisenberg evolution (in the context of QFT in curved spacetimes). However, it does not guarantee that h_I^k forms a square summable sequence over all $\vec{k}$. The necessary and sufficient condition for this to happen, and thus for the Fock quantization of $\tilde{H}_D$ to be well defined on the vacuum, turns out to be that asymptotically [38]

$$\vartheta^k = -i\frac{\pi m}{3l_0^3\omega_k^2}\pi_a e^{iF_2^k} + \theta^k, \qquad \text{with} \qquad \sum_{\vec{k}} \omega_k^2 |\theta^k|^2 < \infty. \tag{98}$$

It is worth noticing that this last condition on the allowed families of fermionic annihilation and creation variables restricts even further the admissible phase space splitting between the fermionic sector and the background. Namely it specifies even further how the assignment of the dynamical content of each sector should be made.

Finally, hereafter we restrict the discussion exclusively to phases G^k such that $\{G^k, H_{|0}\} = 0$, in order not to introduce any artificial asymmetry between the dynamical behavior of the fermionic variables that describe particles and antiparticles (see Equation (93)).

5.3. Hybrid Quantization: Fermionic Backreaction

Let us next summarize the main steps that must be followed for the hybrid quantization of our cosmological system, formed by an inflationary FLRW background coupled to a perturbative Dirac field. As mentioned above, one can freely include metric and inflaton perturbations as well, and discuss a similar phase space splitting and choice of Fock representation for them. We nonetheless ignore them in this review, as they do not necessarily affect the fermionic sector at the considered order of truncation in the action. For details on the treatment of metric and inflaton perturbations in the context of hLQC, we refer the reader to Refs. [35,36,73].

The first step towards the hybrid quantization of the full system is to specify a concrete splitting of phase space with physically good properties, along the aforementioned lines. In other words, one starts by identifying a specific set of fermionic annihilation and creation variables (by means of Equations (73) and (89)) within the family restricted by the asymptotic conditions (97) and (98). In addition to the phase space splitting, such choice fixes also the Fock representation for the fermionic degrees of freedom. Indeed, for their quantization, one just needs to promote these fermionic variables to the corresponding annihilation and creation operators that in turn completely specify the Fock space $\mathcal{F}_D$ from their associated cyclic vacuum state. On the other hand, once a preferred phase space splitting has been identified, the FLRW background spacetime is described by the set of variables $\tilde{a}$, ϕ, and their canonical momenta (see Equations (90) and (91)), that as mentioned above, Poisson commute with the chosen set of annihilation and creation variables, at the classical level. We then adopt a (discrete) loop quantum cosmology representation for the canonical variables that describe the homogeneous background geometry, with operators defined on a Hilbert space that we call $\mathcal{H}_{\text{kin}}^{\text{grav}}$. For specific details on this representation, see Refs. [37,73]. In this review, we only recall its main features when they are relevant for the quantum dynamics of the fermionic sector. In addition, a standard Schrödinger representation is adopted for the homogeneous inflaton and its momentum, with Hilbert space given by $L^2(\mathbb{R}, \mathrm{d}\phi)$, such that the inflaton acts by multiplication and the momentum is represented as $-i\partial_\phi$. The total representation space for the hybrid quantization of the full canonical set of basic variables of our cosmological system is then the tensor product of all the introduced individual spaces, namely $\mathcal{H}_{\text{kin}}^{\text{grav}} \otimes L^2(\mathbb{R}, \mathrm{d}\phi) \otimes \mathcal{F}_D$.

This tensor product space is often called the kinematical space, and it is not the fully physical one. Indeed, the whole system is subject to the zero mode of the Hamiltonian constraint that can be found in Equation (92) and classically generates global time reparameterizations. We implement this symmetry at the quantum level by demanding that physical states be annihilated by the representation of the constraint as an operator on the kinematical Hilbert space[8]. Actually, for mathematical convenience, one often rather imposes a rescaled version of this constraint, obtained through multiplication by the volume $\tilde{V} = \tilde{a}^3 l_0^3$ of the homogeneous FLRW sector. To find physical states in the system, it is, therefore, necessary to specify the corresponding constraint operator and deal with the ambiguities that its representation involves, as it is not a linear function of the canonical variables. In this construction, in particular, we impose normal ordering in the fermionic contribution $\tilde{H}_D$ to the constraint. For details about the remaining ambiguities and how to reasonably fix them in the context of loop quantum cosmology, we refer the reader to Ref. [37].

Let a specific quantum representation of the zero mode of the Hamiltonian constraint (with normal ordering for the fermionic operators) be provided in this way. To search for states of physical interest, such that the influence of the perturbations on the FLRW background can be made controllably small, we look for solutions to the quantum constraint starting from the following ansatz for the allowed wavefunctions Ξ:

$$\Xi = \Gamma(\tilde{V}, \phi)\psi_D(\mathcal{N}_D, \phi). \tag{99}$$

Here, $\tilde{V}$ denotes dependence of the wavefunction on the geometric sector of the homogeneous FLRW background, and $\mathcal{N}_D$ is a generic label indicating the occupancy numbers in the fermionic Fock space. Hence, in our states we can regard Γ as the partial wavefunction that describes the behavior of the FLRW cosmology, whereas ψ_D is the partial state for the fermionic perturbations. We notice that both contributions are allowed to depend on the inflaton. It is also worth noting that

[8] Alternatively, a sufficiently large number of physical states annihilated by the (dual) action of the constraint may live in the dual space of a certain dense subset of the kinematical space.

in case inhomogeneous perturbations of the metric and inflaton were included, this ansatz can be correspondingly generalized, separating the dependence of the total wavefunction in each different type of perturbation. In what concerns the partial FLRW state Γ, we further impose as part of our ansatz that it evolves unitarily with respect to its variation in ϕ (so that we can normalize it in the Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$), with a generator that we call $\hat{\tilde{\mathcal{H}}}_0$ such that

$$-i\partial_\phi\Gamma = \hat{\tilde{\mathcal{H}}}_0\Gamma. \tag{100}$$

We take this generator to be a positive self-adjoint operator and furthermore impose that it gives rise to partial states that are close to exact quantum solutions (i.e., annihilated by the action) of the (rescaled) constraint operator of the homogeneous FLRW background. Explicitly, let us write the constraint operator that we would have for our FLRW model in the absence of perturbations in the form

$$-\frac{1}{2}[\partial_\phi^2 + \hat{\mathcal{H}}_0^{(2)}] \tag{101}$$

where $-\hat{\mathcal{H}}_0^{(2)}$ is the operator that represents the (rescaled) contribution of the inflaton potential and of the homogeneous FLRW geometry [see Equation (84)]. Our restriction on $\hat{\tilde{\mathcal{H}}}_0$ translates into demanding that the action of $(\hat{\tilde{\mathcal{H}}}_0)^2 - \hat{\mathcal{H}}_0^{(2)} - i[\partial_\phi, \hat{\tilde{\mathcal{H}}}_0]$ on Γ be small, let us say at most comparable to terms of quadratic order in the perturbative parameter of our system.

For the wave profiles selected by the above ansatz to potentially become physical states, we must impose that they be annihilated by the (rescaled) constraint operator. Namely the action of the quantum representation of the function (92), rescaled with the homogeneous volume $\tilde{V}$, on states of the form (99) (and satisfying the aforementioned conditions) must be zero. The resulting constraint equation can be greatly simplified, and viewed as an evolution equation on the partial fermionic wavefunction, if the following approximations are applied [37,73]:

(i) The partial state Γ is such that one can ignore transitions in the FLRW geometry mediated by the zero mode of the Hamiltonian constraint. Then, one can apply a kind of mean-field approximation and take the inner product of the constraint equation with Γ, with respect to the Hilbert space $\mathcal{H}_{\mathrm{kin}}^{\mathrm{grav}}$.

(ii) The contribution $\partial_\phi^2\psi_D$ can be neglected when compared with $\langle\hat{\tilde{\mathcal{H}}}_0\rangle_\Gamma\partial_\phi\psi_D$. In other words, the contribution to the inflaton momentum of the fermionic partial state is negligible compared with the contribution of the homogeneous FLRW state. The self-consistency of this approximation can be explicitly checked using the constraint equation [73].

If these approximations hold within our perturbative treatment, then the constraint equation can be recast as the following Schrödinger-like one:

$$i\partial_\phi\psi_D = \left[\frac{\langle\widehat{\tilde{V}\tilde{H}_D}\rangle_\Gamma}{\langle\hat{\tilde{\mathcal{H}}}_0\rangle_\Gamma} + C_D^{(\Gamma)}(\phi)\right]\psi_D, \tag{102}$$

where the hat denotes the hybrid loop representation of the underlying function, and [37,38]

$$C_D^{(\Gamma)} = \frac{\langle\hat{\mathcal{H}}_0^{(2)} + i[\partial_\phi, \hat{\tilde{\mathcal{H}}}_0] - (\hat{\tilde{\mathcal{H}}}_0)^2\rangle_\Gamma}{2\langle\hat{\tilde{\mathcal{H}}}_0\rangle_\Gamma}. \tag{103}$$

This function $C_D^{(\Gamma)}$ encodes, in mean value, how much the partial FLRW state Γ differs from being an exact solution of the unperturbed system. In this sense, it can be understood as a quantum backreaction term between the fermionic sector and the homogeneous background. Moreover, it is worth mentioning that the generator of the fermionic evolution dictated by this Schrödinger equation is a ϕ-dependent operator that only acts on $\mathcal{F}_D$, and depends on the homogeneous background geometry by means of expectation values of FLRW operators on the partial state Γ. Furthermore, this operator is automatically well defined on the vacuum, given the preferred Fock quantization adopted for the fermionic degrees of freedom. Therefore, the introduced approximations in the hybrid quantum constraint equation allow one to recover a QFT regime in a quantum spacetime, with good physical properties.

Solutions to the Schrödinger Equation (102) can be obtained by considering its associated Heisenberg dynamics. For that purpose, it is convenient to introduce the following change of evolution parameter:

$$d\eta_\Gamma = \frac{l_0 \langle \hat{\hat{V}}^{2/3} \rangle_\Gamma}{\langle \hat{\hat{\mathcal{H}}}_0 \rangle_\Gamma} d\phi, \tag{104}$$

which is well defined owing to the positivity of $\hat{\hat{\mathcal{H}}}_0$ and the fact that the volume operator is bounded from below by a strictly positive number in the loop quantization of the FLRW background [37]. With respect to this parameter, the Heisenberg equations associated with Equation (102), evaluated at time $\eta_\Gamma = \eta$, are given by

$$\begin{aligned} d_{\eta_\Gamma} \hat{a}^{(x,y)}_{\vec{k}}(\eta) &= -iF^{(\Gamma)}_k \hat{a}^{(x,y)}_{\vec{k}}(\eta) + G^{(\Gamma)}_k \hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta), \\ d_{\eta_\Gamma} \hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta) &= iF^{(\Gamma)}_k \hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta) - \bar{G}^{(\Gamma)}_k \hat{a}^{(x,y)}_{\vec{k}}(\eta), \end{aligned} \tag{105}$$

where we have introduced the one-parameter family of η_Γ-dependent annihilation and creation operators in the Heisenberg picture, with initial data at some $\eta_\Gamma = \eta_0$ given by the fermionic annihilation and creation operators $\hat{a}^{(x,y)}_{\vec{k}}$ and $\hat{b}^{(x,y)\dagger}_{\vec{k}}$ of our hybrid quantization. In addition, d_{η_Γ} denotes the derivative with respect to the parameter η_Γ. Moreover,

$$F^{(\Gamma)}_k = \frac{2\langle \widehat{\tilde{a}^3 h^k_D} \rangle_\Gamma}{\langle \hat{\tilde{a}}^2 \rangle_\Gamma}, \qquad G^{(\Gamma)}_k = i\frac{\langle \widehat{\tilde{a}^3 h^k_I} \rangle_\Gamma}{\langle \hat{\tilde{a}}^2 \rangle_\Gamma}, \tag{106}$$

where the diagonal mode coefficients h^k_D and the interaction mode coefficients h^k_I of the fermionic Hamiltonian are respectively given in Equations (94) and (96) (up to the elimination of any dependence on the inflaton momentum by identifying $H_{|0}$ with zero, as we have explained). It is worth noting that strictly speaking, these Heisenberg equations for the fermionic modes can be derived without the second approximation (ii) introduced above. In fact, given only the first approximation (i), it suffices that there exists a regime for all the modes in which the annihilation and creation operators find a straightforward counterpart in the Grassmann variables that they represent [36,73].

The resulting evolution from time η_0 to time η of the annihilation and creation operators is a Bogoliubov transformation that can be easily seen to take the form [37]

$$\begin{aligned} \hat{a}^{(x,y)}_{\vec{k}}(\eta) &= \alpha_k(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + \beta_k(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}}, \\ \hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta) &= -\bar{\beta}_k(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + \bar{\alpha}_k(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}}, \end{aligned} \tag{107}$$

where $\alpha_k(\eta_0,\eta_0) = 1$, $\beta_k(\eta_0,\eta_0) = 0$, and, for all η,

$$|\alpha_k(\eta,\eta_0)|^2 + |\beta_k(\eta,\eta_0)|^2 = 1. \tag{108}$$

In particular, recall that we are focusing our attention on phase space splitting and Fock representations of the fermionic degrees of freedom characterized by Equations (97) and (98) in the asymptotic regime of large ω_k. These lead to interacting contributions to the fermionic Hamiltonian such that the beta coefficients of this transformation have the asymptotic behavior

$\beta_k = \mathcal{O}[\text{Max}(\theta^k, \omega_k^{-3})]$, where the function Max[., .] picks out the argument of dominant asymptotic order [38]. Taking into account the second condition in Equation (98), it is clear that these beta coefficients form a square summable sequence, over all $\vec{k}$. It then follows that our quantum Heisenberg dynamics is unitarily implementable on the fermionic Fock space.

The unitary operator that implements the considered Heisenberg evolution can be explicitly constructed [37,38]. Furthermore, it can be checked that its action on the fermionic vacuum state picked out by the hybrid quantization provides a solution to the Schrödinger Equation (102) if the backreaction function is of the form

$$C_D^{(\Gamma)}(\phi) = \frac{l_0 \langle \hat{\tilde{V}}^{2/3} \rangle_\Gamma}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} \sum_{\vec{k},(x,y)} \Big[\Im(\eta_\Gamma) + d_{\eta_\Gamma} c_k^{(x,y)} \Big]. \tag{109}$$

Here, $c_k^{(x,y)}$ are arbitrary real phases of the evolution operator and $\Im$ is certain function with an asymptotic behavior which depends on that of the interaction contribution $G_k^{(\Gamma)}$ (or, equivalently, on that of β_k). For our allowed families of Fock representations of the fermionic degrees of freedom, one can see that this function is of dominant asymptotic order $\mathcal{O}[\text{Max}(\omega_k|\theta^k|^2, \omega_k^{-5})]$. Therefore, our backreaction term relating the FLRW background and the fermionic perturbations in the regime of QFT in a quantum spacetime, attained by the hybrid quantization of the system, turns out to be an absolutely convergent quantity. Thus, one needs not perform any regularization or *subtraction of infinities* to render this backreaction term finite, something that could be done by using the arbitrary phases $c_k^{(x,y)}$ that one can freely add to the evolution operator, but that would imply an unjustified adjustment of an infinite number of quantities.

We end this section with the following remark. The first work [37] that was carried out about the introduction of fermionic perturbations in hLQC employed a choice of annihilation and creation variables analogous to that introduced by D'Eath and Halliwell in Ref. [62]. As mentioned in the previous section, this choice is within the family of unitarily equivalent quantizations that allow for a unitarily implementable dynamics, in the context of QFT in curved spacetimes. The analysis in Ref. [37] shows that with this choice of fermionic variables, the backreaction term $C_D^{(\Gamma)}$ in the hybrid quantum theory fails to be an absolutely convergent quantity and needs to be regularized. This is an example of how the requirement of a unitarily implementable evolution alone is not enough to guarantee nice properties of the hybrid quantization of the full system. In fact, the conditions that are needed for the absolute convergence of $C_D^{(\Gamma)}$ are very similar, but slightly weaker, than those for a proper definition of the fermionic Hamiltonian on the vacuum. Indeed, it is enough that Equation (98) is fulfilled and $\omega_k|\theta^k|^2$ is a summable sequence over all $\vec{k}$ [38]. In this respect, any choice of fermionic variables that leads to a good definition of the Hamiltonian operator on the vacuum automatically guarantees that the quantum fermionic backreaction is finite, without the need for regularization.

6. Fermionic Hamiltonian Diagonalization: Choice of Vacuum State

The restrictions on the definition (73) of fermionic annihilation and creation variables in hybrid quantum cosmology to guarantee: (i) unitarity of the QFT evolution [Equation (97)], and (ii) a well-defined Hamiltonian on the vacuum [Equation (98)], allow us to considerably reduce the possible choices of such variables, at least in the asymptotic regime of large ω_k. However, and even though all the resulting Fock representations are unitarily equivalent, there is still much freedom in identifying a particular set of annihilation and creation variables (even in the asymptotic regime). In other words, there remains ambiguity in the complete characterization of the phase space splitting between the FLRW background and the fermionic sector, as well as of the fermionic vacuum state of the theory. In this section we motivate and adhere to the physical criterion of Hamiltonian diagonalization to try and fix this remaining choice, following a procedure that is specifically adapted to the spatially local structure of the fermionic dynamics.

6.1. Hamiltonian Diagonalization in hLQC

The previously imposed criteria on the allowed choices of fermionic annihilation and creation variables [Equations (97) and (98)] are tailored to have the net effect of diminishing the dominant asymptotic order, in the regime of large ω_k, of the interaction parts h_I^k of the fermionic Hamiltonian $\tilde{H}_D$ [given in Equation (93). Ultimately, this fact is responsible for the unitarity of the fermionic evolution, as well as for a proper definition of the fermionic Hamiltonian on the vacuum. As we have already commented, these interaction parts annihilate and create pairs of particles and antiparticles in the quantum fermionic dynamics. From a physical perspective, one would think that a choice of phase space splitting where the assignment of the dynamical contribution of the FLRW background to the system is such that the fermionic states undergo no annihilation and creation of pairs, would be one that is naturally adapted to the dynamics of the entire cosmological system. This choice should then be such that $h_I^k = 0$, so that the Fock quantization of the resulting fermionic Hamiltonian $\tilde{H}_D$ would have a diagonal action on the n-particle states associated with the selected set of annihilation and creation operators.

According to this line of reasoning, we refer to any choice of fermionic annihilation and creation variables that lead to vanishing interaction terms h_I^k, for all $\vec{k}$, as variables for the Hamiltonian diagonalization. In general, restricting to cases with $f_2^k \neq 0$ (which include all those choices that respect the standard convention for particles and antiparticles in the massless limit [55]), one can readily check that the diagonalization condition $h_I^k = 0$ is fulfilled for all $\vec{k}$ if and only if

$$a\left\{\varphi_k, H_{|0}\right\} + 2i\omega_k\varphi_k + iam\varphi_k^2 - iam = 0, \tag{110}$$

where $f_1^k = f_2^k\varphi_k$. This is a semi-linear partial differential equation which has locally unique solutions, as long as the section of initial conditions is transversal to the flow of the Hamiltonian vector field $\{., H_{|0}\}$ [74]. Naturally, there are several possible families of such solutions for all $\vec{k}$, and each of them completely characterizes (up to the two phases G^k and F_2^k) a different set of fermionic variables for the Hamiltonian diagonalization, in virtue of Equation (89). Explicitly, it holds that

$$|f_2^k|^2 = \frac{1}{1+|\varphi_k|^2}. \tag{111}$$

Let us point out that in fact, the structure of the differential Equation (110) allows for solutions that moreover on the FLRW geometry, can depend also on the inflaton and its canonical momentum. Remarkably, nonetheless, the definition of fermionic annihilation and creation variables resulting from any such choice of coefficients for the Hamiltonian diagonalization can still be completed to become canonical in the entire cosmological system, following an analogous procedure to that discussed in the previous section. We adopt this extended framework for the definition of the fermionic variables in this and the next subsection.

Finally, it is worth noticing that Relation (111) can be used to show that the mode coefficients h_D^k of the resulting diagonal Hamiltonian, for each choice of fermionic variables characterized by a set of solutions to Equation (110) (for all $\vec{k}$), acquire the form [75]

$$2h_D^k = a^{-1}\omega_k + m\mathrm{Re}\left(\varphi_k\right) - \left\{F_2^k, H_{|0}\right\}. \tag{112}$$

6.2. Asymptotic Diagonalization

In the following, we try and fix a preferred solution to Equation (110), using our previous knowledge of the restrictions that unitary evolution and a proper definition of the fermionic Hamiltonian impose, and by looking into the details of this Hamiltonian in the asymptotic regime of large ω_k. For fermionic variables that admit a unitarily implementable evolution, namely when

Equation (97) holds, the interaction coefficients h_I^k of the fermionic Hamiltonian $\tilde{H}_D$ behave asymptotically as

$$h_I^k = \frac{2\omega_k}{a}\vartheta^k + i\frac{2\pi m}{3l_0^3\omega_k}\frac{\pi_a}{a}e^{iF_2^k} + \mathcal{O}[\mathrm{Max}(\vartheta^k, \omega_k^{-2})], \tag{113}$$

where the second summand results from the second Poisson bracket in Equation (96). As we pointed out above, we explicitly see here that demanding condition (98) for a well-defined action of the Fock quantization of the Hamiltonian on the fermionic vacuum is equivalent to diminishing the dominant asymptotic order, in inverse powers of ω_k, of the interaction coefficients. Once this condition is imposed, one arrives at an asymptotic behavior for h_I^k with an analogous structure as in Equation (113). More concretely, its dominant contribution is given by $2\omega_k\theta^k/a$ plus certain specific terms that are proportional to ω_k^{-2}. One can cancel this contribution again by conveniently fixing the dominant asymptotic behavior of θ^k. The resulting interaction coefficient h_I^k displays, once more, a similar asymptotic structure, but with the role of θ^k played by its subdominant contributions and the remaining summands with a lower asymptotic order in powers of ω_k. Owing to the asymptotic structure of the Hamiltonian, this pattern repeats itself at each asymptotic order in inverse powers of ω_k, if one admits an asymptotic expansion of this form and imposes the cancelation of the previous dominant terms in the interaction coefficient h_I^k.

Motivated by these properties of the fermionic Hamiltonian, and taking into account that asymptotically

$$f_2^k = e^{iF_2^k} + \mathcal{O}(\omega_k^{-2}) \tag{114}$$

if the unitary evolution condition (97) is fulfilled, we propose the following asymptotic series as an ansatz for a Hamiltonian diagonalization in the regime of large ω_k:

$$\varphi_k \sim \frac{1}{2\omega_k}\sum_{n=0}^{\infty}\left(-\frac{i}{2\omega_k}\right)^n \gamma_n, \qquad \gamma_0 = ma. \tag{115}$$

Here, the symbol $\sim$ indicates the equality of the asymptotic expansions, and γ_n are functions of the homogeneous FLRW background canonical variables. These are completely fixed in an iterative way if one introduces our ansatz in the interaction coefficients h_I^k of the fermionic Hamiltonian, and imposes that each contribution in inverse powers of ω_k be equal to zero. Specifically, one then obtains [39,75]

$$\gamma_{n+1} = a\left\{H_{|0}, \gamma_n\right\} + ma\sum_{m=0}^{n-1}\gamma_m\gamma_{n-(m+1)}, \qquad \forall n \geq 0, \tag{116}$$

where $\gamma_{-n} \equiv 0$ for all $n > 0$. This is a deterministic recurrence relation that can be used to fix all the functions γ_n, starting from the initial datum γ_0.

It is worth mentioning that the proposed function φ_k for the asymptotic diagonalization of the fermionic Hamiltonian, given by Equations (115) and (116), provides a very specific solution to the general Equation (110), in the sector of unboundedly large ω_k. Such an asymptotic solution can be thought of as a physically preferred solution, inasmuch as it has been obtained by exclusively adhering to local features of the fermionic Hamiltonian. However, despite the strong asymptotic restriction that our requirement sets on the admissible solutions to Equation (110), there may exist many such solutions for all $\vec{k}$ that viewed as functions of ω_k, display the same, preferred asymptotic behavior. It seems therefore most convenient to investigate whether the imposition of certain smoothness conditions on the dependence of any such φ_k on ω_k (e.g., continuity or analyticity) can allow us to fix this solution completely. Indeed, if we were able to ensure this uniqueness, by taking into account relations (89), we would solve the last remaining ambiguity in the choice of fermionic variables for the hybrid description of the system, up to the phases G^k and F_2^k. In other words, once these phases were chosen, we would succeed in specifying a Fock representation (with its associated vacuum state) of the fermionic degrees of freedom, together with a particular splitting of the fermionic and FLRW sectors of the phase space and of their contribution to the dynamics of the entire system. Actually, we have already restricted the phase G^k in a substantial way by demanding it to be a dynamically irrelevant constant in the classical linearized system, after imposing $\{G^k, H_{|0}\} = 0$ to eliminate asymmetries in the evolution of particles and antiparticles. As for the other phase, F_2^k, it can be naturally selected by demanding that the original dynamics that is extracted from the Dirac field by means of the background-dependent transformation (73) be minimal, along the lines detailed in Ref. [40].

We end this subsection by noting that if one specifies a preferred choice of fermionic annihilation and creation variables for the Hamiltonian diagonalization, then one is not only fixing the relevant structures for the hybrid quantization of the cosmological system, but also a concrete Fock representation of the Dirac field, within the framework of QFT in curved spacetimes. This regime is attained when the homogeneous background obeys the Friedmann equations, whereas the fermionic annihilation and creation variables evolve with the dynamics dictated by the fermionic contribution to the Hamiltonian (92). If the interaction terms in this Hamiltonian are zero, then this fermionic dynamics can be straightforwardly solved, namely the annihilation and creation variables just evolve via multiplication of their initial data (at an arbitrary initial time) by a complex phase. With these solutions at hand, if one takes the inverse of the defining transformation of these variables given by Equation (73), and introduces it in the mode expansion of the Dirac field, one immediately obtains a complete basis of solutions for the Dirac equation, in the sense of Equation (7). The constant coefficients of the elements of this basis in the expansion of the field are the annihilation and creation initial data that select a unique Fock representation (and its associated vacuum state) once they are promoted to operators.

6.3. Uniqueness of the Vacuum: Minkowski and de Sitter Spacetimes

In this subsection we focus our discussion on the aforementioned regime of QFT in curved spacetime, and explain how our ansatz for asymptotic diagonalization succeeds in the selection of natural vacuum states in Minkowski and de Sitter spacetimes. In fact, the asymptotic expansion given in Equations (115) and (116) allows us to determine a complete basis of solutions for the Dirac equation (as in Relation (7)) that turns out to correspond to the choice of the Poincaré or the Bunch–Davies vacuum, respectively, when the background cosmology is fixed as the Minkowski or the de Sitter spacetime. Taking into account that when the homogeneous background obeys the Friedmann equations, we have that $a\{., H_{|0}\}$ is simply the derivative with respect to the conformal time, in the considered situations in QFT the recurrence Relation (116) becomes

$$\gamma_{n+1} = -\gamma_n' + ma \sum_{m=0}^{n-1} \gamma_m \gamma_{n-(m+1)}, \qquad \forall n \geq 0. \tag{117}$$

Let us start by considering the case of a background given by the classical Minkowski spacetime. This particularization is easily implemented by setting the scale factor as the unit constant, the inflaton as an arbitrary constant, and its potential equal to zero. Then, we immediately have that $\gamma_0 = m$, while any other γ_n, determined by the recursion Relation (117), has a vanishing time derivative. That iterative equation can be solved by introducing the generating function $G(x) = \sum_{n=0}^{\infty} \gamma_n x^n$ that leads to a quadratic equation with only one solution consistent with the initial datum $\gamma_0 = m$:

$$G(x) = \frac{1}{2mx^2} \left[1 - \sqrt{1 - 4m^2x^2}\right]. \tag{118}$$

Around $x = 0$, this is an analytic function with power series in x characterized by the coefficients γ_n, by construction. Then, comparing this series to our ansatz (115) and employing the uniqueness of the asymptotic expansion, we can directly identify the function φ_k that leads to an asymptotic diagonalization with the following analytic function:

$$\varphi_k = \frac{1}{2\omega_k} G\left(\frac{-i}{2\omega_k}\right) = \frac{\omega_k}{m}\left[\sqrt{1+\frac{m^2}{\omega_k^2}} - 1\right]. \tag{119}$$

Using the relations (89) and (111) that arise from the requirement that the fermionic annihilation and creation variables be defined by means of a canonical transformation, one eventually obtains

$$|f_1^k| = \sqrt{\frac{\xi_k - \omega_k}{2\xi_k}}, \qquad |f_2^k| = \sqrt{\frac{\xi_k + \omega_k}{2\xi_k}}, \tag{120}$$

where $\xi_k = \sqrt{\omega_k^2 + m^2}$. Since the selected function φ_k that permits the Hamiltonian diagonalization is completely independent of time in this case, according to our comments above, it is natural to demand that the phase F_2^k be simply an arbitrary constant, as well as G^k. From Equation (112), one can straightforwardly check that the diagonal coefficients of the resulting fermionic Hamiltonian are then $h_D^k = \xi_k$. A simple inspection of this result, together with Equation (120), immediately reveals that our criterion of asymptotic diagonalization selects indeed the basis of solutions to the Dirac equation in Minkowski spacetime that corresponds to the Poincaré Fock representation of the field. Namely it is the quantization that with a standard convention for particles and antiparticles, separates between positive and negative mass-shell frequencies ξ_k.

Let us show, in addition, how our criterion of asymptotic diagonalization recovers the common notion of Bunch–Davies vacuum for the Dirac field in de Sitter spacetime. In a flat slicing, this spacetime can be understood as a cosmological solution of Friedmann equations obtained by setting the inflaton potential equal to the constant $3H_\Lambda^2/(8\pi)$ and the inflaton momentum equal to zero. Here, H_Λ is the constant Hubble parameter. In conformal time, the expanding scale factor then behaves as

$$a = -\frac{1}{\eta H_\Lambda}, \qquad -\infty < \eta < 0. \tag{121}$$

The analysis of the restrictions that the asymptotic diagonalization imposes on the choice of a fermionic vacuum is easier if one first considers the general differential equation for φ_k in our de Sitter background. It reads

$$\varphi_k' + 2i\omega_k\varphi_k - i\frac{m}{\eta H_\Lambda}\varphi_k^2 + i\frac{m}{\eta H_\Lambda} = 0. \tag{122}$$

The general solution of this equation can be found by introducing a mode-dependent complex time $T_k = -2i\omega_k\eta$ and the following change of variables [75]:

$$\varphi_k = 1 + i\frac{H_\Lambda}{m} T_k \frac{d}{dT_k}\left(\log v_k\right). \tag{123}$$

The function v_k turns out to satisfy a confluent hypergeometric equation in the complex variable T_k that has the general solution

$$\begin{aligned} v_k \;&=\; A\,{}_1F_1\left(-imH_\Lambda^{-1}; 1 - 2imH_\Lambda^{-1}; T_k\right) \\ &+\; B\,T_k^{2imH_\Lambda^{-1}}\,{}_1F_1\left(imH_\Lambda^{-1}; 1 + 2imH_\Lambda^{-1}; T_k\right), \end{aligned} \tag{124}$$

where A and B are integration constants, and ${}_1F_1(.;.;z)$ is the hypergeometric function of type $(1,1)$ that is absolutely convergent for all values of its complex argument z [76].

The asymptotic expansion determined by our criterion of Hamiltonian diagonalization, given in Equations (115) and (117), actually picks out a specific solution of the mentioned hypergeometric equation, up to an irrelevant multiplicative constant, namely a particular ratio between the integration constants A and B. Indeed, the iterative Relation (117), particularized to our de Sitter background, can be seen to lead to coefficients γ_n such that

$$\varphi_{k,\lambda} \sim i\frac{1}{T_k}\sum_{n=0}^{\infty}\left(-\frac{1}{T_k}\right)^n C_n, \tag{125}$$

where C_n are constants that are completely specified by a complicated nonlinear recurrence relation, with the initial value $C_0 = mH_\Lambda^{-1}$ [75]. We need not solve this relation, since the T_k-dependence of the above asymptotic series, together with the known value of C_0, is enough to restrict the associated expansion of v_k in Equation (123) so that

$$v_k \sim T_k^{imH_\Lambda^{-1}}\sum_{n=0}^{\infty}\left(-\frac{1}{T_k}\right)^n v_n, \qquad \text{with} \qquad v_1 = \left(\frac{m}{H_\Lambda}\right)^2 v_0. \tag{126}$$

By introducing this ansatz for the asymptotic behavior of v_k in the confluent hypergeometric equation that it must satisfy, one can determine the coefficients v_n of the asymptotic expansion exclusively in terms of v_0, yielding

$$v_k \sim v_0 T_k^{imH_\Lambda^{-1}}\,{}_2F_0\left(imH_\Lambda^{-1}, -imH_\Lambda^{-1}; -; -T_k^{-1}\right), \tag{127}$$

where ${}_2F_0(.,.;-;z)$ is the hypergeometric function of type $(2,0)$ that has a zero radius of convergence. Even though it formally diverges, its series is known to provide the asymptotic expansion of a very particular type of solution to the confluent hypergeometric equation, namely the Tricomi solution [76]. In fact, using the asymptotic properties of the hypergeometric functions in Equation (124), it is possible to prove that the Tricomi solution is the unique one that has an asymptotic expansion of the form (127). Therefore, after substituting this solution in Relation (123), we immediately see that our procedure of asymptotic Hamiltonian diagonalization allows us to obtain again a unique solution to the general Equation (110), for all wave vectors $\vec{k}$.

In more detail, the Tricomi solution for v_k selected by our criterion of asymptotic diagonalization leads, after several manipulations, to the following function φ_k in Equation (123) [75]:

$$\varphi_k(\eta) = \frac{H^{(1)}_{-\mu}(\omega_k\eta) - iH^{(1)}_{1-\mu}(\omega_k\eta)}{H^{(1)}_{-\mu}(\omega_k\eta) + iH^{(1)}_{1-\mu}(\omega_k\eta)}, \qquad \mu = i\frac{m}{H_\Lambda} + \frac{1}{2}, \tag{128}$$

where $H^{(1)}_\nu$ denotes the Hankel function of the first kind [77]. In turn, using relations (89) and (111), this result determines the coefficients f_1^k, f_2^k, g_1^k, and g_2^k that define the fermionic annihilation and creation variables, up to the phases F_2^k and G^k. We recall that the latter is fixed as an arbitrary constant. As for the former, namely F_2^k, one can select it following the ideas put forward in the previous subsection, so that it minimizes the amount of dynamics extracted by the time-dependent canonical transformation (73). In any case, the details about the time dependence of this phase are irrelevant for the basis of solutions to the Dirac equation that φ_k selects (in the context of QFT in a fixed curved spacetime), as one can straightforwardly check using Equations (73) and (112). Then, after taking into account the diagonal evolution of the annihilation and creation variables dictated by h_D^k in Equation (112), the resulting complete set of solutions for the Dirac equation in which the field decomposes is given by very specific linear combinations of Hankel functions of the first (in the case of antiparticles) and second (in the case of particles) kinds, different for each chirality and helicity [75]. We recall that any such basis decomposition fixes a particular Fock representation of the field. In this case, the basis of solutions turns out to be precisely the one that has been naturally associated in the literature with the fermionic analog of the Bunch–Davies vacuum in de Sitter spacetime [75,78,79].

Therefore, our criterion of asymptotic Hamiltonian diagonalization provides again the vacuum state that is physically accepted as preferred, in this case in a de Sitter background.

We end this section with a final remark. Beyond the well-known background spacetimes analyzed here, namely Minkowski and de Sitter, quantum fields in FLRW cosmologies suffer from the lack of a natural choice of vacuum state, at least if one appeals only to the symmetries of the system to select it. In the case of scalar fields, a common approach to mitigate this issue is the introduction of adiabatic states (see e.g., Refs. [31,80–82]). Their construction is based on an iterative procedure to solve the field equations such that the resulting quantization displays certain local Poincaré-like features. In the case of Dirac fields, there have been at least two notable attempts to generalize the notion of adiabatic states [83,84]. The proposal in Ref. [84] follows closely the construction procedures previously established for scalar fields. In particular, this work introduces an algorithm to iteratively solve the Dirac equation that at each consecutive step, can approach the actual mode solutions up to contributions that are more and more subdominant in the asymptotic regime of large ω_k. An adiabatic state of nth-order is defined by truncating this procedure at the nth-step of the iteration and setting the value of the resulting approximate mode solutions, at an arbitrary time, as the initial data that specify the basis of solutions for the Fock representation of the field. Ref. [85] analyzed the relation between these adiabatic states and our family of unitarily equivalent quantizations of the Dirac field, including those that satisfy the condition of asymptotic diagonalization. It was shown that the representations associated with adiabatic states of all orders belong to the same equivalence class. In particular, the zeroth-order state already corresponds to a representation that admits unitarily implantable evolution, once the time dependence attributed to the FLRW background has been conveniently extracted. In fact, this unitarity guarantees that any two states defined with adiabatic initial data at different times are unitarily equivalent, so that the choice of initial time for the definition of the adiabatic states is not a relevant ambiguity. Furthermore, the first-order adiabatic state directly leads to a Fock quantization of the Dirac field in the family selected by imposing that the fermionic Hamiltonian for the annihilation and creation variables be well defined on the vacuum. The question of whether higher-order adiabatic states give rise to representations that behave, in the asymptotic regime of large ω_k, increasingly closer to the one(s) selected by our criterion of asymptotic Hamiltonian diagonalization is yet an open issue.

7. Conclusions

In this work, we have reviewed some recent investigations, carried out by us and our collaborators, about the physical motivation and use of certain criteria capable to ensure the uniqueness of the Fock quantization of fields in cosmological systems, specialized to the case of fermions described by Dirac fields. The presented results have been applied to the study of the hybrid quantization of the primordial Universe with perturbations that contain all the fermionic degrees of freedom described by a Dirac field (and may also include other matter field perturbations and metric perturbations).

We have first considered the Fock quantization of the CARs for Dirac fields in conformally ultrastatic three-dimensional spacetimes, as well as in cosmological FLRW spacetimes in four dimensions, with spherical or toroidal spatial hypersurfaces. We have characterized the set of vacua that are invariant under the physical symmetries of the Dirac equation in these spacetimes. These symmetries include the continuous isometries of the spatial hypersurfaces, enlarged with the spin rotations generated by the helicity in the case of FLRW cosmologies with sections of toroidal topology.

For all the Fock representations associated with the above set of invariant vacua, we have proven that there exists a subset that admits unitary implementability of the dynamics on the Fock space. This evolution comes from the Dirac equation, after extracting from the fermionic field some of its time variation that can be attributed to the dependence on the variables that describe the spacetime background. In the Heisenberg picture, the extracted part is regarded as explicitly time-dependent, and therefore is not included in the proper quantum dynamics of the annihilation and creation operators. In fact, this extraction is necessary to achieve the unitary implementability of the quantum evolution. It must be restricted, nonetheless, by the condition that the evolution remaining from the original Dirac equation be not trivialized.

After determining all the Fock representations that are allowed by the criteria of invariance under the symmetries of the equations of motion and of a nontrivial unitary implementability of the dynamics, we have shown that all these representations are unitarily equivalent for each of the spacetime scenarios that we have considered, provided that one fixes a convention to distinguish between particles and antiparticles of the Dirac field. In other words, our well-motivated conditions of unitarity and invariance guarantee the uniqueness of the Fock representation, up to unitary equivalence.

This uniqueness result has the immediate consequence of also specifying a unique concept of quantum dynamics for the fermionic annihilation and creation operators, modulo unitary redefinitions. Indeed, our analysis allows us to fully characterize the functions of the spacetime background that need to be removed from the time dependence of the fields, at least in the ultraviolet limit of large eigenvalues of the Dirac operator on the spatial hypersurfaces. This characterization can alternatively be understood as the determination of which field excitations are the particles and antiparticles that preserve their coherence over time.

We have provided an optimal description, with an eye to its quantization, of the phase space of a homogeneous and isotropic cosmology coupled to a homogeneous scalar field (that acts as an inflaton in General Relativity) and with fermionic perturbations, when the Einstein-Dirac action is truncated at quadratic perturbative order. For the fermionic sector of the phase space, we have used our previous result about the Fock representation of a Dirac field to select a quantization of the fermionic degrees of freedom, up to unitary modifications. Hence, for the fermionic field, we have chosen certain annihilation and creation variables that are related with the Dirac modes through a canonical transformation that depends on the homogeneous and isotropic background, and that supports a unitarily implementable Heisenberg dynamics when the background is viewed as a fixed entity. This leads to a specific splitting of the phase space between the background degrees of freedom and the fermionic content. A particular consequence is the modification of the contribution to the global Hamiltonian constraint associated with the fermionic perturbations. We have taken advantage of this modification and, going beyond the criterion of unitary dynamics for the selection of the fermionic variables, we have employed the remaining freedom in the background dependence of this choice to obtain other desirable properties in the quantization of our system. One property that we have investigated is a proper definition of the fermionic Hamiltonian operator on the set of finite particle/antiparticle states constructed from the vacuum. On the other hand, the discussed splitting of the phase space also implies a change in the canonical variables that describe the homogeneous background, to preserve the symplectic canonical structure of the system at the perturbative order of our truncation. The corresponding change in the background variables amounts to the correction of the original ones with terms that are quadratic in the perturbations.

Using the above description of the phase space, the only nontrivial constraint that needs to be imposed quantum mechanically is the zero mode of the Hamiltonian constraint. This global constraint interrelates the different physically relevant sectors of the phase space, namely the geometric FLRW sector, for which a loop representation is adopted, the inflaton, with a Schrödinger-like representation, and the fermionic perturbations, for which one takes a Fock representation in the selected family (in addition, it is possible to include scalar and tensor perturbations, described by perturbative gauge invariants, with Fock representations that can be picked out as well with our proposed criteria). In order to single out this preferred family of Fock representations, in addition to the invariance under the symmetries of the field equations and the unitary implementability of the Heisenberg dynamics, we have chosen a convention for the distinction between particles and antiparticles which smoothly connects with the standard convention of QFT when the mass of the field vanishes.

We have shown how to impose the operator that represents the zero mode of the Hamiltonian constraint of our perturbed cosmological system on states for which the dependence on the different sectors of the phase space, except the inflaton, becomes separable. In this way, we have been able to find mild conditions under which the imposition of the constraint turns out to be essentially equivalent to a certain master constraint equation on the fermionic perturbations. Given our perturbative hierarchy, these conditions amount to have negligible FLRW geometry transitions mediated by the zero mode of the Hamiltonian for the partial wave function that describes such a homogeneous geometry in our state. The resulting equation is special since the dependence on the FLRW geometry only persists by the inclusion of expectation values over that geometry. With an additional approximation on the variation of the partial wave function of the fermionic perturbations with respect to the inflaton, that can be checked at least for self-consistency, one can deduce from this master constraint on the perturbations a Schrödinger equation for the partial state that describes the fermionic content. This Schrödinger equation involves the quantum backreaction that the fermionic perturbations produce on the FLRW geometry.

Moreover, within our approximations, it is possible to solve the quantum dynamics dictated by the commented master constraint equation on the perturbative fermionic modes. We have reviewed how such dynamics can be implemented on our Fock space. The resulting evolution depends, in particular, on the FLRW geometry, but this is so exclusively through expectation values that turn out to be different for each fermionic mode and that are well defined thanks to the loop representation adopted in the scheme of hLQC. These facts, together with ultraviolet properties, guarantee the unitary implementability of the fermionic Heisenberg dynamics. One can construct the associated unitary evolution operator that is generated by the fermionic Hamiltonian that appears in the Schrödinger equation that has been derived. Actually, we have seen that the requirement that this Hamiltonian be well defined on the vacuum is enough to guarantee a finite fermionic backreaction on the FLRW background, without the need for any regularization. On the other hand, the unitarity of the fermionic dynamics translates into a finite production of pairs of particles and antiparticles in the evolved vacuum.

We have gone one step beyond and employed the still remaining freedom in the determination of the Fock representation of the fermionic degrees of freedom, and their splitting from the FLRW sector of the phase space, to demand an additional feature in the fermionic Hamiltonian, namely that it become diagonal in terms of the fermionic annihilation and creation variables in the asymptotic region of large wave numbers of the modes, in the sense that it do not contain interactions in that region that produce pairs of particles and antiparticles. We have seen that this condition indeed fixes asymptotically the choice of vacuum state. Furthermore, we have argued in favor of the uniqueness of the vacuum selected by means of this asymptotic Hamiltonian diagonalization when extended to all wave numbers by suitable smoothness conditions. In this respect, we have demonstrated the uniqueness in the case of standard QFT in Minkowski and de Sitter spacetimes, treated as fixed backgrounds, showing in addition that the vacua that are picked out by the diagonalization procedure are the Poincaré and the Bunch–Davies vacua, respectively. For more general backgrounds, either of classical or quantum nature, our proposal can potentially serve to attain a well-defined and unique choice of vacuum state with especially good physical and mathematical properties.

Finally, we have commented on the relation between adiabatic states and the vacua selected by our criteria. For iterative constructions of fermionic adiabatic states, all of them turn out to belong to the unitary equivalence class of Fock states that incorporate symmetry invariance and allow for a unitarily implementable dynamics. Moreover, states of first or higher adiabatic order belong to the family of Fock states picked out by the additional requirement of a fermionic Hamiltonian with a well-defined action on the dense set of finite particle/antiparticle states, and therefore it is ensured that they lead also to a finite fermionic backreaction. As for the issue of Hamiltonian diagonalization, it is an open question whether higher-order adiabatic states give rise to representations in which the vacuum state increasingly approaches our choice in the asymptotic regime of large wave numbers.

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Nonoscillating vacuum states and the quantum homogeneity and isotropy hypothesis in loop quantum cosmology

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We study the compatibility of the quantum homogeneitiy and isotropy hypothesis (QHIH), proposed by Ashtekar and Gupt to restrict the choice of vacuum state for the cosmological perturbations in loop quantum cosmology (LQC), with the requirement that the selected vacuum should lead to a power spectrum that does not oscillate. We inspect in close detail the procedure that these authors followed to construct a set of states satisfying the QHIH, and how a preferred vacuum can be determined within this set. We find a step that is not univocally specified in this procedure, in relation with the replacement of the set of states that was originally allowed by the QHIH with an alternative set that is more manageable. In fact, the first of these sets does not contain the state that has been used in most of the implementations of the QHIH to the analysis of the power spectrum of the perturbations in LQC. We focus our attention on the original set picked out by the QHIH and investigate whether some of its elements may display a nonoscillatory behavior. We show that, to the extent to which the techniques used in this paper apply, this possibility is feasible. Thus, the two aforementioned criteria for the physical restriction of the vacuum state in LQC are compatible with each other and not exclusive.

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I. INTRODUCTION

In order to extract useful predictions from a physical theory, sometimes it does not suffice to determine the dynamical equations that rule the evolution of the system and analyze their properties. Choosing initial conditions can be just as important as these dynamical laws, especially for scenarios that cannot be reproduced in a controlled way in a laboratory (such as, e.g., gravitational systems). In these cases, any successful theory should incorporate a procedure to determine suitable initial conditions, based on reasonable justifications and leading to phenomenologically sensible results. A situation in which this issue is particularly important is in the study of the evolution of primordial cosmological perturbations. These perturbations are believed to be the seeds of the temperature anisotropies that can be observed in the cosmic microwave background (CMB) [1–4]. Beyond the standard cosmological paradigm, there is a growing hope that the power spectrum of the CMB radiation may keep some traces of the quantum geometry phenomena that would have taken place when the Universe was extremely young and in this manner provide a way to falsify the predictions of quantum cosmology formalisms that describe the behavior of those early epochs [5–8].

Many attempts have been made to include quantum gravity effects in the analysis of primordial perturbations in cosmology (see, e.g., [9–28]). Most of these works adopt a Fock representation for the linear fields corresponding to the gauge-invariant perturbations. Then, the choice of initial conditions is equivalent to selecting a preferred Fock vacuum state. A natural starting point is to demand that this vacuum state remains invariant under the spatial isometries of the homogeneous background (either treated as a classical or a quantum entity). Nonetheless, since the cosmological background is not stationary, these symmetries are usually not enough to pick out a unique vacuum, but only to restrict the choice within a family of states, unitarily equivalent among them in an optimal scenario, if the selection criteria have been wisely imposed [29,30]. Within that family, one of the most common proposals is to choose the Bunch-Davies vacuum at the onset of inflation, especially if there is an inflationary phase that admits a slow-roll description. The Bunch-Davies state is arguably the most natural vacuum in de Sitter spacetime, which is believed to provide a good approximation for the

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cosmological expansion in such an inflationary phase [2,31]. However, this state is not well adapted to the cosmological evolution if there are relevant regimes previous to slow-roll inflation with physical phenomena that can affect the primordial perturbations. For instance, this may happen for perturbation modes with wavelengths of the order of the characteristic scales associated with the quantum gravity processes that may have affected the Universe well before inflation, out of the domains of applicability of classical general relativity. To take those primeval epochs into account, we must have some level of understanding of the underlying quantum geometry. Several candidate formalisms have been suggested to describe quantum gravity regimes in cosmology. Among them, we will focus our attention on loop quantum cosmology (LQC) [32–34], which is a nonperturbative quantization of cosmological systems based on the background-independent canonical theory of loop quantum gravity [35,36]. In LQC, for certain quantum states with interesting classical properties at large volumes, the big bang singularity becomes replaced with a quantum bounce [37,38].

Within these bouncing regimes of LQC, the choices of vacuum state for the perturbations that were first employed to extract predictions from the theory correspond to the so-called adiabatic states [19,39]. Adiabatic states [40,41] are constructed iteratively from a zeroth-order state and, for sufficiently high order, they have the physically appealing property of permitting the renormalization of the stress-energy tensor. The adiabatic iterative process, however, is not mathematically robust and breaks down in certain circumstances. In addition, the motivation for using adiabatic conditions around a bounce of quantum origin is not completely clear from a theoretical point of view [42–44]. A more recent proposal for the choice of a vacuum, with a more elaborated motivation, has been given by Ashtekar and Gupt [45,46] in the context of the so-called dressed-metric approach to the study of primordial perturbations in LQC (see, e.g., Refs. [16,19,20,47]). According to this proposal, one chooses the state with a maximal classical behavior at the end of inflation among those that fulfill the so-called quantum homogeneity and isotropy hypothesis (QHIH). This is an extension into the quantum realm of Penrose's Weyl curvature hypotesis [48,49], which states that the Weyl curvature should vanish at the big bang. The vacuum state selected so far using this QHIH has been seen to lead to a primordial power spectrum that is highly oscillatory in the dressed-metric approach to LQC, with respect to the wave number of the Fourier modes of the perturbations [46]. When these oscillations are suitably averaged, this power spectrum shows good agreement with the current CMB observations, and it may even provide a way to alleviating certain anomalies reported by the Planck satellite [6,7]. Nonetheless, it has been argued that these oscillations might come from an evolution of the proposed vacuum in the preinflationary epoch that blurs the information about the genuine effects of the LQC bounce on the perturbations [50,51]. To deal with the problem of these superimposed oscillations in the power spectrum, Martín de Blas and Olmedo put forward an alternative proposal, implemented numerically, which selects a vacuum state with a nonoscillatory (NO) spectrum [50]. This NO-vacuum was originally introduced in the context of the so-called hybrid approach to LQC (see Ref. [52] for a comprehensive review on the topic). Recent investigations have identified some analytical conditions that must be satisfied by a vacuum displaying NO properties, and that restrict its asymptotic behavior for infinitely large wave numbers [51,53].

The aim of this work is to investigate the relationship and compatibility between the QHIH and the NO-proposal as two criteria to restrict the choice of vacuum state in the context of hybrid LQC. In order to do this, we start by revisiting the mathematical conditions that define the admissible states according to the QHIH in a bouncing quantum cosmological scenario, indicating the steps where there appear ambiguities when the original proposal of Ashtekar and Gupt [45] is put into practice [46]. This construction starts by defining a ball of states that satisfies the QHIH in an interval around the quantum bounce, that is regarded as the Planck regime. In more detail, this interval is defined, for the sake of concreteness, as the period in which the density of the Universe is higher than 10^{-4} in Planck units. Then, according to Ashtekar and Gupt, a preferred state should be selected within this ball such that it has maximal classical behavior at the end of inflation. However, because of the numerical complications in the imposition of these requirements, an alternative but much more manageable definition of the ball of admissible states was finally adopted in Ref. [46]. In the present work we show that this alternative definition leads to a different set of states to the original QHIH ball, raising the question of whether the Ashtekar-Gupt state selected in this manner actually lives in such original ball. We find that the answer is in the negative, at least in the hybrid approach to LQC. We recall that this state has highly oscillatory properties in the case of the dressed-metric approach to LQC, and it can be reasonably expected that it also displays this behavior in hybrid LQC.[1] Our result then opens the possibility that the preferred vacuum state that would arise from the original QHIH considerations may be compatible with the demand of an NO-behavior. With this motivation in mind and using the results of Ref. [51], we derive certain necessary conditions for the simultaneous satisfaction of an NO-behavior and the QHIH. Employing these conditions, we then examine the possibility that the Ashtekar-Gupt proposal may eventually lead to the choice of an NO-vacuum. Our result is that, without additional inputs, the two proposals are compatible.

[1]This is because both approaches share a classical preinflationary period that tends to produce oscillations in the evolution of the vacuum state, if this vacuum is not carefully chosen [43].

The structure of this paper is as follows. In Sec. II we take a close look at the definition of the QHIH given in Ref. [45] and the Ashtekar-Gupt vacuum selected in Ref. [46]. In Sec. III we identify a loose step in the passage from the theoretical construction of the ball of QHIH states, where this vacuum should reside, to its practical implementation. Furthermore, we derive certain compatibility conditions between the ball introduced in Ref. [45] and an NO-behavior. Section IV considers the analog in the hybrid approach to LQC of the Ashtekar-Gupt vacuum that was finally selected in Ref. [46], proving that it does not belong to the original QHIH ball of states of Ref. [45]. In view of this result, in this section we also study the compatibility conditions between the original QHIH and an NO-behavior in hybrid LQC, showing that they are not exclusive. Section V contains our conclusions and further comments. Throughout this paper, we work in Planck units, setting $\hbar = c = G = 1$.

II. CONSTRUCTION OF THE ASHTEKAR-GUPT VACUUM

Given a real-valued function $s(\eta)$, where η is a time coordinate, let us consider all complex solutions of the following family of differential equations:

$$\mu_k'' + (k^2 + s)\mu_k = 0, \qquad k \in \mathbb{R}^+, \tag{2.1}$$

that satisfy the normalization condition,

$$\mu_k \bar{\mu}_k' - \mu_k' \bar{\mu}_k = i. \tag{2.2}$$

Here, the prime denotes the derivative with respect to the time η and the overhead bar indicates complex conjugation. On the other hand, let us consider a purely inhomogeneous real scalar field on $\mathbb{R}^4$ with Fourier coefficients labeled by a real wave vector $\vec{k} \in \mathbb{R}^3 - \{\vec{0}\}$ and satisfying Eq. (2.1) with $k = |\vec{k}|$. It is well known that any complete set $\{\mu_k\}_{k\in\mathbb{R}^+}$ of normalized solutions univocally defines a quantum Fock representation of the considered real scalar field [54]. Now, since Eq. (2.1) is linear and real, we may write its general complex solution as a linear combination of a particular solution and its complex conjugate [which are functionally independent in virtue of Eq. (2.2)]. It then follows that any two choices of basis elements, $\tilde{\mu}_k$ and μ_k, may be related to each other through a linear Bogoliubov transformation,

$$\tilde{\mu}_k(\eta) = \alpha_k(\tilde{\mu}_k, \mu_k)\mu_k(\eta) + \beta_k(\tilde{\mu}_k, \mu_k)\bar{\mu}_k(\eta). \tag{2.3}$$

The normalization condition (2.2) holds provided that the constant Bogoliubov coefficients satisfy

$$|\alpha_k(\tilde{\mu}_k, \mu_k)|^2 - |\beta_k(\tilde{\mu}_k, \mu_k)|^2 = 1, \qquad \forall\, k \in \mathbb{R}^+. \tag{2.4}$$

A choice of solutions $\{\mu_k\}_{k\in\mathbb{R}^+}$ is often called a basis of positive-frequency solutions, and it completely specifies a vacuum state from which the Fock space can be constructed. Henceforth, we refer to the vacuum state selected by a specific basis $\{\mu_k\}_{k\in\mathbb{R}^+}$ as $|0_\mu\rangle$.

In cosmological perturbation theory, both classically as well as for several approaches to quantum cosmology, an equation of the form (2.1) typically dictates the propagation of the mode coefficients of the real Mukhanov-Sasaki field that describes the gauge-invariant scalar perturbations [55–57]. Therefore, this equation is frequently called the Mukhanov-Sasaki equation. Moreover, the dynamics of the tensor perturbations are also ruled by an equation of this type [2]. The function $s(\eta)$ is commonly referred to as the (effective) mass of the perturbations, and it can be given as a function of the geometrical variables of the background on classical solutions or alternatively on quantum background states [19,25]. In this context, any choice of basis of positive-frequency solutions (or, equivalently, of their initial conditions) amounts to the choice of a specific vacuum state in the Fock quantization of the perturbations.

Let us define $\mu_k^{\eta_0}$ as the solution to Eq. (2.1) determined by the following initial conditions at any given time η_0:

$$\mu_k^{\eta_0}(\eta_0) = \frac{1}{\sqrt{2k}}, \qquad \mu_k^{\eta_0\prime}(\eta_0) = -i\sqrt{\frac{k}{2}}. \tag{2.5}$$

The basis constructed from such solutions $\mu_k^{\eta_0}$ for all k gives rise to the so-called adiabatic state of zeroth-order, $|0_{\mu^{\eta_0}}\rangle$ [41]. The family of adiabatic states of zeroth-order parametrized by η_0 has some interesting physical properties, as we have succinctly commented in the Introduction. One of these properties is that $|0_{\mu^{\eta_0}}\rangle$ is the unique state that exactly fulfills at time η_0 the QHIH formulated in Refs. [45,46]. In the case of tensor perturbations, this condition can be understood as an instantaneous quantum generalization of Penrose's Weyl curvature hypothesis that takes into account and minimizes the quantum uncertainties of the operators representing the Weyl tensor at η_0. Owing to the similarities between the dynamics of the tensor and scalar perturbations, the QHIH has also been proposed in order to select a preferred family of quantum states for the Mukhanov-Sasaki field [46].

Actually, the space of states allowed in the analysis of Ashtekar and Gupt is larger than the family of adiabatic states of zeroth-order that we have introduced. This is to cope with the fact that the dynamical evolution of the quantum field states is nontrivial in cosmological scenarios, something that leads to an instability of the instantaneous QHIH condition as time evolves. Explicitly, the QHIH is fulfilled at time η_0 by a normalized solution $\tilde{\mu}_k$ of Eq. (2.1) if and only if [45]

$$\Lambda_k(\tilde{\mu}, \eta_0) = 1, \qquad \Lambda_k(\tilde{\mu}_k, \eta) = k|\tilde{\mu}_k(\eta)|^2 + \frac{1}{k}|\tilde{\mu}_k'(\eta)|^2. \tag{2.6}$$

As commented above, this condition alone fixes $\tilde{\mu}_k = \mu_k^{\eta_0}$ (up to a constant phase that does not affect the definition of the corresponding vacuum). In fact, one may write Λ_k in terms of beta coefficients for Bogoliubov transformations to adiabatic states,

$$\Lambda_k(\tilde{\mu}_k, \eta) = 1 + 2|\beta(\tilde{\mu}_k, \mu_k^{\eta})|^2. \quad (2.7)$$

This implies that $\Lambda_k(\mu_k^{\eta_0}, \eta) > 1$ in general, for any $\eta \neq \eta_0$. In view of this property of the cosmological system, Ashtekar and Gupt generalized the instantaneous QHIH condition to a dynamical one by requiring that physically admissible vacuum states should belong to the set [45,46],

$$B = \{|0_{\tilde{\mu}}\rangle | \Lambda_k(\tilde{\mu}_k, \eta) \leq z_k, \quad \forall\, k \in \mathbb{R}^+, \eta \in I\}, \quad (2.8)$$

where I is certain compact interval of time, and we have defined the supremum,[2]

$$z_k = \sup_{\eta_0, \eta_1 \in I} \Lambda_k(\mu_k^{\eta_0}, \eta_1). \quad (2.9)$$

We will refer to the family of states B as the *total* Weyl uncertainty ball. Obviously, its construction depends on the choice of interval I. Since the QHIH is a generalization of Penrose's Weyl curvature hypothesis, which should only be applied in the high-curvature regime of spacetime, it is natural to demand that this interval coincides with the period where important quantum cosmological phenomena take place (the so-called Planck regime). Specifically, in Ref. [45] this interval was defined as the epoch in which the density of the Universe is higher than 10^{-4} Planck units.

In order to extract robust physical predictions from the theory, one needs to single out a preferred vacuum state within B by demanding a suitable behavior. According to Ref. [46], this preferred state must minimize the quantum dispersions of the field operators at the end of inflation, so that the state has optimal classical properties at times when the quantum effects should be negligible. In practice, it is a complicated task to find such a state starting from B (even from a numerical perspective). This difficulty was circumvented in Ref. [46] by instead searching for the vacuum among states that live in *instantaneous* Weyl uncertainty balls B_{η_0}, defined as follows:

$$B_{\eta_0} = \{|0_{\tilde{\mu}}\rangle | \Lambda_k(\tilde{\mu}_k, \eta_0) \leq z_k^{\eta_0} \quad \forall\, k \in \mathbb{R}^+\}, \quad (2.10)$$

where

$$z_k^{\eta_0} = \sup_{\eta \in I} \Lambda_k(\mu_k^{\eta}, \eta_0). \quad (2.11)$$

[2] This definition is consistent as long as $s(\eta)$ has no singularities in I. This is the case for LQC, where $s(\eta)$ is obtained from well-defined expectation values of quantum geometry operators.

According to Ref. [46], the state $|0_{\nu^{\eta_0}}\rangle$ that minimizes the quantum field dispersions at the end of inflation, within the instantaneous Weyl uncertainty ball B_{η_0}, has the form,

$$\nu_k^{\eta_0}(\eta) = \sqrt{1 + (r_k^{\eta_0})^2}\,\mu_k^{\eta_0}(\eta) + r_k^{\eta_0} e^{-i\theta_k^{\eta_0}} \bar{\mu}_k^{\eta_0}(\eta), \quad (2.12)$$

where

$$(r_k^{\eta_0})^2 = \frac{1}{2}(z_k^{\eta_0} - 1), \qquad \theta_k^{\eta_0} = \pi - 2 \arg[\mu_k^{\eta_0}(\eta_{\rm end})], \quad (2.13)$$

where $\eta_{\rm end}$ marks the end of inflation, $r_k^{\eta_0} \geq 0$, and arg denotes the argument of the complex quantity. Considering then all instantaneous Weyl uncertainty balls in the Planck regime, we have a one-parameter family of states that minimize the quantum dispersions at $\eta_{\rm end}$. The state corresponding to the global minimum is the unique Ashtekar-Gupt vacuum.[3]

III. QHIH: AMBIGUITIES IN ITS IMPLEMENTATION AND COMBINATION WITH THE NO-PROPOSAL

A. Difference between balls of states

As we have commented, the actual construction of the Ashtekar-Gupt vacuum state put forward in Ref. [46] does not start from the total Weyl uncertainty ball of states B, but rather from the union of instantaneous balls, $\cup_{\eta_0 \in I} B_{\eta_0}$. An important question that immediately arises is whether the two sets of states are equal. If this were the case, then the procedure followed in Ref. [46] to find the state with a maximally classical behavior at the end of inflation would be, without question, consistent with the QHIH originally proposed in Ref. [45] (and actually used as a motivation in Ref. [46]). In the following, we show that the answer is in the negative.

We begin by using Eq. (2.6) to rewrite the definition of B and B_{η_0} in terms of beta coefficients,

$$B_{\eta_0} = \{|0_{\tilde{\mu}}\rangle \,||\beta_k(\tilde{\mu}_k, \mu_k^{\eta_0})|^2 \leq \sup_{\eta \in I} |\beta_k(\mu_k^{\eta}, \mu_k^{\eta_0})|^2 \quad \forall\, k \in \mathbb{R}^+\}, \quad (3.1)$$

[3] In principle, there is no guarantee that there exists such global minimum simultaneously for all k. If this did not happen, one may instead choose the state $|0_{\nu^{\eta_0}}\rangle$ that minimizes a (suitably defined) average of the quantum dispersions over all of the modes. Alternatively, one may construct a new state by picking out each positive-frequency solution, among the two-parameter family $\{\nu_k^{\eta_0}\}$, that minimizes the quantum dispersions for each k separately. Unfortunately, by its construction, one cannot generally assure that the state that would result from this last procedure belongs to any of the instantaneous balls B_{η_0}. So, we will not consider this possibility in this paper.

$$B = \{|0_{\tilde{\mu}}\rangle \,|\, |\beta_k(\tilde{\mu}_k, \mu_k^{\eta})|^2 \leq \sup_{\eta_0,\eta_1 \in I} |\beta_k(\mu_k^{\eta_0}, \mu_k^{\eta_1})|^2 \quad \forall\, k \in \mathbb{R}^+, \quad \forall\, \eta \in I\}. \tag{3.2}$$

Given a compact interval I and any positive k there exist times η_-^k and η_+^k in I such that

$$|\beta_k(\mu_k^{\eta_-^k}, \mu_k^{\eta_+^k})|^2 = \sup_{\eta_0,\eta_1 \in I} |\beta_k(\mu_k^{\eta_0}, \mu_k^{\eta_1})|^2. \tag{3.3}$$

Considering a *fixed* (but otherwise generic) wave number $\tilde{k}$, let us then define a state $|0_{\mu^S}\rangle$ such that

$$\mu_k^S(\eta) = \bar{\alpha}_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}})\mu_k^{\eta_+^{\tilde{k}}}(\eta) + \beta_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}})\bar{\mu}_k^{\eta_+^{\tilde{k}}}(\eta). \tag{3.4}$$

This state belongs to the instantaneous ball $B_{\eta_+^{\tilde{k}}}$, which is by definition contained in the union $\bigcup_{\eta_0 \in I} B_{\eta_0}$. In order to show this, we first notice that

$$|\beta_k(\mu_k^S, \mu_k^{\eta_+^{\tilde{k}}})| = |\beta_k(\mu_k^{\eta_-^{\tilde{k}}}, \mu_k^{\eta_+^{\tilde{k}}})|, \tag{3.5}$$

as one can check using the general property $|\beta_k(\tilde{\mu}_k, \mu_k)| = |\beta_k(\mu_k, \tilde{\mu}_k)|$, which follows from Eqs. (2.3) and (2.4). Thus, for any k and taking into account the definition of supremum, it holds that

$$|\beta_k(\mu_k^S, \mu_k^{\eta_+^{\tilde{k}}})|^2 \leq \sup_{\eta \in I} |\beta_k(\mu_k^{\eta}, \mu_k^{\eta_+^{\tilde{k}}})|^2. \tag{3.6}$$

This inequality can at most be saturated, as it happens e.g., for $k = \tilde{k}$. Hence we conclude that, according to the definition of instantaneous ball given in Eq. (3.1), the state $|0_{\mu^S}\rangle$ belongs to $B_{\eta_+^{\tilde{k}}}$ as we wanted to show.

Now, we can write the basis element $\mu_k^{\eta_+^{\tilde{k}}}$ in terms of the Bogoliubov coefficients that relate it to $\mu_k^{\eta_-^{\tilde{k}}}$,

$$\mu_k^{\eta_+^{\tilde{k}}}(\eta) = \alpha_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}})\mu_k^{\eta_-^{\tilde{k}}}(\eta) + \beta_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}})\bar{\mu}_k^{\eta_-^{\tilde{k}}}(\eta). \tag{3.7}$$

Composing the transformations (3.7) and (3.4), we see that

$$\beta_k(\mu_k^S, \mu_k^{\eta_-^{\tilde{k}}}) = 2\bar{\alpha}_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}})\beta_k(\mu_k^{\eta_+^{\tilde{k}}}, \mu_k^{\eta_-^{\tilde{k}}}). \tag{3.8}$$

Therefore, focusing our discussion on the mode $k = \tilde{k}$, we have that

$$|\beta_{\tilde{k}}(\mu_{\tilde{k}}^S, \mu_{\tilde{k}}^{\eta_-^{\tilde{k}}})|^2 = 4|\alpha_{\tilde{k}}(\mu_{\tilde{k}}^{\eta_+^{\tilde{k}}}, \mu_{\tilde{k}}^{\eta_-^{\tilde{k}}})|^2 |\beta_{\tilde{k}}(\mu_{\tilde{k}}^{\eta_+^{\tilde{k}}}, \mu_{\tilde{k}}^{\eta_-^{\tilde{k}}})|^2 \geq 4 \sup_{\eta_0,\eta_1 \in I} |\beta_{\tilde{k}}(\mu_{\tilde{k}}^{\eta_0}, \mu_{\tilde{k}}^{\eta_1})|^2, \tag{3.9}$$

where we have used that the squared norm of the alpha-coefficient is never smaller than the unit because of the normalization condition (2.4). This inequality straightforwardly implies that $|0_{\mu^S}\rangle$ does not belong to B, and hence we have that $B \neq \bigcup_{\eta_0 \in I} B_{\eta_0}$. Of course, this does not mean that the intersection of these two sets is empty. In fact, we clearly have that any adiabatic state of zeroth-order $|0_{\mu^\eta}\rangle$, with $\eta \in I$, automatically belongs to both sets.

B. Nonoscillatory requirements for states in the Weyl uncertainty ball

The primordial power spectrum of the perturbations in a state $|0_{\tilde{\mu}}\rangle$ can be obtained from the evaluation of $|\tilde{\mu}_k|^2$ at the end of slow-roll inflation. The dynamical evolution of the perturbations from their initial conditions in the Planck regime to this stage when inflation ends can leave imprints that are potentially observable in the CMB. In particular, any oscillatory behavior of the amplitude of the positive-frequency solutions during the preinflationary evolution may affect the spectrum and, in this way, produce oscillations in it. These oscillations may be superimposed to the genuine imprints of the preinflationary dynamics of the Universe on the spectrum, including quantum gravity modifications, and blur them [51]. With this motivation in mind, Martín de Blas and Olmedo proposed a criterion to select a state with nonoscillatory behavior, called the NO-vacuum, which minimizes the oscillations in the spectrum over the interval between the time where the initial conditions are imposed and the onset of inflation [50]. The implementation of this criterion was generally numerical, in the way in which it was originally introduced.

More recently, it has been possible to derive some necessary conditions that an NO-vacuum has to satisfy. In detail, given an NO-vacuum $|0_{\mu^{NO}}\rangle$ (the existence of which is supported at least from a numerical perspective), we can write the squared amplitude of the basis of positive-frequency solutions associated with any other state $|0_{\tilde{\mu}}\rangle$ as [51],

$$|\tilde{\mu}_k|^2 = \frac{1}{2}|\mu_k^{NO}|^2[A + B + (A - B)\cos(2\phi_k) + 2C\sin(2\phi_k)], \quad \phi_k' = \frac{1}{2}|\mu_k^{NO}|^{-2}, \tag{3.10}$$

where A, B, and C are real constants, with $C^2 = AB - 1$. As long as there exists a sufficiently long regime in the evolution of the perturbations in which $2||\mu_k^{NO}|'|\mu_k^{NO}|| < 1$, it follows from this formula that any other NO-vacuum state must have constants A and B lying in a close neighborhood of the unit. The existence of such a regime is expected in any preinflationary cosmological evolution that resembles the Einsteinian one for a universe with a massless scalar field at low energy densities, as it is the case e.g., in interesting LQC scenarios [43,47]. This is because, in low-curvature regimes of general relativity where the energy density of the inflaton is dominated by its kinetic contribution, the mass $s(\eta)$ is a very slowly varying function of time [51,58].

Following these considerations, we can regard as a necessary condition for any candidate to be an NO-vacuum $|0_{\mu^{NO}}\rangle$ that it must satisfy $2||\mu_k^{NO}|'|\mu_k^{NO}|| < 1$ at least for all times η near the end of the Planck regime. Explicitly, if we write the basis of positive-frequency solutions $\{\mu_k^{NO}\}$ in the form [51],

$$\mu_k^{NO} = \frac{1}{\sqrt{-2\mathrm{Im}(h_k)}} e^{i\int_{\eta_1}^{\eta} d\tilde{\eta}\,\mathrm{Im}(h_k)(\tilde{\eta})}, \tag{3.11}$$

where η_1 is a reference time, irrelevant for the choice of vacuum state, and h_k is a solution to the Riccati equation

$$h_k' = k^2 + s + h_k^2 \tag{3.12}$$

with strictly negative imaginary part, then the aforementioned necessary condition on an NO-vacuum can be equivalently expressed as

$$|\mathrm{Re}(h_k)(\eta)| = \epsilon_k(\eta)|\mathrm{Im}(h_k)(\eta)| \quad \text{with} \quad 0 < \epsilon_k(\eta) < 1, \tag{3.13}$$

$$\left|\frac{k^2 + s(\eta)}{\mathrm{Im}(h_k)(\eta)} - [1+\epsilon_k^2(\eta)]\mathrm{Im}(h_k)(\eta)\right| < 1, \tag{3.14}$$

at least for all times η at the end of the Planck regime. Actually, we expect the above expressions involving h_k to be much smaller than the unity, in particular for the resulting value of ϵ_k.

One can use the Bogoliubov transformation between the NO-vacuum and a zeroth-order adiabatic state $|0_{\mu^\eta}\rangle$ to obtain that

$$|\mu_k^{NO}(\eta)| = \frac{1}{\sqrt{2k}}|\alpha_k(\mu_k^{NO},\mu_k^\eta) + \beta_k(\mu_k^{NO},\mu_k^\eta)|,$$
$$|\mu_k^{NO\prime}(\eta)| = \sqrt{\frac{k}{2}}|\alpha_k(\mu_k^{NO},\mu_k^\eta) - \beta_k(\mu_k^{NO},\mu_k^\eta)|. \tag{3.15}$$

These identities, combined with Eqs. (3.12) and (3.13), imply that

$$2\Lambda_k(\mu_k^{NO},\eta) = \frac{k}{|\mathrm{Im}(h_k)(\eta)|} + [1+\epsilon_k^2(\eta)]\frac{|\mathrm{Im}(h_k)(\eta)|}{k} \tag{3.16}$$

for times η at the end of the Planck regime.

Hence, given an interval I defining this Planck regime, a state satisfying the first necessary NO-vacuum condition (3.13) can belong to the total Weyl uncertainty ball B only if

$$\frac{k}{|\mathrm{Im}(h_k)(\eta)|} + [1+\epsilon_k^2(\eta)]\frac{|\mathrm{Im}(h_k)(\eta)|}{k} \leq 2z_k, \tag{3.17}$$

for all η at the end of I [and with $\epsilon_k(\eta)$ being small]. This inequality can be solved and leads to the following restriction:

$$[1+\epsilon_k^2(\eta)]|\mathrm{Im}(h_k)(\eta)| \in \left[kz_k - k\sqrt{z_k^2 - [1+\epsilon_k^2(\eta)]},\, kz_k + k\sqrt{z_k^2 - [1+\epsilon_k^2(\eta)]}\right]. \tag{3.18}$$

On the other hand, the second necessary condition (3.14) for an NO-vacuum is satisfied if and only if

$$[1+\epsilon_k^2(\eta)]|\mathrm{Im}(h_k)(\eta)| \in \left(\frac{1}{2}\sqrt{1+4[k^2+s(\eta)][1+\epsilon_k^2(\eta)]} - \frac{1}{2}, \frac{1}{2}\sqrt{1+4[k^2+s(\eta)][1+\epsilon_k^2(\eta)]} + \frac{1}{2}\right). \tag{3.19}$$

Recalling that ϵ_k is expected to be much smaller than the unity for an NO-vacuum, at leading order we can ignore the contribution of this parameter in the above expressions. With this approximation, it follows that the two necessary conditions for an NO-vacuum can only be compatible with the QHIH (as formulated in terms of the total ball B) if

$$\left[kz_k - k\sqrt{z_k^2-1},\, kz_k + k\sqrt{z_k^2-1}\right] \bigcap \left(\frac{1}{2}\sqrt{1+4[k^2+s(\eta)]} - \frac{1}{2}, \frac{1}{2}\sqrt{1+4[k^2+s(\eta)]} + \frac{1}{2}\right) \neq \emptyset, \tag{3.20}$$

for all instants of time η near the end of I. It is worth remarking that this interval I should cover all of the Planck regime, so that it smoothly connects with a kinetically dominated universe where, according to general relativity, the mass $s(\eta)$ varies very slowly over time.

One can similarly obtain a consistency requirement for a state that satisfies the necessary NO-vacuum conditions in order that it also belongs to the instantaneous Weyl uncertainty balls B_{η_0} for times η_0 close to the end of I: it suffices to replace η with η_0 and z_k with $z_k^{\eta_0}$ in Eq. (3.20).

Nonetheless, we will mainly focus our attention on the consistency of the nonoscillatory behavior with the QHIH formulated in terms of the total ball B. This is so because of two reasons. The first one is that this is the original formulation of the QHIH, motivated in Ref. [45] on fundamental issues. The second one is that, for the alternative formulation of the QHIH given in Ref. [46], our current analytic knowledge of the NO-vacua only allows us to study the consistency requirement on solid grounds for instantaneous Weyl uncertainty balls B_{η_0} defined at times η_0 that are near the end of the Planck regime.

IV. QHIH IN HYBRID LQC: COMPATIBILITY WITH THE NO-PROPOSAL

Our previous discussion is valid for any choice of mass $s(\eta)$ for the perturbations, provided that it is nonsingular in the time interval of interest, and that it varies slowly at the end of this interval. In the following we will focus our attention on the case that this mass is given by the evaluation on effective LQC backgrounds of the result of a hybrid quantization of the perturbed inflationary cosmology. In this hybrid approach, the Friedmann-Lemaître-Robertson-Walker (FLRW) background is quantized according to LQC, while the perturbations are treated with typical techniques of quantum field theory in curved spacetimes, more specifically by adopting a Fock description. If we consider certain quantum states for the background in LQC that are highly peaked in bouncing trajectories, the evaluation of background operators on these quantum states can be well approximated by considering the evaluation of their classical analogs on the peak trajectories. Actually, these peak trajectories follow the evolution dictated by an effective Hamiltonian constraint on the FLRW background. In this background, inflation is driven by a homogeneous scalar field subject to a potential, that we will particularize to a quadratic one for simplicity. In this setting, any background solution is completely fixed by the value of the inflaton field at an arbitrary initial time, e.g., at the bounce, and of its mass m. From a phenomenological point of view, in order to obtain power spectra that are compatible with the observations but still are capable of including traces of the LQC effects, the typical effective solutions that turn out to be interesting present a classical era shortly after the bounce in which the kinetic energy of the inflaton greatly dominates over its potential, era that extends almost until the onset of inflation [43,47]. This type of solutions is obtained for initial values of the inflaton at the bounce and values of its mass close to $\phi_B = 0.97$ and $m = 1.2 \times 10^{-6}$, data that we will adopt from now on for our analyses [43,58]. In the hybrid approach, the gauge-invariant perturbations that propagate on the above LQC backgrounds follow dynamical equations of the form (2.1).

We can numerically integrate the background evolution with the aforementioned initial conditions to obtain the value of the mass $s(\eta)$, and then apply the procedure that we have explained in Sec. II to determine the Ashtekar-Gupt vacuum in hybrid LQC. For this numerical integration, we use Verner's "most efficient" $9/8$ Runge-Kutta method (with a lazy nineth-order interpolant) [59,60]. To implement this procedure, we first need to characterize the Planck regime in a precise manner. According to the definition given by Ashtekar and Gupt, which requires values of the inflaton energy density above 10^{-4}, the conformal times that define the considered regime are $I_{PL} = [-4.2, 4.2]$ (with $\eta = 0$ corresponding to the bounce). Employing the interval $I = I_{PL}$, we can obtain values of the upper bounds $z_k^{\eta_0}$, for all $\eta_0 \in I_{PL}$, and z_k, which respectively define the instantaneous and total Weyl uncertainty balls B_{η_0} and B. As in the case of the dressed-metric approach to LQC [45,46], these bounds rapidly approach the unit for Fourier scales k that are much larger than the Planck scale, which is the characteristic order of magnitude of the spacetime curvature around the bounce in LQC. This behavior reflects the fact that the effects of the cosmological evolution on a zeroth-order adiabatic state are negligible in the ultraviolet regime, and hence the ultraviolet scales approximately remain in this vacuum state, thus satisfying the QHIH at all times. On the other hand, for scales of the Planck order and smaller, the effects of the cosmological evolution on the dynamics of a zeroth-order adiabatic state become increasingly important, and as a consequence the bounds $z_k^{\eta_0}$ and z_k grow above one in the infrared regime.

With the obtained values of the bounds $z_k^{\eta_0}$ that characterize the instantaneous uncertainty balls B_{η_0} in hybrid LQC, we can determine the initial conditions that correspond to the one-parameter family of states $|0_{\nu^{\eta_0}}\rangle$ with maximal classical behavior at the end of inflation. Indeed, in view of Eqs. (2.12) and (2.13) determining such states, the only additional data that we need are the phases of the adiabatic solutions $\mu_k^{\eta_0}$ at the end of inflation, which we compute numerically. As we explained in Sec. II, the vacuum state that Ashtekar and Gupt would propose as preferred, according to Ref. [46], should lie in the resulting family of states. Recalling that the QHIH was originally formulated in terms of the total uncertainty ball B which, as we have shown in Sec. III A, is different to the union of instantaneous balls $\bigcup_{\eta_0\in I_{PL}} B_{\eta_0}$, the following question naturally arises: does the family of states $\{|0_{\nu^{\eta_0}}\rangle\}_{\eta_0\in I_{PL}}$ actually belong to B, within the hybrid LQC framework? According to the definition given in Eq. (2.8) for this total ball, the considered states belong to B if and only if, for each $\eta_0 \in I_{PL}$, we have

$$(z_k)^{-1} \max_{\eta\in I_{PL}} \Lambda_k(\nu_k^{\eta_0}, \eta) \leq 1, \tag{4.1}$$

for all $k \in \mathbb{R}^+$. In Fig. 1 we plot this function of η_0 for two representative values of k, showing that the above

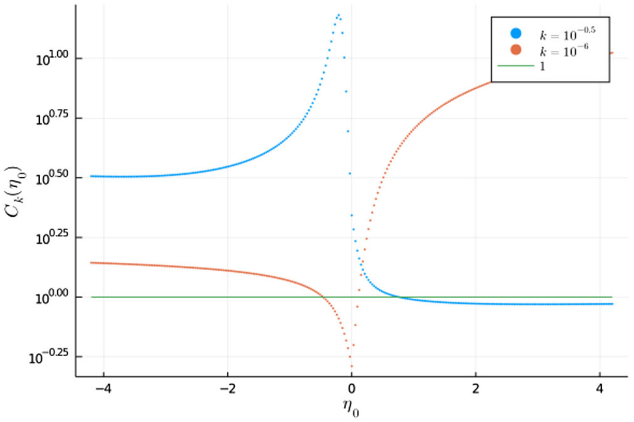

FIG. 1. The quantity $C_k(\eta_0) = (z_k)^{-1} \max_{\eta\in I_{PL}} \Lambda_k(\nu_k^{\eta_0}, \eta)$ compared with 1 for $k = 10^{-6}$ and $k = 10^{-0.5}$. There exists no value of η_0 such that the two curves remain below or equal to 1, a fact that implies that no state $\nu_k^{\eta_0}$ lives in B.

requirement cannot be met for any time η_0 in the Planck regime. Therefore, in the case of hybrid LQC, the vacuum state proposed by Ashtekar and Gupt in Ref. [46] does not belong to the total Weyl uncertainty ball that was originally motivated by the QHIH. From this perspective, the oscillatory behavior that is expected for this vacuum (taking into account its analog in dressed-metric LQC) does not imply an incompatibility between the NO-criterion and the original implementation of the QHIH when combined with a maximal classical behavior at the end of inflation.

This result further supports our decision to focus the attention on vacua belonging to the total uncertainty ball B,

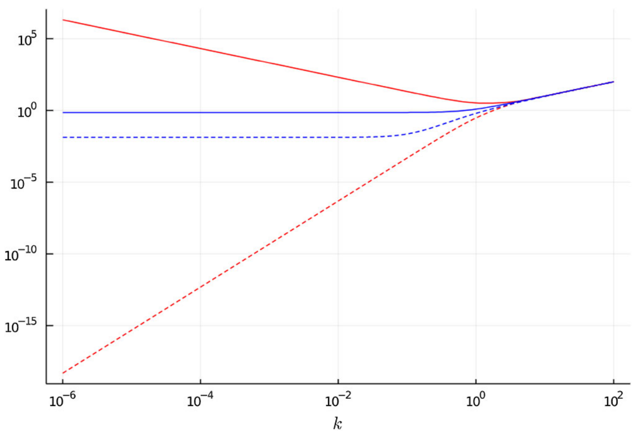

FIG. 2. The bounds imposed by the Weyl uncertainty ball, $k(z_k - \sqrt{z_k^2 - 1})$ and $k(z_k + \sqrt{z_k^2 - 1})$, in red dashed and solid lines respectively, compared with the bounds imposed by the NO-condition, $\frac{1}{2}\sqrt{1 + 4[k^2 + s(\eta)]} - \frac{1}{2}$ and $\frac{1}{2}\sqrt{1 + 4[k^2 + s(\eta)]} + \frac{1}{2}$, in blue dashed and solid lines respectively, for different modes k. These are evaluated for the mass $s(\eta)$ obtained in the hybrid approach to LQC, where $I = I_{PL} = [-4.2, 4.2]$ and $\eta = 4.2$, time near which the mass varies slowly. The intersection given by these bounds is not empty for any k.

when studying the compatibility of the QHIH with the necessary NO-vacuum conditions in hybrid LQC. According to our discussion in Sec. III B, in order to do this we just have to particularize the intervals appearing in Eq. (3.20) to the case of hybrid LQC and check that their intersection is nonempty. All the ingredients needed for this test, namely the mass $s(\eta)$ and the upper bound z_k, are readily available from our previous computations. In Fig. 2 we plot the curves that limit these two intervals at the representative time $\eta = 4.2$ that marks the end of the Planck regime I_{PL}. We clearly see that their intersection is not empty, indicating the compatibility between the QHIH and the NO-criterion for the choice of a vacuum state of the cosmological perturbations in hybrid LQC. Actually, in the infrared regime (which is where oscillations can appear for the considered type of states [43]) the z_k-independent interval related with the NO-condition is contained in the interval that corresponds to the original version of the QHIH. Therefore, it follows that any state that is an NO-vacuum satisfies this version of the QHIH at least at the end of the Planck regime.

V. CONCLUSIONS

With a combination of analytical and numerical means, we have investigated the compatibility between the QHIH proposed by Ashtekar and Gupt [45,46] and the NO-proposal for the choice of initial conditions on primordial perturbations in quantum cosmology [50,51]. In order to do this, we have examined in detail the construction that Ashtekar and Gupt employed to determine their vacuum state, and we have discussed a step that is not univocal and its consequences. In addition, we have derived some analytical conditions that a vacuum state must satisfy to comply with the original formulation of the QHIH introduced in Ref. [45] and with the NO-condition. We have followed the Asthekar-Gupt proposal, adapted to hybrid LQC, in the phenomenologically interesting case with a kinetically dominated preinflationary era. We have shown that the vacuum selected by the Ashtekar-Gupt construction in fact lies outside the ball of states that satisfy the QHIH according to the prescription of Ref. [45], where it was motivated as a quantum generalization of Penrose's Weyl curvature hypothesis. Because of this, we have focused our attention on the properties of the states in this last ball, showing that the original formulation of the QHIH is perfectly compatible with an NO-behavior.

More specifically, our starting point has been a careful revisitation of the entire Ashtekar-Gupt proposal, applicable for any real-valued (and nonsingular) function that plays the role of a time-dependent mass in the dynamical equations of the Fourier modes of the perturbations, which have the form of generalized harmonic oscillator equations. By translating Penrose's hypothesis to the quantum realm, one then defines a Weyl uncertainty ball for the states of the perturbations such that they all fulfill the QHIH in a specific interval of time [45]. Since this hypothesis is formulated for high-curvature regimes, this interval is chosen as the Planck regime in which quantum gravity effects are truly important. To extract meaningful predictions, a unique preferred state must be chosen from the ball obtained for the Planck interval: this is the state with a maximal classical behavior at times when quantum effects have become irrelevant, e.g., the end of inflation for concreteness. Finding this state directly with numerical methods is a very complicated task. As an alternative route, in Ref. [46] Ashtekar and Gupt opted to instead consider instantaneous Weyl uncertainty balls, defined at each instant of time in the studied interval. In this manner, one characterizes in an analytical way a one-parameter family of states, namely, one with maximal classical behavior for each instantaneous ball. Among them, one should numerically find the state with best classical properties and identify it with the Ashtekar-Gupt vacuum.

The need to replace the ball of states originally determined by the QHIH by its instantaneous counterparts can give rise to questions about the real habitat of the Ashtekar-Gupt vacuum and to ambiguities in its construction, if these balls are different. In fact, in this work we have shown that the original Weyl uncertainty ball is actually different to the union of all its instantaneous counterparts. It is worth remarking that our proof is independent of the specific form of the mass of the perturbations, the choice of compact interval for the definition of the Planck regime, and the wave number of the Fourier mode. In addition, we notice that our proof does not exclude the fact that the two considered sets of states, even if different, have a nonempty intersection (e.g., adiabatic states of zeroth-order do belong to both sets). For a fixed functional form of the time-dependent mass of the perturbations, it is then legitimate to ask whether any of the states with maximal classical behavior in the instantaneous balls belongs to the original Weyl uncertainty ball. To get an answer in the case of the mass function derived in hybrid LQC, we have explicitly evaluated all these possible vacuum candidates of Ashtekar-Gupt type and shown that they do not belong to the ball obtained with the original implementation of the QHIH.

On the other hand, a physically relevant question one may ask to any viable choice of vacuum state is whether or not it leads to a highly oscillatory power spectrum. This oscillatory behavior can be considered an undesirable property inasmuch as it may blur away any modification to the primordial power spectrum that is ultimately caused by quantum geometry corrections [51]. Actually, it is clear from the analysis carried out by Ashtekar and Gupt that these oscillations indeed appear in the dressed-metric approach for their choice of vacuum [46] (and a similar behavior can be expected for hybrid LQC). Our result shows, nonetheless, that in hybrid LQC this vacuum is outside of the ball of states that was introduced to comply with the fundamentals of the QHIH. This new perspective has led us to wonder whether the basic requirements on this set of admissible states are compatible with a nonoscillatory behavior of (at least) a subset of them. In order to answer this question, we have derived an analytical compatibility condition between these two types of requirements and then have proceeded to check it in hybrid LQC. The result is satisfactory, from a theoretical perspective. Not only the QHIH is compatible with an NO-behavior but, furthermore, any NO-vacuum fulfills the QHIH at least at the end of the Planck regime.

The conclusions of this work are an important advance towards the theoretical motivation and determination of a preferred vacuum for the perturbations and the extraction of the corresponding physical predictions in (loop) quantum cosmology. Given two well-motivated criteria for the restriction of physically sound vacuum states (the QHIH proposed by Ashtekar and Gupt and the NO-criterion proposed by Martín de Blas and Olmedo), both of which lead to predictions that are compatible with observations [6,50,58], testing and ensuring their compatibility is a key step to understand which physical conditions determine the quantum state of the primordial perturbations that explains the power spectrum that we observe nowadays in the CMB. This knowledge is paramount to investigate and falsify on a robust basis the phenomenological predictions that follow from any theory of quantum cosmology, since an inappropriate choice of vacuum state can hide or misreflect the imprints that the genuine quantum cosmological dynamics may have left on the primordial fluctuations.

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Correction: Equation (2.12) contained an error that had consequences for the numerical computation in Fig. 1. Both the equation and figure have been been fixed.

Backreaction of fermionic perturbations in the Hamiltonian of hybrid loop quantum cosmology

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We discuss the freedom available in hybrid loop quantum cosmology to define canonical variables for the matter content and investigate whether this can be used to derive a quantum field theory with good properties for the matter sector. We study a primordial, inflationary, cosmological spacetime with inhomogeneous perturbations at lowest nontrivial order, and focus our attention on the contribution of minimally coupled fermionic perturbations of Dirac type. Within the framework of the hybrid quantization, we analyze the different possible separations of the homogeneous background and the inhomogeneous perturbations, by means of canonical transformations that mix the two separated sectors. These possibilities provide a family of sets of annihilation and creationlike fermionic variables, each of them with a different associated contribution to the total Hamiltonian. In all cases, imposing the quantum constraints and introducing a Born-Oppenheimer approximation, one can derive a Schrödinger equation for the fermionic part of the wave functions. The resulting evolution turns out to be generated, for each of the allowed choices of variables, by a version of the fermionic contribution to the Hamiltonian which is obtained by evaluating all the dependence on the homogeneous geometry at quantum expectation values. This equation contains a term that encodes the backreaction of the fermionic perturbations on the quantum dynamics of the homogeneous sector. We analyze this backreaction by solving the associated Heisenberg evolution of the fermionic annihilation and creation operators. Then, we identify the conditions that the choice of those operators must satisfy in order to lead to a finite backreaction. Finally, we discuss further restrictions on this choice so that the fermionic Hamiltonian that dictates the Schrödinger dynamics is densely defined in Fock space.

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I. INTRODUCTION

In conventional quantum theories of matter fields, one employs, in one way or another, some type of renormalization or regularization procedure to obtain physically acceptable results. Such techniques are especially well understood when it comes to (perturbatively) describing the nongravitational interactions contained in the standard model of particle physics. Nonetheless, the issue exceeds this traditional framework in high energy physics. Actually, divergences become even more severe when one considers matter fields propagating in generally curved spacetimes, as it is allowed by Einstein's theory. In those cases, one usually considers that the matter fields are coupled gravitationally to the spacetime, which is viewed as a classical entity. Besides, one frequently neglects the contribution of the fields to the dynamics of the spacetime geometry itself. In such scenarios, infinities generically arise in the quantum theories that describe the matter fields. This problem has been studied in depth over the last decades (see, e.g., Refs. [1–11]), and it is commonly believed that the reasons behind it can be traced to the treatment of the spacetime as a classical, continuum background.[1] In particular, this type of spacetime description triggers the appearance of ill-defined products of field operators, which typically include the building blocks of the free field Hamiltonian in the considered background (and thus of the energy in stationary situations).

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[1]We are deliberately avoiding any mention to the so-called infrared divergences in quantum field theory. If necessary, they can be prevented by, e.g., considering topologically compact spatial hypersurfaces in the considered spacetimes.

Despite the considerable effort devoted to develop covariant renormalization techniques, even for free fields in curved spacetimes, one could be tempted to believe that, instead of recurring to those schemes for the "substraction of infinities," a formalism that satisfactorily accounts for the presumable quantum nature of the spacetime would be able to prevent the occurrence of divergencies in the first place. In this sense, the role that a theory of quantum gravity might play in surpassing the limits of predictability of our current theoretical models could be twofold, actually, because it might also cure the problem of formation of spacetime singularities that is intrinsic to classical general relativity [12].

A promising candidate for the quantization of Einstein's theory is the nonperturbative and canonical formalism known as loop quantum gravity [13]. To make direct contact with physically feasible models, the techniques developed in this formalism have been used, suitably combined with more conventional Fock quantization methods, in order to describe certain types of inhomogeneous spacetimes quantum mechanically. This procedure has been given the name of hybrid quantization, and it has been primarily applied to cosmological scenarios [14–18]. Essentially, this hybrid approach is based on a convenient splitting of the cosmological phase space into two sectors: a purely homogeneous one, that is represented in a quantum mechanical way by employing methods that are inspired in loop quantum gravity, and an inhomogeneous sector, for which a suitable Fock representation is adopted. In fact, the application of loop quantum gravity techniques to the quantization of homogeneous cosmologies, often known as loop quantum cosmology [19–21], has been shown to lead to a quite general resolution of the cosmological singularities predicted by general relativity [22,23]. Remarkably, the big bang singularity is replaced with a bounce in the trajectories followed by the peaks of a wide class of quantum states in the homogeneous cosmologies studied so far in the literature (see, e.g., Refs. [24–26]).

The hybrid quantization approach extends to inhomogeneous models the expectation that, with a loop quantum cosmology representation of the homogeneous sector of the geometry, one should be able to solve (at least) the most severe singularities of a genuine cosmological nature. At the same time, this hybrid strategy gives hope for the possibility that a suitably chosen Fock representation for the inhomogeneous sector of the phase space may complete the quantum description of the system in a divergence-free way. This possibility is motivated by the existing freedom in performing canonical transformations within the entire phase space, transformations that assign different dynamical roles to the homogeneous sector of the system and to the rest of matter and gravitational degrees of freedom (d.o.f.). Indeed, these transformations change the part of the total Hamiltonian (constraint) that, while retaining the coupling with the homogeneous sector, generates the dynamics of the inhomogeneous, fieldlike d.o.f.. Given that each sector of the phase space is quantized in a different type of representation, it is then possible that a suitable choice of canonical transformation and Fock representation for the inhomogeneities may yield a quantum description that is free of the divergences that would otherwise appear in standard quantum field theory in curved spacetimes. In particular, this procedure would allow us to handle properly (at least certain forms of) the matter-geometry backreaction in a quantum mechanical way.

The aim of this work is to provide solid ground for our expectations by showing, in a specific cosmological system, that one can attain such a well-defined quantum hybrid description without the need of any regularization. The case that we discuss here is an inflationary homogeneous and isotropic cosmology in the presence of Dirac fermions, considered as perturbations. The hybrid quantization of this system was introduced in Ref. [27], allowing also for the presence of scalar and tensor perturbations of the metric and of the inflaton field, and after truncating the action at second order in all the perturbations. As far as the Dirac perturbations are concerned, the splitting of the (truncated) phase space adopted in that reference was inspired by the pioneer work in Ref. [28] about fermions in quantum cosmology, developed in the context of quantum geometrodynamics. It was seen in Ref. [27] that, by adopting a separation of variables between the homogeneous part of the geometry, on the one hand, and the inhomogeneities, on the other hand, in the dependence of the quantum states (separation that can be viewed as a kind of Born-Oppenheimer *ansatz* in which the inflaton field plays the role of an internal time), it is possible to derive a quantum evolution for the fermionic perturbations that is ruled by a Schrödinger-like equation. Actually, the resulting dynamics is generated by the fermionic contribution to the total Hamiltonian (constraint), converting the coupling of the fermionic perturbations with the homogeneous geometry into expectation values of the corresponding geometric operators. In addition, the expectation value of this total Hamiltonian supplies information about the backreaction of the fermions (and of the rest of perturbations) on the homogeneous background. This information is given by the difference between the average of two operators on the homogeneous part of the state, difference that tells us whether such a quantum state is an exact solution of the unperturbed model or not. It was then proven in the cited work that the discussed evolution of the fermionic perturbations can be implemented unitarily in Fock space. Furthermore, explicit solutions were found by constructing an evolution operator and evolving the fermionic vacuum with it. However, it was shown that the mentioned Hamiltonian contribution of the fermionic d.o.f. intrinsically leads to divergences (of an ultraviolet nature), with an infinite backreaction, unless one introduces a convenient regularization procedure.

In this article, we present an alternative and, at the same time, rather generic description of the system that resolves the problem of the divergences encountered in Ref. [27]. We do so by employing in our benefit the commented freedom in adopting different dynamical splittings between the homogeneous geometric background and the fermionic perturbations, related by canonical transformations. It suffices to restrict our discussion to choices of annihilation and creationlike variables for the fermionic fields such that, when the spacetime background is considered to be classical and the fermions are treated in the context of quantum field theory in curved spacetimes, the quantum dynamics becomes unitarily implementable in Fock space (while being nontrivial according to the evolution dictated by the Dirac equation) [29]. It has been shown that all such variables define unitarily equivalent Fock representations of the Dirac field, once a convention for the notions of particles and antiparticles has been set [29]. In fact, the variables introduced in Ref. [28] and then used in Ref. [27] satisfy this unitarity condition. We characterize here the set of such annihilation and creationlike variables for which the description of the system is free of the divergences of standard quantum field theory. From a conceptual viewpoint, this result may have important implications. Moreover, it will shed light on the problem of the choice of a unique vacuum for the Dirac field in quantum cosmology (among all those available in our unitary class of Fock representations) with good physical properties.

The structure of the paper is the following. In Sec. II we summarize the description of the classical system presented in Ref. [27], and then introduce a more general class of annihilation and creationlike variables for the Dirac field than those adopted in that reference. With those definitions at hand, we compute the Hamiltonian that generates the associated fermionic dynamics. We start Sec. III with a brief review of the procedure to derive the corresponding Schrödinger equation for the fermionic d.o.f., after adopting a kind of Born-Oppenheimer ansatz for the physical states. In addition, we analyze the ultraviolet properties of the fermionic dynamics and deduce the conditions that the annihilation and creationlike variables must fulfil in order that their backreaction be finite. Finally, we further impose that the Hamiltonian that drives this evolution be a well-defined operator on the fermionic vacuum and, as a consequence, a densely defined operator in Fock space. We conclude in Sec. IV with a summary of our results and a brief outlook.

II. THE CLASSICAL SYSTEM

In this section we use the conventions and notation of Ref. [27]. We refer the reader to that work for specific derivations and formulas. The starting point for the construction of the system is a Friedmann-Lemaître-Robertson-Walker (FLRW) spacetime with flat and compact spatial hypersurfaces (isomorphic to a three-torus, T^3). We employ spatial coordinates adapted to the homogeneity. The matter content is given by a homogenous scalar field subject to a potential (that, classically, would play the role of the inflaton), and a Dirac field, both of them minimally coupled. The Dirac field is treated entirely as a perturbation. Besides, we can introduce perturbations of the metric and of the scalar field, as discussed in Refs. [27,30,31].

More specifically, we truncate our perturbed system so that its Einstein-Dirac action is at most quadratic in all the perturbations [28,32]. Our canonical formulation is obtained from the symplectic structure and from the Hamiltonian associated with this truncated action. Within this truncation scheme, and regardless of the consideration or not of additional perturbations, the Dirac field couples exclusively to the homogeneous tetrad that describes the FLRW sector of the cosmology, because the Dirac action is already quadratic in the fermionic field. This fact immediately implies that the fermionic d.o.f. are gauge invariant, at the considered perturbative order. Namely, they commute under Poisson brackets with the linear perturbative (Hamiltonian and diffeomorphisms) constraints of the relativistic system. On the other hand, together with an Abelianization of these linear perturbative constraints and suitable momenta of them, it is possible to construct a completely gauge-invariant parametrization of the sector of the phase space that contains the physical information about the metric and scalar field perturbations, as explained in Refs. [30,31]. In particular, this information can be encoded in a set of variables that consists of the well-known tensor and Mukhanov-Sasaki gauge invariants [33–37]. To arrive at this description of the perturbations, one introduces linear transformations on the original perturbative variables, transformations which depend on the homogeneous sector of the phase space. It is then possible to complete the change of variables to include this homogeneous sector as well and obtain a canonical set for the entire system, again at the considered truncation order in perturbations. As a result, the new canonical variables for the homogeneous d.o.f. acquire a (spatially integrated) correction which is quadratic in the metric and inflaton perturbations. In the case of the Dirac field, given its consideration as a perturbation and the fact that its contribution to the action is quadratic, one finds within our truncation scheme that the expression of the Dirac Hamiltonian in terms of the new homogeneous tetrads amounts just to a minimal coupling of the fermions directly with such new variables.

To exploit the spatial symmetries associated with the homogeneous foliation of the unperturbed sector of our model, that is, the FLRW cosmology, it is most convenient to expand the perturbations in spatial modes (of the Laplace-Beltrami or Dirac operators) on T^3. For the fermionic content, in particular, each of the two chiral components of the Dirac field may be expanded in a complete set of eigenspinors of the Dirac operator on T^3, after imposing the time gauge on the homogeneous tetrads (e.g., by considering a diagonal gauge) [28]. The spectrum of that operator is discrete and characterized by eigenvalues $\pm\omega_k = \pm 2\pi|\vec{k}+\vec{\tau}|/l_0$, where l_0 is the compactification length of the tori, $\vec{k}\in\mathbb{Z}^3$, and $2\vec{\tau}$ can be any of the constant vectors that form the standard orthonormal basis of the lattice $\mathbb{Z}^3$ and that characterize each of the eight possible spin structures on T^3 [38,39]. Since ω_k grows like $|\vec{k}|$ when this quantity tends to infinity, the density of states with eigenvalues in an interval $(\omega_k, \omega_k+\Delta\omega_k]$ grows asymptotically as $\omega_k^2\Delta\omega_k$ multiplied by a constant. Then, let us consider the Dirac field multiplied by the rescaling factor $e^{3\alpha/2}$, where α is, up to an additive constant, the logarithm of the scale factor of the FLRW cosmology, once we have corrected it with quadratic contributions of the perturbations as we have commented above. In the expansion of the left-handed component of such rescaled Dirac field, we call $m_{\vec{k}}$ and $\bar{r}_{\vec{k}}$, up to a multiplicative constant $[4\pi/(3l_0)]^{-3/4}$, the time-dependent coefficients of the eigenspinors of the Dirac operator on T^3 with respective eigenvalues ω_k and $-\omega_k$. Similarly, $\bar{s}_{\vec{k}}$ and $t_{\vec{k}}$ respectively denote the coefficients, up to the mentioned constant factor, of the complex conjugates of the eigenspinors with eigenvalues ω_k and $-\omega_k$ in the expansion of the right-handed component of the rescaled Dirac field. All of these eigenspinor coefficients are taken as Grassmann variables [40], in order to capture the anticommuting nature of the field. Besides, each of them forms a canonical pair with its complex conjugate, with a Dirac bracket (obtained after eliminating second-class constraints that relate the Dirac field with its momentum) equal to $-i$, and vanishing anticommutation relations with the rest of coefficients. Introducing these mode decompositions in the action, one obtains the fermionic contribution to the total Hamiltonian. This contribution is quadratic in the fermionic variables, and is given by a sum over all modes, which decouple from each other. It comes multiplied by the homogeneous lapse function N_0, so we call it $N_0 H_D$. As expected, this fermionic term adds to the zero mode of the Hamiltonian constraint, which is therefore the only constraint affected.

A. Instantaneous diagonalization of the Dirac Hamiltonian

As commented in the introduction, and partially motivated by the work of D'Eath and Halliwell [28], the following annihilation and creationlike variables were chosen in Ref. [27] for the description of the fermionic d.o.f.:

$$\breve{a}^{(x,y)}_{\vec{k}} = \sqrt{\frac{\xi_k-\omega_k}{2\xi_k}}x_{\vec{k}} + \sqrt{\frac{\xi_k+\omega_k}{2\xi_k}}\bar{y}_{-\vec{k}-2\vec{\tau}},$$
$$\bar{\breve{b}}^{(x,y)}_{\vec{k}} = \sqrt{\frac{\xi_k+\omega_k}{2\xi_k}}x_{\vec{k}} - \sqrt{\frac{\xi_k-\omega_k}{2\xi_k}}\bar{y}_{-\vec{k}-2\vec{\tau}}, \tag{2.1}$$

where $(x_{\vec{k}}, y_{\vec{k}})$ is any of the ordered pairs $(m_{\vec{k}}, s_{\vec{k}})$ or $(t_{\vec{k}}, r_{\vec{k}})$, and $\breve{a}^{(x,y)}_{\vec{k}}$ and $\bar{\breve{b}}^{(x,y)}_{\vec{k}}$ correspond to annihilationlike variables for particles and creationlike variables for antiparticles, respectively. Besides, an overbar denotes complex conjugation, and we have defined

$$\xi_k = \sqrt{\omega_k^2 + \tilde{M}^2 e^{2\alpha}}, \tag{2.2}$$

where $\tilde{M} = 2M\sqrt{\pi/(3l_0^3)}$ is the mass M of the Dirac field up to a multiplicative constant [27]. Notice that then the square roots appearing in Eq. (2.1) are always well defined and real. The variables (2.1) are distinguished (apart from irrelevant redefinitions among degenerate modes) by the fact that they diagonalize H_D (if one ignores the $\vec{k}=\vec{\tau}$ mode[2]). This diagonalization means that no term containing creation or annihilation of particle-antiparticle pairs appears in the resulting expression of H_D. More specifically, if we call $H_{\vec{k}}$, with $\vec{k}\neq\vec{\tau}$, each of the terms in the sum that forms H_D, we get

$$H_{\vec{k}} = \frac{e^{-\alpha}}{2}\sum_{(x,y)}[\xi_k(\bar{\breve{a}}^{(x,y)}_{\vec{k}}\breve{a}^{(x,y)}_{\vec{k}} - \breve{a}^{(x,y)}_{\vec{k}}\bar{\breve{a}}^{(x,y)}_{\vec{k}} + \bar{\breve{b}}^{(x,y)}_{\vec{k}}\breve{b}^{(x,y)}_{\vec{k}} - \breve{b}^{(x,y)}_{\vec{k}}\bar{\breve{b}}^{(x,y)}_{\vec{k}})], \tag{2.3}$$

where the sum over (x,y) is over the pairs (m,s) and (t,r). Although this diagonalization might seem appealing, it turns out that the introduction of these annihilation and creationlike variables gives rise to the appearance of an additional, nondiagonal, quadratic contribution to the fermionic part of the Hamiltonian of the system. This is due to the fact that the definition (2.1) is a background-dependent linear transformation of the fermionic mode coefficients, inasmuch as it involves the homogeneous variable α. In fact, it is not hard to see that the transformation is canonical when restricted to the fermionic sector of the phase space. However if, adopting the strategy of the hybrid approach, one wants a transformation that respects the canonical symplectic structure of the entire set of d.o.f. at the considered order of truncation, then the momentum of α must be modified with the addition of a factor that is quadratic in the fermionic perturbations, according to our previous comments. If we call $\breve{\pi}_\alpha$ this new canonical momentum, the expression of the total Hamiltonian in terms of the new canonical variables is functionally the same as in terms of the old homogeneous ones, but with an additional sum over $\vec{k}$ of the following contributions [27]:

[2]This particular contribution to H_D is only present when a trivial spin structure is chosen on T^3, and it corresponds to $\omega_k = 0$. We safely ignore it throughout this work since, owing to the compactness of the spatial sections, it can be isolated from the rest of contributions and be handled without producing infrared divergences.

$$-iN_0\sum_{(x,y)}\frac{\tilde{M}\omega_k}{2\xi_k^2}e^{-2\alpha}\breve{\pi}_\alpha(\breve{a}_{\vec{k}}^{(x,y)}\breve{b}_{\vec{k}}^{(x,y)}+\bar{\breve{a}}_{\vec{k}}^{(x,y)}\bar{\breve{b}}_{\vec{k}}^{(x,y)}). \quad (2.4)$$

The coefficient of each of these "interaction" terms, that produce the creation and annihilation of pairs, decays asymptotically as ω_k^{-1}. As shown in Ref. [27], this asymptotic behavior is transmitted to the quantum theory [at least in regimes where the state for the homogeneous geometry experiences (almost) no transition mediated by the total Hamiltonian, so that the geometric information can be encoded in expectation values on this state]. This asymptotic behavior, together with the specific dependence on ω_k, α, and $\tilde{M}$ of the part of $H_{\vec{k}}$ which is asymptotically dominant, is what at the end of the day guarantees that the fermionic quantum dynamics can be implemented unitarily in Fock space. Nonetheless, the fact that the discussed interaction terms decay as ω_k^{-1} in the ultraviolet regime, and not faster, is precisely what leads to a possibly divergent backreaction on the state of the homogenous geometry. Indeed, such backreaction was seen to be a sum over $\vec{k}$ of terms of dominant order equal to ω_k^{-3}, which is not absolutely convergent, given the quadratic growth of the density of states (see e.g., Refs. [41,42] for additional details concerning the convergence of mode-dependent series in T^3).

B. Alternative choices of fermionic variables

In order to explore whether other choices of fermionic variables may elude the appearance of divergences in the quantum field theory treatment, in this section we consider a rather generic family of alternative definitions of annihilation and creationlike variables for the Dirac field. For this purpose, we exploit the freedom to perform linear canonical transformations of the fermionic variables that depend on the homogeneous background geometry. In doing it, we are contemplating the possibility of considering different dynamical splittings between the background geometry and the genuine fermionic d.o.f. This possibility comes naturally on stage when one aims at constructing a quantum mechanical description of the system as a whole, following a hybrid scheme in which the homogeneous sector of the phase space is represented in a fundamentally different manner.

Obviously, when one adopts this perspective, the choice of fermionic variables is affected by a vast ambiguity. This ambiguity can be viewed as twofold. On the one hand, there are certainly many ways of redefining the dynamical behavior of the fermionic excitations (and, correspondingly, of the cosmological variables) by plugging different dependencies on α and its momentum π_α in the linear canonical transformations that define the fermionic variables. On the other hand, even after a dynamical splitting has been set, choices of fermionic annihilation and creationlike variables related by constant transformations can give rise to different, and in many cases inequivalent, Fock representations, each with its associated vacuum. Actually, both types of ambiguities can be analyzed simultaneously, restricting to choices that respect the dynamical decoupling between modes, by introducing generic annihilation and creationlike variables of the form

$$a_{\vec{k}}^{(x,y)}=f_1^{\vec{k},(x,y)}(\alpha,\pi_\alpha)x_{\vec{k}}+f_2^{\vec{k},(x,y)}(\alpha,\pi_\alpha)\bar{y}_{-\vec{k}-2\vec{\tau}},$$
$$\bar{b}_{\vec{k}}^{(x,y)}=g_1^{\vec{k},(x,y)}(\alpha,\pi_\alpha)x_{\vec{k}}+g_2^{\vec{k},(x,y)}(\alpha,\pi_\alpha)\bar{y}_{-\vec{k}-2\vec{\tau}}, \quad (2.5)$$

where, to satisfy the standard canonical anticommutation relations, one must have [27]

$$g_1^{\vec{k},(x,y)}=e^{iJ_{\vec{k}}^{(x,y)}}\bar{f}_2^{\vec{k},(x,y)}, \quad g_2^{\vec{k},(x,y)}=-e^{iJ_{\vec{k}}^{(x,y)}}\bar{f}_1^{\vec{k},(x,y)}, \quad (2.6)$$

$$f_2^{\vec{k},(x,y)}=e^{iF_2^{\vec{k},(x,y)}}\sqrt{1-|f_1^{\vec{k},(x,y)}|^2}, \quad (2.7)$$

with $J_{\vec{k}}^{(x,y)}$ and $F_2^{\vec{k},(x,y)}$ being some (possibly background-dependent) phases. Clearly, the choice (2.1) is one of these many different sets of annihilation and creationlike variables.

Despite all the freedom allowed in the definitions (2.5), one can restrict the selection of annihilation and creationlike variables to a single privileged family of unitarily equivalent choices by imposing some physically desirable properties. In this sense, a satisfactory criterion is the imposition that the dynamics of the annihilation and creationlike variables can be implemented as unitary transformations in Fock space (for dynamics that are not rendered trivial with respect to the evolution dictated by the Dirac equation and when the Dirac field is treated as a test field propagating on the FLRW cosmology). This condition, together with the invariance of the vacuum under the continuous isometries of the toroidal sections of the homogeneous cosmology, and a standard convention for the notions of particles and antiparticles, indeed leads to a family of unitarily equivalent Fock representations [29]. Actually, the set of annihilation and creationlike variables defined in Eq. (2.1) belongs to this privileged family (this was precisely the motivation to adopt that set in Ref. [27]). Going beyond this particular choice, which we recall diagonalizes H_D, it turns out that the family of fermionic variables (2.5)–(2.7) that satisfies the explained selection criterion is totally specified by the following asymtpotic behavior in the limit of large ω_k:

$$f_1^{\vec{k},(x,y)}=\sqrt{\frac{\xi_k-\omega_k}{2\xi_k}}+\frac{\tilde{M}e^\alpha}{2\omega_k}[e^{iF_2^{\vec{k},(x,y)}}-1]+\theta_{\vec{k}}^{(x,y)} \quad \text{with} \quad \sum_{\vec{k}}|\theta_{\vec{k}}^{(x,y)}|^2<\infty. \quad (2.8)$$

More specifically, the sequence $\{\theta_{\vec{k}}^{(x,y)}\}_{\vec{k}\in\mathbb{Z}^3}$ must contain an infinite subsequence that is $o(\omega_k^{-1})$, where the symbol $o(.)$ means asymptotically negligible with respect to its argument. In fact, given the asymptotic behavior of the Dirac eigenvalues and of their density of states, and hence the generic nonsummability of the sequence ω_k^{-3} over all $\vec{k} \in \mathbb{Z}^3$, it is not hard to convince oneself that $\theta_{\vec{k}}^{(x,y)}$ must have the following asymptotic behavior. For a nonempty and infinite subset $\tilde{\mathbb{Z}}^3 \subset \mathbb{Z}^3$, the functions $\theta_{\vec{k}}^{(x,y)}$ with $\vec{k} \in \tilde{\mathbb{Z}}^3$ must be $o(\omega_k^{-3/2})$. In addition to this, there might exist a complementary subset $\mathbb{Z}^3_\uparrow$ of infinite cardinal such that the sequence $\{\theta_{\vec{k}}^{(x,y)}\}_{\vec{k}\in\mathbb{Z}^3_\uparrow}$, while being square summable, is of asymptotic order $\omega_k^{-3/2}$ or higher.

On the other hand, let us recall that both $F_2^{\vec{k},(x,y)}$ and $\theta_{\vec{k}}^{(x,y)}$ may be functions of the homogeneous FLRW variables (α, π_α). For the sake of concreteness in our analysis and adopting in the following the notation $\{h_l\} = \{f_l, g_l\}$, with $l = 1,\ 2$, for any of the functions that determine the fermionic variables, we restrict ourselves to functional dependencies such that

$$\partial_\alpha^n h_l^{\vec{k},(x,y)} = \mathcal{O}(h_l^{\vec{k},(x,y)}), \partial_{\pi_\alpha}^n h_l^{\vec{k},(x,y)} = \mathcal{O}(h_l^{\vec{k},(x,y)}), \quad (2.9)$$

for integers n at least up to 3 (and where the derivatives act order by order in the asymptotic expansion for large ω_k, at least for the relevant orders in our discussion). Here, a contribution is $\mathcal{O}(.)$ when it is of the asymptotic order of the corresponding argument (or smaller). Our restriction excludes, in particular, the possibility of absorbing in the phases of $h_1^{\vec{k},(x,y)}$ and $h_2^{\vec{k},(x,y)}$ any of the dominant oscillations in conformal time that the Dirac field displays in the limit of large ω_k when it is treated as a test field obeying the Dirac equation in a classical FLRW cosmology.

Similar to the situation found in the previous subsection, the family of annihilation and creationlike variables defined by Eqs. (2.5)–(2.7), together with condition (2.8), is obtained by means of an (α, π_α)-dependent transformation that is canonical within the fermionic sector of the phase space. In order to be canonical in the entire truncated system, as desired e.g., in the hybrid quantization strategy, the geometric variables (α, π_α) of the homogeneous sector must be replaced with a new, corrected, canonical pair $(\tilde{\alpha}, \tilde{\pi}_\alpha)$. Concretely, the corrections $\Delta\tilde{\alpha} = \tilde{\alpha} - \alpha$ and $\Delta\tilde{\pi}_\alpha = \tilde{\pi}_\alpha - \pi_\alpha$ that determine these new variables are quadratic in the fermionic perturbations, and are given by [27]

$$\Delta\tilde{\alpha} = \frac{i}{2}\sum_{\vec{k},(x,y)} [(\partial_{\pi_\alpha} x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_{\pi_\alpha} \bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_{\pi_\alpha} y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_{\pi_\alpha} \bar{y}_{\vec{k}})y_{\vec{k}}], \quad (2.10)$$

$$\Delta\tilde{\pi}_\alpha = -\frac{i}{2}\sum_{\vec{k},(x,y)} [(\partial_\alpha x_{\vec{k}})\bar{x}_{\vec{k}} + (\partial_\alpha \bar{x}_{\vec{k}})x_{\vec{k}} + (\partial_\alpha y_{\vec{k}})\bar{y}_{\vec{k}} + (\partial_\alpha \bar{y}_{\vec{k}})y_{\vec{k}}]. \quad (2.11)$$

Taking into account the quadratic order of our perturbative truncation, one then concludes that the expression of the total Hamiltonian of the cosmological system in terms of these new variables can be obtained by directly substituting the new pair $(\tilde{\alpha}, \tilde{\pi}_\alpha)$ in its functional dependence on (α, π_α), and replacing the Dirac Hamiltonian $N_0 H_D$ with

$$N_0 \tilde{H}_D = N_0[H_D + e^{-3\tilde{\alpha}}\tilde{\pi}_\alpha \Delta\tilde{\pi}_\alpha - 8\pi e^{3\tilde{\alpha}} V(\phi)\Delta\tilde{\alpha}]. \quad (2.12)$$

Here, $V(\phi)$ is (up to a multiplicative constant [27]) the potential of the homogeneous inflaton field ϕ, and all the dependence of H_D, $\Delta\tilde{\alpha}$, and $\Delta\tilde{\pi}_\alpha$ on the homogeneous pair (α, π_α) must again be evaluated at $(\tilde{\alpha}, \tilde{\pi}_\alpha)$. In order to arrive at this corrected fermionic Hamiltonian, a well-controlled redefinition of the homogeneous lapse function must be performed, adding to it a sum over modes of certain terms that are quadratic in the fermionic perturbations [27].

Let us notice that, in terms of the family of annihilation and creationlike variables (2.5)–(2.8) that we are considering, the Dirac contribution H_D to the Hamiltonian does no longer, in general, display a diagonal form as it did before [see Eq. (2.3)]. In fact, one may obtain the new expression of H_D by inserting in Eq. (2.3) the Bogoliubov transformation

$$\breve{a}_{\vec{k}}^{(x,y)} = \kappa_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)} + \lambda_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)},$$
$$\bar{\breve{b}}_{\vec{k}}^{(x,y)} = e^{-iJ_{\vec{k}}^{(x,y)}}[\bar{\kappa}_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)} - \bar{\lambda}_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)}], \quad (2.13)$$

that relates the old variables $\{\breve{a}_{\vec{k}}^{(x,y)}, \bar{\breve{b}}_{\vec{k}}^{(x,y)}\}$ employed in Refs. [27,28] with the more general family considered here. It is not hard to check that relations (2.6) and (2.7) guarantee that this is indeed a Bogoliubov transformation in the fermionic phase space, so that in particular we have $|\kappa_{\vec{k}}^{(x,y)}|^2 + |\lambda_{\vec{k}}^{(x,y)}|^2 = 1$. A straightforward computation then shows that

$$H_{\vec{k}} = \frac{e^{-\tilde{\alpha}}}{2}\sum_{(x,y)}[\tilde{\xi}_k(1 - 2|\lambda_{\vec{k}}^{(x,y)}|^2)(\bar{a}_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)} - a_{\vec{k}}^{(x,y)}\bar{a}_{\vec{k}}^{(x,y)} + \bar{b}_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)}\bar{b}_{\vec{k}}^{(x,y)}) - 4\tilde{\xi}_k(\kappa_{\vec{k}}^{(x,y)}\bar{\lambda}_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - \bar{\kappa}_{\vec{k}}^{(x,y)}\lambda_{\vec{k}}^{(x,y)}\bar{a}_{\vec{k}}^{(x,y)}\bar{b}_{\vec{k}}^{(x,y)})], \quad (2.14)$$

where $\tilde{\xi}_k$ stands for the result of replacing α directly with $\tilde{\alpha}$ in the definition (2.2) of ξ_k. Besides, we recall that H_D is the sum over all modes $\vec{k} \neq \vec{\tau}$ of the corresponding Hamiltonian term $H_{\vec{k}}$.

Apart from the mentioned contributions to H_D, interaction terms that cause the creation and annihilation of pairs in all modes arise again from the corrections that are proportional to $\Delta\tilde{\alpha}$ and $\Delta\tilde{\pi}_\alpha$ in the expression (2.12) of the fermionic Hamiltonian $N_0\tilde{H}_D$. All those terms can be computed using Eqs. (2.10) and (2.11) after imposing the asymptotic relations (2.8). Then, one can regard the resulting fermionic Hamiltonian as a sum over all $\vec{k} \in \mathbb{Z}^3$ of some functions $N_0 \tilde{H}_{\vec{k}}$ that possess a quite specific asymptotic behavior. One obtains

$$\begin{aligned}\tilde{H}_{\vec{k}} = \sum_{(x,y)} \bigg[\left(\frac{e^{-\tilde{\alpha}}}{2} \tilde{\xi}_k + h_D^{\vec{k}} \right) (\bar{a}_{\vec{k}}^{(x,y)} a_{\vec{k}}^{(x,y)} - a_{\vec{k}}^{(x,y)} \bar{a}_{\vec{k}}^{(x,y)} \\ + \bar{b}_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)}) \\ + h_J^{\vec{k}} (\bar{b}_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} - b_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)}) \\ + e^{i(J_{\vec{k}}^{(x,y)} - F_2^{\vec{k},(x,y)})} e^{-\tilde{\alpha}} (2\omega_k \bar{\theta}_{\vec{k}}^{(x,y)} + \bar{h}_I^{\vec{k}}) a_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)} \\ - e^{-i(J_{\vec{k}}^{(x,y)} - F_2^{\vec{k},(x,y)})} e^{-\tilde{\alpha}} (2\omega_k \theta_{\vec{k}}^{(x,y)} + h_I^{\vec{k}}) \bar{a}_{\vec{k}}^{(x,y)} \bar{b}_{\vec{k}}^{(x,y)} \bigg],\end{aligned} \quad (2.15)$$

where we have defined

$$\begin{aligned} h_J^{\vec{k}} = -4\pi e^{3\tilde{\alpha}} V(\phi) \partial_{\tilde{\pi}_\alpha} J_{\vec{k}}^{(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \\ - \frac{1}{2} e^{-3\tilde{\alpha}} \tilde{\pi}_\alpha \partial_{\tilde{\alpha}} J_{\vec{k}}^{(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha). \end{aligned} \quad (2.16)$$

To avoid complicating the notation in excess, we denote the partial derivatives with respect to the homogeneous geometry evaluated at $(\tilde{\alpha}, \tilde{\pi}_\alpha)$ directly by $\partial_{\tilde{\alpha}}$ and $\partial_{\tilde{\pi}_\alpha}$. Besides, $h_D^{\vec{k}}$ is a real function that, in the asymptotic regime of large ω_k, is given by

$$\begin{aligned} h_D^{\vec{k}} = 4\pi e^{4\tilde{\alpha}} V(\phi) \partial_{\tilde{\pi}_\alpha} F_2^{\vec{k},(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \\ + \frac{1}{2} e^{-2\tilde{\alpha}} \tilde{\pi}_\alpha \partial_{\tilde{\alpha}} F_2^{\vec{k},(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \\ + \mathcal{O}(\mathrm{Max}[\omega_k^{-2}, (\theta_{\vec{k}}^{(x,y)})^2]). \end{aligned} \quad (2.17)$$

In this asymptotic regime, we also have for $\vec{k} \in \mathbb{Z}^3_\uparrow$,

$$h_I^{\vec{k}} = \mathcal{O}(\mathrm{Max}[\omega_k^{-1}, \theta_{\vec{k}}^{(x,y)}, \omega_k (\theta_{\vec{k}}^{(x,y)})^3]), \quad (2.18)$$

while, for $\vec{k} \in \tilde{\mathbb{Z}}^3$,

$$\begin{aligned} h_I^{\vec{k}} = i e^{-2\tilde{\alpha}} \tilde{\pi}_\alpha \bigg[\frac{\tilde{M} e^{\tilde{\alpha}}}{2\omega_k} e^{iF_2^{\vec{k},(x,y)}} + \partial_{\tilde{\alpha}} \theta_{\vec{k}}^{(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \\ - i\theta_{\vec{k}}^{(x,y)} \partial_{\tilde{\alpha}} F_2^{\vec{k},(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \bigg] \\ + 8\pi i e^{4\tilde{\alpha}} V(\phi) [\partial_{\tilde{\pi}_\alpha} \theta_{\vec{k}}^{(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha) \\ - i\theta_{\vec{k}}^{(x,y)} \partial_{\tilde{\pi}_\alpha} F_2^{\vec{k},(x,y)} (\tilde{\alpha}, \tilde{\pi}_\alpha)] + \mathcal{O}(\omega_k^{-2}). \end{aligned} \quad (2.19)$$

The function Max[., .] picks out the argument of dominant asymptotic order. To arrive at these expressions, we have made a convenient use of condition (2.9). Given the standard convention for the assignation of particles and antiparticles, this is the only relevant restriction that we impose on the family of annihilation and creationlike variables, apart from the physically appealing requirement of a quantum dynamics that is compatible with the symmetries of the homogeneous cosmology and is unitarily implementable, in the context of quantum field theory in curved spacetimes.

III. BACKREACTION TERM IN THE HAMILTONIAN

The asymptotic characterization that we have carried out of the fermionic part $\tilde{H}_D$ in the zero mode of the Hamiltonian constraint allows for a rather general passage to the quantum theory, without the need to specify a particular choice of fermionic annihilation and creationlike variables [among those allowed by Eqs. (2.8) and (2.9)]. With that freedom in mind, we now briefly summarize the hybrid quantization of the system and display the equations that result for the fermionic perturbations when one adopts a kind of Born-Oppenheimer ansatz for the quantum states. We recall that the phase space of the system has been split into the following sectors. First of all, there is the homogeneous background, with canonical variables that, after being perturbatively corrected, describe the homogeneous FLRW geometry and the homogeneous inflaton. Secondly, we have the information about the scalar and tensor perturbations, encoded in the tensor and Mukhanov-Sasaki gauge invariants, as well as in the linear perturbative constraints of the system, together with their canonical momenta. Finally, the fermionic d.o.f. are characterized by variables of the form (2.5)–(2.7) subject to the conditions (2.8) [and (2.9)]. All of these sectors are jointly subject to the zero mode of the Hamiltonian constraint, formed from the constraint of the unperturbed inflationary model (but evaluated now in the new, corrected, background variables) by adding to it terms that are quadratic in the gauge-invariant perturbations. In particular, $\tilde{H}_D$ provides the fermionic contribution to this global constraint. In the hybrid approach, one then adopts some suitably chosen quantum representations for each of the different sectors, each of them with its corresponding Hilbert or Fock space, and introduces some well-defined operator(s) on the resulting tensor product space to represent the constraint(s), imposed quantum mechanically. This is highly nontrivial, given the fact that the zero mode of the Hamiltonian constraint mixes the homogeneous sector, which is provided with a quantum gravity-inspired representation, with all the rest.

In this work, we do not worry about the specific details of the representation chosen for the tensor and Mukhanov-Sasaki perturbations, or about their associated part of the zero mode of the Hamiltonian constraint. It suffices to say that they are described with a suitable Fock representation (for additional details, see e.g., Refs. [27,30,43]). As for the Abelianized, linear perturbative constraints, their imposition can be made straightforward, since they are part of the constructed set of canonical variables. They just restrict the quantum states not to depend on their canonical momenta, which are purely gauge d.o.f. The remaining sectors that are relevant for our study are then the homogeneous background and the fermionic perturbations. For the former, we select a loop quantum cosmology-inspired representation [22,25]. In short, this means that, instead of working with the canonical pair $(\tilde{\alpha}, \tilde{\pi}_\alpha)$, one performs a canonical transformation to obtain a new pair that describes (up to corrections that are quadratic in perturbations) the physical volume of the universe V and its canonical momentum. This latter variable contains, in turn, the information about the Ashtekar-Barbero connection for the homogeneous sector. The volume variable and the complex exponentiation of its momentum are then the functions of the homogeneous geometry that are represented quantum mechanically, adopting what is known as a polymeric representation. It is common to construct it on a Hilbert space formed from eigenstates of the volume, with the discrete inner product [21]. We denote this polymeric Hilbert space as $\mathcal{H}^{\text{grav}}_{\text{kin}}$. On the other hand, for the inflaton field ϕ and its momentum we choose a standard Schrödinger representation, with Hilbert space given by the space of square integrable functions of the inflaton, $L^2(\mathbb{R}, d\phi)$. And for the fermionic perturbations we consider the Fock representation associated with any choice of annihilation and creationlike variables within the family defined by Eqs. (2.5)–(2.9). We call $\mathcal{F}_D$ the corresponding Fock space. Besides $\hat{a}^{(x,y)}_{\vec{k}}$ and $\hat{b}^{(x,y)\dagger}_{\vec{k}}$ respectively denote the annihilation operators of particle excitations and the creation operators of antiparticle excitations, with their adjoints acting reversely. Let us recall that all the possible Fock representations chosen in this way are unitarily equivalent. However, as we have seen in the previous section, the fermionic Hamiltonian, and in particular its asymptotic tail in the mode decomposition with respect to the eigenspinors of the Dirac operator in T^3, can experience significant changes when choosing different annihilation and creationlike variables in the considered family. It is this freedom what we now exploit in order to see whether we can avoid the appearance of ultraviolet divergences in the quantum theory.

With the representation space fixed as the tensor product of all the mentioned spaces, the construction of an operator for the zero mode of the Hamiltonian constraint involves some additional choices. For the representation of the nonpolynomic functions of the homogeneous variables that appear in the different contributions to the constraint, we refer the reader to the prescriptions listed in Refs. [27,43]. It suffices to say here that it is possible to define them in such a way that the action of the constraint divides the space $\mathcal{H}^{\text{grav}}_{\text{kin}}$ into separable sectors (called superselection sectors) which provide a strictly positive lower bound for the homogeneous volume V [22]. On the other hand, we impose normal ordering for the annihilation and creation operators that represent the Fock quantized perturbations.

A. Schrödinger and Heisenberg equations

In order to find solutions to the zero mode of the Hamiltonian constraint, namely states that are annihilated by its (adjoint) action, we follow the strategy of Refs. [27,30,43] and adopt a convenient ansatz as follows. We consider states with a wave function in which the dependence on the homogeneous geometry and on each of the perturbative sectors can be factorized in a different term. On the other hand, all of these factors, that can be regarded as wave functions for each of the corresponding sectors, are allowed to depend on the homogeneous inflaton, ϕ, which then plays the role of an internal time for the total system. We generically call $\Gamma(V, \phi)$ the part of the wave function that contains the information about the homogeneous geometry, while $\psi_D(\mathcal{N}_D, \phi)$ denotes the part with dependence on the fermionic d.o.f. The abstract notation $\mathcal{N}_D$ refers to the occupation numbers of all the fermionic particles and antiparticles. Moreover, as an ingredient of our ansatz, we restrict our considerations to normalized states Γ in $\mathcal{H}^{\text{grav}}_{\text{kin}}$ with a unitary evolution in ϕ, which furthermore is generated by a positive operator $\hat{\tilde{\mathcal{H}}}_0$,

$$-i\partial_\phi \Gamma(V, \phi) = \hat{\tilde{\mathcal{H}}}_0 \Gamma(V, \phi). \tag{3.1}$$

Besides, the above generator is chosen so that the action of $(\hat{\tilde{\mathcal{H}}}_0)^2 + \partial^2_\phi$ on Γ differs from the corresponding action of the constraint of the unperturbed FLRW cosmology at most in a quadratic contribution of the perturbations.

With this ansatz for the states, we impose the Hamiltonian constraint (conveniently densitized in the homogeneous volume). Then, if in the state Γ we can ignore any transition in the homogeneous geometry mediated by the action of our quantum Hamiltonian constraint, and the contribution of the perturbations to the momentum of the inflaton is negligible with respect to that of Γ (estimated as the expectation value of $\hat{\tilde{\mathcal{H}}}_0$), we arrive at a collection of Schrödinger-like equations, with respect to ϕ, one for each of the partial wave functions of the system on the different perturbative sectors. For details about the calculations and involved approximations, we refer the reader to Refs. [27,30]. Here we are interested in the equation that rules the evolution of the fermionic wave function ψ_D with respect to ϕ. This equation was deduced in Ref. [27] for the particular choice (2.1) of annihilation and creationlike variables. Adapting the derivation to the family of fermionic variables considered here, we get

$$\begin{aligned} i\partial_\phi \psi_D(\mathcal{N}_D, \phi) &= \frac{l_0 \langle \widehat{V^{2/3} e^{\tilde{\alpha}} \tilde{H}_D} \rangle_\Gamma - C^{(\Gamma)}_D(\phi)}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} \psi_D(\mathcal{N}_D, \phi) \\ &\equiv \mathcal{H}^{(\Gamma)}_D(\phi) \psi_D(\mathcal{N}_D, \phi). \end{aligned} \tag{3.2}$$

Here, the hat over classical observables indicates their corresponding representation as operators, according to the prescriptions of the works that we have already mentioned. Besides, the brackets $\langle . \rangle_\Gamma$ stand for the expectation value in Γ, taken with respect to the inner product in $\mathcal{H}_{\text{kin}}^{\text{grav}}$. Since the momentum of ϕ does not appear in $\tilde{H}_D$, the right-hand side of (3.2) represents a ϕ-dependent operator (or a family of operators labeled by ϕ, as one prefers) acting on the fermionic sector. Hence, one may interpret this operator as the (*effective*) Hamiltonian that generates the evolution of the fermionic d.o.f. in the time ϕ. This Hamiltonian, $\mathcal{H}_D^{(\Gamma)}(\phi)$, captures the most relevant features of the quantum background spacetime by means of the expectation values on Γ and the specific quantum representation of the geometry that is employed.

On the other hand, the function $C_D^{(\Gamma)}(\phi)$, added to similar contributions that arise from the scalar and tensor perturbations, provides the mean value in Γ of the difference between $(\hat{\tilde{\mathcal{H}}}_0)^2 + \partial_\phi^2$ and the Hamiltonian constraint of the unperturbed model[3] [27]. Thus, it can be understood as the fermionic contribution to the quantum backreaction on the homogeneous background, inasmuch as the mentioned difference actually measures how much Γ departs from an exact solution of the unperturbed system.

Since the term $\tilde{H}_D$ is a sum over all possible fermionic modes, the Schrödinger equation (3.2) may be decomposed in a collection of individual equations, one for each of the modes. The fermionic contribution to the backreaction, $C_D^{(\Gamma)}(\phi)$, then depends on the behavior of the mode solutions. In fact, one does not always get a well-defined fermionic backreaction without applying regularization techniques. This issue critically depends on the asymptotic tail of the fermionic Hamiltonian $\mathcal{H}_D^{(\Gamma)}(\phi)$, when expressed as a sum over modes. And therefore it depends on the set of annihilation and creationlike variables chosen to describe the fermionic d.o.f. Thus, in order to analyze the possible divergence of $C_D^{(\Gamma)}(\phi)$, we study the solutions to Eq. (3.2). In doing this, it is most convenient to view the Hamiltonian $\mathcal{H}_D^{(\Gamma)}(\phi)$ as the generator of some Heisenberg-like dynamics for the fermionic annihilation and creation operators. In fact, from Eq. (3.2) one can easily get the associated Heisenberg equations, taking into account the decomposition of $\tilde{H}_D$ as a sum over modes of the functions $\tilde{H}_{\vec{k}}$ that have an asymptotic behavior determined by Eq. (2.15). In more detail, if we introduce the following state-dependent change to a conformal time,

$$d\eta_\Gamma = \frac{l_0 \langle \hat{V}^{2/3} \rangle_\Gamma}{\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma} d\phi, \tag{3.3}$$

which is well-defined thanks to the positivity of $\hat{\tilde{\mathcal{H}}}_0$ and the lower positive bound on the volume in each superselection sector of loop quantum cosmology, we obtain the following Heisenberg equations, evaluated at $\eta_\Gamma = \eta$:

$$\begin{aligned} d_{\eta_\Gamma} \hat{a}_{\vec{k}}^{(x,y)}(\eta, \eta_0) &= -i F_{\vec{k}}^{(\Gamma)} \hat{a}_{\vec{k}}^{(x,y)}(\eta, \eta_0) + G_{\vec{k}}^{(\Gamma)} \hat{b}_{\vec{k}}^{(x,y)\dagger}(\eta, \eta_0), \\ d_{\eta_\Gamma} \hat{b}_{\vec{k}}^{(x,y)\dagger}(\eta, \eta_0) &= i (F_{\vec{k}}^{(\Gamma)} + \tilde{J}_{\vec{k}}^{(\Gamma)}) \hat{b}_{\vec{k}}^{(x,y)\dagger}(\eta, \eta_0) \\ &\quad - \bar{G}_{\vec{k}}^{(\Gamma)} \hat{a}_{\vec{k}}^{(x,y)}(\eta, \eta_0), \end{aligned} \tag{3.4}$$

where, in the asymptotic regime of large ω_k,

$$\tilde{J}_{\vec{k}}^{(\Gamma)} = \frac{\langle \widehat{2 e^{\tilde{\alpha}} V^{2/3} h_J^{\vec{k}}} \rangle_\Gamma}{\langle \hat{V}^{2/3} \rangle_\Gamma}, \tag{3.5}$$

$$F_{\vec{k}}^{(\Gamma)} = \frac{\langle \widehat{V^{2/3} \xi_k} \rangle_\Gamma + 2 \langle \widehat{e^{\tilde{\alpha}} V^{2/3} h_D^{\vec{k}}} \rangle_\Gamma}{\langle \hat{V}^{2/3} \rangle_\Gamma}, \tag{3.6}$$

$$G_{\vec{k}}^{(\Gamma)} = \frac{2 i \omega_k \langle \widehat{e^{i(F_2^{\vec{k},(x,y)} - J_{\vec{k}}^{(x,y)})} V^{2/3} \theta_{\vec{k}}^{(x,y)}} \rangle_\Gamma + i \langle \widehat{e^{i(F_2^{\vec{k},(x,y)} - J_{\vec{k}}^{(x,y)})} V^{2/3} h_I^{\vec{k}}} \rangle_\Gamma}{\langle \hat{V}^{2/3} \rangle_\Gamma}. \tag{3.7}$$

The factors $h_J^{\vec{k}}$, $h_D^{\vec{k}}$, and $h_I^{\vec{k}}$ are given in Eqs. (2.16)–(2.19). Provided that our prescriptions for the representation of the homogeneous geometry promote real functions to (at least) symmetric operators, we have that $F_{\vec{k}}^{(\Gamma)}$ and $\tilde{J}_{\vec{k}}^{(\Gamma)}$ are real. In addition, we assume that the state Γ is such that all the considered functions admit asymptotic expansions in the limit of infinitely large ω_k. The coefficients of these expansions are expectation values in Γ of mode-independent operators. Actually, for our discussion, it suffices that the expansions exist up to terms of the order of a certain inverse power of ω_k.

The Heisenberg equations determine a family of annihilation and creation operators parametrized by different values η of η_Γ, once one fixes as initial data at $\eta_\Gamma = \eta_0$ the annihilation and creation operators $\hat{a}_{\vec{k}}^{(x,y)}$ and $\hat{b}_{\vec{k}}^{(x,y)\dagger}$ that appear in the fermionic Hamiltonian (together with their adjoints). It is straightforward to see that each such family of operators, $\hat{a}_{\vec{k}}^{(x,y)}(\eta, \eta_0)$ and $\hat{b}_{\vec{k}}^{(x,y)\dagger}(\eta, \eta_0)$, can be obtained by means of a Bogoliubov transformation from the initial ones, $\hat{a}_{\vec{k}}^{(x,y)}$ and $\hat{b}_{\vec{k}}^{(x,y)\dagger}$. In order to analyze the properties of

[3]We notice here a typo in Ref. [27], where $C_D^{(\Gamma)}(\phi)$ and the rest of the backreaction contributions in Eqs. (6.5)–(6.7) of that paper should appear divided by $\langle \hat{\tilde{\mathcal{H}}}_0 \rangle_\Gamma$.

that transformation, we follow a strategy that is close to the one developed in Ref. [27] for the particular choice of variables (2.1). In the present and more general case, nonetheless, the analysis has some peculiarities that affect the asymptotic regime of large ω_k. So, let us study in detail this asymptotic behavior.

We first introduce the following fermionic operators, motivated in part by the previous definitions (2.5)–(2.7) of the annihilation and creationlike variables and by the dominant asymptotic term in $F^{(\Gamma)}_{\vec{k}}$,

$$\hat{x}_{\vec{k}}(\eta,\eta_0) = f^{(\Gamma)}_{1,k}\hat{a}^{(x,y)}_{\vec{k}}(\eta,\eta_0) + e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}} f^{(\Gamma)}_{2,k}\hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta,\eta_0),$$
$$\hat{y}^{\dagger}_{-\vec{k}-2\vec{\tau}}(\eta,\eta_0) = f^{(\Gamma)}_{2,k}\hat{a}^{(x,y)}_{\vec{k}}(\eta,\eta_0) - e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}} f^{(\Gamma)}_{1,k}\hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta,\eta_0), \qquad (3.8)$$

where

$$f^{(\Gamma)}_{1,k} = \sqrt{\frac{\tilde{F}^{(\Gamma)}_{k} - \omega_k}{2\tilde{F}^{(\Gamma)}_{k}}}, \qquad f^{(\Gamma)}_{2,k} = \sqrt{\frac{\tilde{F}^{(\Gamma)}_{k} + \omega_k}{2\tilde{F}^{(\Gamma)}_{k}}},$$
$$\tilde{F}^{(\Gamma)}_{k} = \frac{\langle V^{2/3}\hat{\xi}_k\rangle_\Gamma}{\langle \hat{V}^{2/3}\rangle_\Gamma}. \qquad (3.9)$$

Notice that $f^{(\Gamma)}_{1,k}$ and $f^{(\Gamma)}_{2,k}$ are both real functions for sufficiently large ω_k, given the asymptotic behavior of ξ_k, and they satisfy $|f^{(\Gamma)}_{1,k}|^2 + |f^{(\Gamma)}_{2,k}|^2 = 1$. These newly introduced operators inherit the following dynamics from Eq. (3.4):

$$d_{\eta_\Gamma}\hat{x}_{\vec{k}}(\eta,\eta_0) = i\left[\omega_k\left(1+\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right) + P^{(\Gamma)}_{\vec{k}}\right]\hat{x}_{\vec{k}}(\eta,\eta_0) + H^{(\Gamma)}_{\vec{k}}\hat{y}^{\dagger}_{-\vec{k}-2\vec{\tau}}(\eta,\eta_0),$$
$$d_{\eta_\Gamma}\hat{y}^{\dagger}_{-\vec{k}-2\vec{\tau}}(\eta,\eta_0) = -i\left[\omega_k\left(1+\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right) + P^{(\Gamma)}_{\vec{k}}\right]\hat{y}^{\dagger}_{-\vec{k}-2\vec{\tau}}(\eta,\eta_0) - \bar{H}^{(\Gamma)}_{\vec{k}}\hat{x}_{\vec{k}}(\eta,\eta_0), \qquad (3.10)$$

with the definitions

$$P^{(\Gamma)}_{\vec{k}} = \frac{\sqrt{(\tilde{F}^{(\Gamma)}_{k})^2 - \omega_k^2}}{\tilde{F}^{(\Gamma)}_{k}}\Im\left(G^{(\Gamma)}_{\vec{k}} e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}}\right), \qquad (3.11)$$

$$H^{(\Gamma)}_{\vec{k}} = -G^{(\Gamma)}_{\vec{k}} e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}} - i\sqrt{(\tilde{F}^{(\Gamma)}_{k})^2 - \omega_k^2}\left(1+\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right) + \frac{\omega_k(\tilde{F}^{(\Gamma)}_{k})'}{2\tilde{F}^{(\Gamma)}_{k}\sqrt{(\tilde{F}^{(\Gamma)}_{k})^2 - \omega_k^2}} + iQ^{(\Gamma)}_{\vec{k}}, \qquad (3.12)$$

$$Q^{(\Gamma)}_{\vec{k}} = \frac{\tilde{F}^{(\Gamma)}_{k} + \omega_k}{\tilde{F}^{(\Gamma)}_{k}}\Im\left(G^{(\Gamma)}_{\vec{k}} e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}}\right). \qquad (3.13)$$

Here, the prime denotes the derivative with respect to η_Γ and $\Im(.)$ is the imaginary part. Employing now the compact notation $\{\hat{z}_{\vec{k}}\} = \{\hat{x}_{\vec{k}}, \hat{y}_{-\vec{k}-2\vec{\tau}}\}$ and introducing the rescaled operators $\hat{\tilde{z}}_{\vec{k}} = (iH^{(\Gamma)}_{\vec{k}})^{-1/2}\hat{z}_{\vec{k}}$, these all turn out to satisfy the same second order equation,

$$\hat{\tilde{z}}''_{\vec{k}} = -[\tilde{\omega}^2_{\vec{k}} + |H^{(\Gamma)}_{\vec{k}}|^2 - i\tilde{\omega}'_{\vec{k}}]\hat{\tilde{z}}_{\vec{k}}, \qquad (3.14)$$

where

$$\tilde{\omega}_{\vec{k}} = \omega_k\left(1+\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right) + P^{(\Gamma)}_{\vec{k}} + \frac{i}{2}(\ln H^{(\Gamma)}_{\vec{k}})'. \qquad (3.15)$$

It can be checked that two independent solutions of the linear differential equation (3.14) are $\tilde{z}^l_{\vec{k}} = \exp[-i(-1)^l\tilde{\Theta}^l_{\vec{k}}]$ with

$$\tilde{\Theta}^l_{\vec{k}}(\eta_0) = 0, \qquad (\tilde{\Theta}^l_{\vec{k}})' = \tilde{\omega}_{\vec{k}} + \Lambda^l_{\vec{k}}, \qquad l = 1,2, \qquad (3.16)$$

where $\Lambda^l_{\vec{k}}$ are the solutions of the Ricatti equation

$$(\Lambda^l_{\vec{k}})' = i(-1)^l[(\Lambda^l_{\vec{k}})^2 + 2\tilde{\omega}_{\vec{k}}\Lambda^l_{\vec{k}}] - u^l_{\vec{k}}, \qquad (3.17)$$

$$u^l_{\vec{k}} = i(-1)^l|H^{(\Gamma)}_{\vec{k}}|^2 + [(-1)^l + 1]\tilde{\omega}'_{\vec{k}}, \qquad (3.18)$$

with initial conditions $\Lambda^l_{\vec{k}}(\eta_0) = 0$. The corresponding independent solutions for $\hat{z}_{\vec{k}}$, after undoing the scaling, are then given by $z^l_{\vec{k}} = \exp[-i(-1)^l\Theta^l_{\vec{k}}]$, where

$$\Theta^l_{\vec{k}} = \omega_k(\eta-\eta_0) + \frac{i}{2}[(-1)^l+1]\ln\left(\frac{H^{(\Gamma)}_{\vec{k}}}{H^{(\Gamma),0}_{\vec{k}}}\right) + \omega_k\int_{\eta_0}^{\eta} d\eta_\Gamma \left(\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right) + \int_{\eta_0}^{\eta} d\eta_\Gamma(\Lambda^l_{\vec{k}} + P^{(\Gamma)}_{\vec{k}}). \tag{3.19}$$

From now on, we use a superindex or a subindex 0 (on occasions preceded by a coma) to denote evaluation at $\eta_\Gamma = \eta_0$. With the above independent solutions of the second order equation at hand, the relation between $\hat{x}_{\vec{k}}$ and $\hat{y}^\dagger_{-\vec{k}-2\vec{\tau}}$ (or their adjoints) implied by the first order equations (3.10), and the relation of these operators with the annihilation and creation operators in the Heisenberg picture, we can readily derive the dynamical Bogoliubov transformation of the latter as

$$\hat{a}^{(x,y)}_{\vec{k}}(\eta,\eta_0) = \alpha_{\vec{k}}(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + \beta_{\vec{k}}(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}},$$
$$\hat{b}^{(x,y)\dagger}_{\vec{k}}(\eta,\eta_0) = -e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}}\bar{\beta}_{\vec{k}}(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}^{(\Gamma)}_{\vec{k}}}\bar{\alpha}_{\vec{k}}(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}}, \tag{3.20}$$

where the alpha and beta coefficients take the expressions

$$\alpha_{\vec{k}} = \left[f^{(\Gamma)}_{1,k}(f^{(\Gamma),0}_{1,k} - f^{(\Gamma),0}_{2,k}\zeta_{\vec{k}})e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma\tilde{\Lambda}^1_{\vec{k}}} - f^{(\Gamma)}_{2,k}f^{(\Gamma),0}_{1,k}\bar{\zeta}_{\vec{k}}\frac{\bar{H}^{(\Gamma)}_{\vec{k}}}{\bar{H}^{(\Gamma),0}_{\vec{k}}}e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma\bar{\tilde{\Lambda}}^2_{\vec{k}}}\right]e^{i\omega_k\left[\eta-\eta_0+\int_{\eta_0}^{\eta} d\eta_\Gamma\frac{F^{(\Gamma)}_{\vec{k}}-\tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right]}$$
$$+\left[f^{(\Gamma)}_{2,k}(f^{(\Gamma),0}_{1,k}\bar{\zeta}_{\vec{k}} + f^{(\Gamma),0}_{2,k})e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma\bar{\tilde{\Lambda}}^1_{\vec{k}}} + f^{(\Gamma)}_{1,k}f^{(\Gamma),0}_{2,k}\zeta_{\vec{k}}\frac{H^{(\Gamma)}_{\vec{k}}}{H^{(\Gamma),0}_{\vec{k}}}e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma\tilde{\Lambda}^2_{\vec{k}}}\right]e^{-i\omega_k\left[\eta-\eta_0+\int_{\eta_0}^{\eta} d\eta_\Gamma\frac{F^{(\Gamma)}_{\vec{k}}-\tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right]}, \tag{3.21}$$

$$\beta_{\vec{k}} = \left[f^{(\Gamma)}_{1,k}(f^{(\Gamma),0}_{2,k} + f^{(\Gamma),0}_{1,k}\zeta_{\vec{k}})e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma\tilde{\Lambda}^1_{\vec{k}}} - f^{(\Gamma)}_{2,k}f^{(\Gamma),0}_{2,k}\bar{\zeta}_{\vec{k}}\frac{\bar{H}^{(\Gamma)}_{\vec{k}}}{\bar{H}^{(\Gamma),0}_{\vec{k}}}e^{i\int_{\eta_0}^{\eta} d\eta_\Gamma\bar{\tilde{\Lambda}}^2_{\vec{k}}}\right]e^{i\omega_k\left[\eta-\eta_0+\int_{\eta_0}^{\eta} d\eta_\Gamma\frac{F^{(\Gamma)}_{\vec{k}}-\tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right]}$$
$$+\left[f^{(\Gamma)}_{2,k}(f^{(\Gamma),0}_{2,k}\bar{\zeta}_{\vec{k}} - f^{(\Gamma),0}_{1,k})e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma\bar{\tilde{\Lambda}}^1_{\vec{k}}} - f^{(\Gamma)}_{1,k}f^{(\Gamma),0}_{1,k}\zeta_{\vec{k}}\frac{H^{(\Gamma)}_{\vec{k}}}{H^{(\Gamma),0}_{\vec{k}}}e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma\tilde{\Lambda}^2_{\vec{k}}}\right]e^{-i\omega_k\left[\eta-\eta_0+\int_{\eta_0}^{\eta} d\eta_\Gamma\frac{F^{(\Gamma)}_{\vec{k}}-\tilde{F}^{(\Gamma)}_{k}}{\tilde{F}^{(\Gamma)}_{k}}\right]}. \tag{3.22}$$

Here, we have defined

$$\zeta_{\vec{k}} = \frac{iH^{(\Gamma),0}_{\vec{k}}}{2\omega_k[1+(F^{(\Gamma),0}_{\vec{k}} - \tilde{F}^{(\Gamma),0}_{k})/\tilde{F}^{(\Gamma),0}_{k}] + i(\ln H^{(\Gamma)}_{\vec{k}})'_0 + 2P^{(\Gamma),0}_{\vec{k}}}, \tag{3.23}$$

$$\tilde{\Lambda}^l_{\vec{k}} = \Lambda^l_{\vec{k}} + P^{(\Gamma)}_{\vec{k}}. \tag{3.24}$$

B. Unitarity and backreaction

The Bogoliubov transformation of the annihilation and creation operators that implements the Heisenberg dynamics dictated by Eq. (3.4) may be used to obtain solutions of the associated Schrödinger equation (3.2) [27]. In order to do so, nonetheless, it is necessary that the transformation admits a unitary implementation in the fermionic Fock space $\mathcal{F}_D$, for all values of initial and final times, η_0 and η. If this is the case, one can construct the unitary operator that integrates the Heisenberg equation. Evolving with it the Fock vacuum defined by the initial operators $\{\hat{a}^{(x,y)}_{\vec{k}}, \hat{b}^{(x,y)}_{\vec{k}}\}$, one indeed arrives at a solution of the Schrödinger equation. Other solutions can be similarly found starting with the initial n-particle states.

Actually, the considered Bogoliubov transformation is unitarily implementable in Fock space if and only if the sequence $\{\beta_{\vec{k}}(\eta,\eta_0)\}_{\vec{k}\in\mathbb{Z}^3}$ is square summable [44,45]. This summability exclusively depends on the asymptotic behavior of the beta coefficients, in the regime of large ω_k, provided that they are regular in their dependence on η and η_0 for all $\vec{k}\in\mathbb{Z}^3$. This should be the case with the adopted loop representation of the homogeneous geometry (and suitable operator prescriptions), assuming that $\theta^{(x,y)}_{\vec{k}}$ is taken as a smooth function of the geometric d.o.f. Therefore, we are interested in the asymptotic behavior of all functions and quantities appearing in Eq. (3.22). On the one hand, as it was shown in Ref. [27], we have

$$\tilde{F}_{\vec{k}}^{(\Gamma)} = \omega_k + \frac{M^2}{2l_0^2\omega_k} W_1^{(\Gamma)} + \mathcal{O}(\omega_k^{-3}), \qquad W_1^{(\Gamma)} = \frac{\langle \hat{V}^{4/3}\rangle_\Gamma}{\langle \hat{V}^{2/3}\rangle_\Gamma}, \tag{3.25}$$

where we recall that M is the bare mass of the Dirac field. Then,

$$f_{1,k}^{(\Gamma)} = \frac{M}{2l_0\omega_k}\sqrt{W_1^{(\Gamma)}} + \mathcal{O}(\omega_k^{-3}),$$
$$f_{2,k}^{(\Gamma)} = 1 - \frac{M^2}{8l_0^2\omega_k^2} W_1^{(\Gamma)} + \mathcal{O}(\omega_k^{-4}). \tag{3.26}$$

On the other hand, from the asymptotic behavior of $h_D^{\vec{k}} = \mathcal{O}(1)$ and $h_I^{\vec{k}}$, that follows from Eqs. (2.17)–(2.19) together with condition (2.9), we get

$$\frac{F_{\vec{k}}^{(\Gamma)} - \tilde{F}_{\vec{k}}^{(\Gamma)}}{\tilde{F}_{\vec{k}}^{(\Gamma)}} = \frac{2\langle e^{\tilde{\alpha}}\widehat{V^{2/3}h_D^{\vec{k}}}\rangle_\Gamma}{\langle \widehat{V^{2/3}\xi_k}\rangle_\Gamma} = \mathcal{O}(\omega_k^{-1}),$$
$$P_{\vec{k}}^{(\Gamma)} = \mathcal{O}q\left(G_{\vec{k}}^{(\Gamma)}\omega_k^{-1}\right) = \mathcal{O}(\mathrm{Max}[\omega_k^{-2}, \theta_{\vec{k}}^{(x,y)}]), \tag{3.27}$$

and therefore

$$H_{\vec{k}}^{(\Gamma)} = -\bar{G}_{\vec{k}}^{(\Gamma)} e^{-i\int_{\eta_0}^{\eta} d\eta_\Gamma \tilde{J}_{\vec{k}}^{(\Gamma)}} + \frac{M}{l_0}\sqrt{W_1^{(\Gamma)}}\left[-i\left(1 + \frac{2\langle e^{\tilde{\alpha}}\widehat{V^{2/3}h_D^{\vec{k}}}\rangle_\Gamma}{\langle \widehat{V^{2/3}\xi_k}\rangle_\Gamma}\right) + \frac{1}{4\omega_k}(\ln W_1^{(\Gamma)})'\right] + \mathcal{O}(\mathrm{Max}[\omega_k^{-2}, G_{\vec{k}}^{(\Gamma)}\omega_k^{-2}]), \tag{3.28}$$

so that

$$\zeta_{\vec{k}} = \frac{M}{2l_0\omega_k}\sqrt{W_1^{(\Gamma),0}} - \frac{i}{2\omega_k}\bar{G}_{\vec{k}}^{(\Gamma),0} + \mathcal{O}(\mathrm{Max}[\omega_k^{-m}, G_{\vec{k}}^{(\Gamma)}\omega_k^{-2}]), \tag{3.29}$$

where $m = 2$ for $\vec{k} \in \mathbb{Z}_\uparrow^3$, whereas $m = 3$ for $\vec{k} \in \tilde{\mathbb{Z}}^3$. The remaining functions that we have to analyze in order to derive the asymptotic behavior of $\beta_{\vec{k}}(\eta, \eta_0)$ are the solutions $\Lambda_{\vec{k}}^l$ of the Ricatti equation (3.17). Their behavior depends drastically on the function $u_{\vec{k}}^l$, given in Eq. (3.18). It is not difficult to see that, provided condition (2.9) holds for second order derivatives, all the contributions to those functions are of asymptotic order $\mathcal{O}(1)$, except possibly for $|H_{\vec{k}}^{(\Gamma)}|^2$. For this specific quantity, a look at Eq. (3.28) reveals that one gets a contribution that may grow as $\omega_k^2(\theta_{\vec{k}}^{(x,y)})^2$. In particular, it is $\mathcal{O}(1)$ if $\theta_{\vec{k}}^{(x,y)} = \mathcal{O}(\omega_k^{-1})$. Recalling the characterization of the possible asymptotic behavior allowed for $\theta_{\vec{k}}^{(x,y)}$, described in the previous section, we have the following scenarios:

(a) For $\vec{k} \in \tilde{\mathbb{Z}}^3$ or $\vec{k} \in \mathbb{Z}_{\uparrow,1}^3 \subset \mathbb{Z}_\uparrow^3$, with $\theta_{\vec{k}}^{(x,y)} = \mathcal{O}(\omega_k^{-1})$ in $\mathbb{Z}_{\uparrow,1}^3$, the source term $u_{\vec{k}}^l$ of the Ricatti equation (3.17) is asymptotically $\mathcal{O}(1)$ and the solutions $\Lambda_{\vec{k}}^l$ satisfy

$$\int_{\eta_0}^{\eta} d\eta_\Gamma \Lambda_{\vec{k}}^l = -(-1)^l \frac{i}{2\omega_k}\int_{\eta_0}^{\eta} d\eta_\Gamma u_{\vec{k}}^l + \mathcal{O}(\omega_{\vec{k}}^{-2}) = \mathcal{O}(\omega_{\vec{k}}^{-1}), \tag{3.30}$$

similarly as it happened in Ref. [27]. This can be checked by solving Eq. (3.17), with vanishing initial condition and after ignoring the nonlinear term, by means of a repeated integration by parts [taking into account condition (2.9)]. With the result, one can estimate the order of the ignored term, obtaining Eq. (3.30).

(b) For tuples $\vec{k}$ in the complement (up to a finite subset) $\mathbb{Z}_{\uparrow,2}^3$ of $\mathbb{Z}_{\uparrow,1}^3$ in $\mathbb{Z}_\uparrow^3$, that is such that $\omega_k^{-1} = o(\theta_{\vec{k}}^{(x,y)})$, we use that $u_{\vec{k}}^l = \mathcal{O}(\omega_k^2[\theta_{\vec{k}}^{(x,y)}]^2)$. Let us notice, however, that it is only the imaginary part of $u_{\vec{k}}^l$ that gives a growing contribution in the asymptotic regime of large ω_k, as can be seen from definition (3.18). It follows that one may again compute the solutions of the linear part of the Ricatti equation (3.17), that we call $\lambda_{\vec{k}}^l$, with vanishing initial conditions. In this way, one finds

$$\int_{\eta_0}^{\eta} d\eta_\Gamma \Re(\lambda_{\vec{k}}^l) = \frac{1}{2\omega_k}\int_{\eta_0}^{\eta} d\eta_\Gamma |H_{\vec{k}}^{(\Gamma)}|^2 + o(1),$$
$$\int_{\eta_0}^{\eta} d\eta_\Gamma \Im(\lambda_{\vec{k}}^l) = o(1), \tag{3.31}$$

where $\Re(.)$ is the real part. Taking into account this behavior, and iteratively repeating the same analysis for the subdominant contributions to $\lambda_{\vec{k}}^l$ in the solution $\Lambda_{\vec{k}}^l$ of the entire Ricatti equation, one can show that, asymptotically,

$$\int_{\eta_0}^{\eta} d\eta_\Gamma \Re(\Lambda_{\vec{k}}^l) = \gamma_{\vec{k}} + o(1),$$
$$\int_{\eta_0}^{\eta} d\eta_\Gamma \Im(\Lambda_{\vec{k}}^l) = o(1), \tag{3.32}$$

where $\gamma_{\vec{k}}$ does not depend on l. Therefore, in particular, in the asymptotic regime of large ω_k,

$$e^{-i(-1)^l\int_{\eta_0}^{\eta}d\eta_\Gamma\Lambda^l_{\vec{k}}} = e^{-i(-1)^l\int_{\eta_0}^{\eta}d\eta_\Gamma\Re(\Lambda^l_{\vec{k}})}[1+o(1)]. \tag{3.33}$$

Employing all this asymptotic information, we can easily show that the alpha and beta coefficients (3.21) and (3.22) have the following behavior for infinitely large ω_k:

$$\alpha_{\vec{k}}(\eta,\eta_0) = e^{-i\omega_k(\eta-\eta_0)-i\int_{\eta_0}^{\eta}d\eta_\Gamma\Xi_1^{\vec{k}}} + o(1), \tag{3.34}$$

$$\beta_{\vec{k}}(\eta,\eta_0) = \frac{i}{2\omega_k}\{G^{(\Gamma),0}_{\vec{k}}e^{-i\omega_k(\eta-\eta_0)-i\int_{\eta_0}^{\eta}d\eta_\Gamma\Xi_1^{\vec{k}}} - G^{(\Gamma)}_{\vec{k}}e^{i\omega_k(\eta-\eta_0)+i\int_{\eta_0}^{\eta}d\eta_\Gamma[\tilde{J}^{(\Gamma)}_{\vec{k}}+\Xi_2^{\vec{k}}]}\} + \delta_{\vec{k}}, \tag{3.35}$$

$$\delta_{\vec{k}} = \mathcal{O}(\mathrm{Max}[\omega_k^{-3}, G^{(\Gamma)}_{\vec{k}}\omega_k^{-2}]) \quad \text{when } \vec{k}\in\tilde{\mathbb{Z}}^3, \delta_{\vec{k}} = o(G^{(\Gamma)}_{\vec{k}}\omega_k^{-1}) \quad \text{when } \vec{k}\in\mathbb{Z}^3_\uparrow, \tag{3.36}$$

where we have defined, with $l = 1, 2$,

$$\Xi_l^{\vec{k}} = \omega_k\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{\vec{k}}}{\tilde{F}^{(\Gamma)}_{\vec{k}}} \quad \text{for } \vec{k}\in\tilde{\mathbb{Z}}^3\cup\mathbb{Z}^3_{\uparrow,1},$$

$$\Xi_l^{\vec{k}} = \omega_k\frac{F^{(\Gamma)}_{\vec{k}} - \tilde{F}^{(\Gamma)}_{\vec{k}}}{\tilde{F}^{(\Gamma)}_{\vec{k}}} + \Re(\Lambda^l_{\vec{k}}) \quad \text{for } \vec{k}\in\mathbb{Z}^3_{\uparrow,2}. \tag{3.37}$$

Then, in all cases, we have that

$$\beta_{\vec{k}}(\eta,\eta_0) = \mathcal{O}(\mathrm{Max}[\omega_k^{-3}, G^{(\Gamma)}_{\vec{k}}\omega_k^{-1}]). \tag{3.38}$$

Since the sequences that define any of the two quantities in the Max function are square summable over $\mathbb{Z}^3$ [see the definition of $G^{(\Gamma)}_{\vec{k}}$, together with the asymptotic expression for $h^{\vec{k}}_I$ and condition (2.8)], we can conclude that the transformations implied by the Heisenberg equations (3.4) are unitarily implementable in Fock space.

A comment is in order at this point. In our previous analysis, we have assumed that $H^{(\Gamma)}_{\vec{k}} \neq 0$. If this were not the case, it is not hard to convince oneself that the beta coefficients of the dynamical Bogoliubov transformation would be of the same asymptotic order as ω_k^{-1}, given the behavior of $f^{(\Gamma)}_{1,k}$ and $f^{(\Gamma)}_{2,k}$. However, from Eq. (3.28) one can check that, for $H^{(\Gamma)}_{\vec{k}}$ to vanish, $\theta^{(x,y)}_{\vec{k}}$ must be precisely of order $\mathcal{O}(\omega_k^{-1})$. Since $\theta^{(x,y)}_{\vec{k}}$ forms a square summable sequence by assumption, that might only happen for $\vec{k}$ in some subset of $\mathbb{Z}^3_\uparrow$ where any sequence that is $\mathcal{O}(\omega_k^{-1})$ turned out to be square summable. Therefore, the Heisenberg dynamics would also be unitarily implementable in this particular case. Taking this into account, our following analysis about the backreaction can be applied to all possible scenarios.

Once we have confirmed the unitarity of the Heisenberg dynamics determined by our quantum expectation values over the homogeneous geometry, which do not even need to correspond to a background described by effective loop quantum cosmology, we can proceed to construct solutions of the associated Schrödinger equation (3.2) by evolving the initial Fock vacuum with the corresponding unitary operator. In order to do so, we follow the strategy of Ref. [27], conveniently generalized to the present situation but avoiding the repetition of redundant computations. First of all, given the asymptotic formula (3.34), it is most convenient to split the operator that implements the Heisenberg dynamics into the composition of two unitaries. The first one incorporates the dominant η_Γ-dependent phase of the alpha coefficients; namely, it is the unitary operator associated with the Bogoliubov transformation

$$\hat{a}^{(x,y)}_{\vec{k}} \to e^{-i\omega_k(\eta-\eta_0)-i\int_{\eta_0}^{\eta}d\eta_\Gamma\Xi_1^{\vec{k}}}\hat{a}^{(x,y)}_{\vec{k}},$$
$$\hat{b}^{(x,y)\dagger}_{\vec{k}} \to e^{i\omega_k(\eta-\eta_0)+i\int_{\eta_0}^{\eta}d\eta_\Gamma[\tilde{J}^{(\Gamma)}_{\vec{k}}+\Xi_1^{\vec{k}}]}\hat{b}^{(x,y)\dagger}_{\vec{k}}. \tag{3.39}$$

The second unitary operator then completes the dynamical transformation (3.20) by implementing the linear mapping

$$\hat{a}^{(x,y)}_{\vec{k}} \to \tilde{\alpha}_{\vec{k}}(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + \tilde{\beta}_{\vec{k}}(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}},$$
$$\hat{b}^{(x,y)\dagger}_{\vec{k}} \to -\bar{\tilde{\beta}}_{\vec{k}}(\eta,\eta_0)\hat{a}^{(x,y)}_{\vec{k}} + \bar{\tilde{\alpha}}_{\vec{k}}(\eta,\eta_0)\hat{b}^{(x,y)\dagger}_{\vec{k}}, \tag{3.40}$$

with

$$\tilde{\alpha}_k(\eta,\eta_0) = e^{i\omega_k(\eta-\eta_0)+i\int_{\eta_0}^{\eta}d\eta_\Gamma\Xi_1^{\vec{k}}}\alpha_k(\eta,\eta_0),$$
$$\tilde{\beta}_k(\eta,\eta_0) = e^{-i\omega_k(\eta-\eta_0)-i\int_{\eta_0}^{\eta}d\eta_\Gamma[\tilde{J}^{(\Gamma)}_{\vec{k}}+\Xi_1^{\vec{k}}]}\beta_k(\eta,\eta_0). \tag{3.41}$$

This latter operator can be written in the form $e^{-\hat{T}}$, with [27]

$$\hat{T} = \sum_{\vec{k}\neq\vec{\tau},(x,y)}[\Delta_{\vec{k}}\hat{a}^{(x,y)\dagger}_{\vec{k}}\hat{b}^{(x,y)\dagger}_{\vec{k}} - \bar{\Delta}_{\vec{k}}\hat{b}^{(x,y)}_{\vec{k}}\hat{a}^{(x,y)}_{\vec{k}} - i\rho_{\vec{k}}(\hat{a}^{(x,y)\dagger}_{\vec{k}}\hat{a}^{(x,y)}_{\vec{k}} + \hat{b}^{(x,y)\dagger}_{\vec{k}}\hat{b}^{(x,y)}_{\vec{k}}) + ic^{(x,y)}_{\vec{k}}], \tag{3.42}$$

where $c^{(x,y)}_{\vec{k}}\in\mathbb{R}$ is an undetermined phase, and we have chosen the following parametrization of the (modified) Bogoliubov coefficients:

$$\tilde{\alpha}_{\vec{k}} = \cos\sqrt{|\Delta_{\vec{k}}|^2 + \rho_{\vec{k}}^2} + i\rho_{\vec{k}} \frac{\sin\sqrt{|\Delta_{\vec{k}}|^2 + \rho_{\vec{k}}^2}}{\sqrt{|\Delta_{\vec{k}}|^2 + \rho_{\vec{k}}^2}},$$

$$\tilde{\beta}_{\vec{k}} = -\Delta_{\vec{k}} \frac{\sin\sqrt{|\Delta_{\vec{k}}|^2 + \rho_{\vec{k}}^2}}{\sqrt{|\Delta_{\vec{k}}|^2 + \rho_{\vec{k}}^2}}. \quad (3.43)$$

An analogous calculation to that presented in Ref. [27], taking now due care of the additional phase contribution $\tilde{J}_{\vec{k}}^{(\Gamma)}$, shows that the evolution of the fermionic Fock vacuum by the combined action of the two introduced unitary operators indeed gives rise to solutions of the Schrödinger equation (3.2), provided that

$$C_D^{(\Gamma)}(\phi) = l_0 \langle \hat{V}^{2/3} \rangle_\Gamma \sum_{\vec{k},(x,y)} [\Im(G_{\vec{k}}^{(\Gamma)} \bar{\Delta}_{\vec{k}}) - d_{\eta_\Gamma} c_{\vec{k}}^{(x,y)}]. \quad (3.44)$$

This is the fermionic contribution to the backreaction. In the rest of this section, we analyze the convergence of this fermionic backreaction by using our asymptotic analyses above. In fact, one might always set the quantity $C_D^{(\Gamma)}$ equal to 0 by means of an appropriate choice of $c_{\vec{k}}^{(x,y)}$, i.e., by conveniently tuning the phase of the solutions ψ_D to the Schrödinger equation, even if the total sum of these phases could then diverge. Ignoring this fine-tuning of the phases, and hence avoiding the possible resummation of two individually divergent quantities, we focus our attention on the terms that depend on $\bar{\Delta}_{\vec{k}}$. From our previous definitions and considerations, it is not difficult to check that $\tilde{\alpha}_{\vec{k}} = 1 + o(1)$ in the asymptotic regime of large ω_k. Therefore, the parametrization (3.43) implies that the asymptotically dominant term in $\Delta_{\vec{k}}$ is the same as for $\tilde{\beta}_{\vec{k}}$. Using Eq. (3.35) and the asymptotic behavior of $\Re(\Lambda_{\vec{k}}^l)$ shown in Eq. (3.32), we then obtain

$$\Im(G_{\vec{k}}^{(\Gamma)} \bar{\Delta}_{\vec{k}}) = \frac{1}{2\omega_k} \Bigg\{ |G_{\vec{k}}^{(\Gamma)}|^2 - \Re[G_{\vec{k}}^{(\Gamma)} \bar{G}_{\vec{k}}^{(\Gamma),0}] \cos\left[2\omega_k(\eta - \eta_0) + \int_{\eta_0}^{\eta} d\eta_\Gamma (\tilde{J}_{\vec{k}}^{(\Gamma)} + 2\Xi_1^{\vec{k}})\right] + \Im[G_{\vec{k}}^{(\Gamma)} \bar{G}_{\vec{k}}^{(\Gamma),0}] \sin\left[2\omega_k(\eta - \eta_0) + \int_{\eta_0}^{\eta} d\eta_\Gamma (\tilde{J}_{\vec{k}}^{(\Gamma)} + 2\Xi_1^{\vec{k}})\right] \Bigg\} + \tilde{\delta}_{\vec{k}}, \quad (3.45)$$

where the subdominant terms $\tilde{\delta}_{\vec{k}}$ are of the asymptotic order of $\delta_{\vec{k}} G_{\vec{k}}^{(\Gamma)}$, with the behavior of $\delta_{\vec{k}}$ being given in Eq. (3.36). Hence, to ensure that the backreaction is finite, without the need of introducing a divergent phase in the fermionic part of the states, we only have to impose that the sum over $\vec{k} \in \mathbb{Z}^3$ of the contributions in Eq. (3.45) be absolutely convergent. In particular, this condition eliminates any ambiguity that might affect the nonabsolute sum, given the possibility of attaining conditional convergences. Besides, we naturally require that this contribution to the backreaction is well defined independently of the choice of homogeneous state Γ, and for all times η. Taking into account the different asymptotic behaviors allowed for $\theta_{\vec{k}}^{(x,y)}$, we contemplate the following cases:

(i) For tuples $\vec{k} \in \mathbb{Z}_\uparrow^3$, we have from Eqs. (2.15) and (2.18) that $G_{\vec{k}}^{(\Gamma)}$ is of the same order as $\omega_k \theta_{\vec{k}}^{(x,y)}$. The subdominant term $\tilde{\delta}_{\vec{k}}$ in Eq. (3.45) is then asymptotically negligible compared to $[G_{\vec{k}}^{(\Gamma)}]^2 \omega_k^{-1}$, since $\theta_{\vec{k}}^{(x,y)}$ is of order $\omega_k^{-3/2}$ or higher in this case. Besides, with our assumptions [including condition (2.9)], the time-dependent oscillations in Eq. (3.45) cannot be compensated, at dominant order, with the first term. Hence, we conclude that the contribution to the backreaction is absolutely summable over the considered modes, independently of Γ, if and only if the sequence $\{\omega_k |\theta_{\vec{k}}^{(x,y)}|^2\}_{\vec{k} \in \mathbb{Z}_\uparrow^3}$ is summable (regardless of the values of the canonical variables for the homogeneous geometry on which $\theta_{\vec{k}}^{(x,y)}$ may depend). The sufficiency of this condition for the oscillating terms in Eq. (3.45) follows, in particular, from the use of the Cauchy-Schwarz inequality.

(ii) On the other hand, for $\vec{k} \in \tilde{\mathbb{Z}}^3$, we recall that $\omega_k \theta_{\vec{k}}^{(x,y)}$ must be negligible compared to $\omega_k^{-1/2}$. Employing the asymptotic expressions (2.15) and (2.19), we conclude that $G_{\vec{k}}^{(\Gamma)}$ is either of the same order as $\omega_k \theta_{\vec{k}}^{(x,y)}$ or of order ω_k^{-1}, whichever is dominant, unless these two types of contributions are of the same order and cancel each other. If this cancellation did not happen, at least for a nonempty infinite subset $\tilde{\mathbb{Z}}_1^3 \subseteq \tilde{\mathbb{Z}}^3$, it is not difficult to realize that the terms (3.45) would not be absolutely summable over $\tilde{\mathbb{Z}}^3$, given the asymptotic growth of the density of states with the Dirac eigenvalue ω_k. Therefore, it is necessary that the term $2\omega_k \theta_{\vec{k}}^{(x,y)}$ in $\tilde{H}_{\vec{k}}$ cancels any possible contribution of order ω_k^{-1} in $h_I^{\vec{k}}$, up to terms that are $o(\omega_k^{-1})$. Imposing this requirement, and recalling condition (2.9), we must have that, for $\vec{k} \in \tilde{\mathbb{Z}}_1^3$,

$$\theta_{\vec{k}}^{(x,y)} = -i \frac{\tilde{M} e^{-\alpha}}{4\omega_k^2} \pi_\alpha e^{iF_2^{\vec{k},(x,y)}} + \vartheta_{\vec{k}}^{(x,y)}, \qquad (3.46)$$

where $\vartheta_{\vec{k}}^{(x,y)} = o(\omega_k^{-2})$. This is a necessary condition for the absolute convergence of the terms (3.45) in $\tilde{\mathbb{Z}}^3$. Inserting this behavior into the interacting part of $\tilde{H}_{\vec{k}}$, and considering its relation with $G_{\vec{k}}^{(\Gamma)}$, one can show that this latter quantity has the same asymptotic order, for $\vec{k} \in \tilde{\mathbb{Z}}_1^3$, as the dominant contribution among the terms $\omega_k \vartheta_{\vec{k}}^{(x,y)}$ and ω_k^{-2}. The latter type of term automatically provides, when introduced in Eq. (3.45), a convergent series in $\tilde{\mathbb{Z}}_1^3$. Thus, following analogous arguments to those explained in our previous case, we reach the conclusion that the sufficient condition in $\tilde{\mathbb{Z}}^3$ for the absolute convergence of the considered fermionic backreaction is that

$$\sum_{\vec{k} \in \tilde{\mathbb{Z}}_1^3} \omega_k |\vartheta_{\vec{k}}^{(x,y)}|^2 < \infty \qquad (3.47)$$

and that the sequence $\{\mathrm{Max}[\omega_k^{-3}, \omega_k |\theta_{\vec{k}}^{(x,y)}|^2]\}_{\vec{k} \in \tilde{\mathbb{Z}}_2^3}$ be summable if the complement $\tilde{\mathbb{Z}}_2^3$ of $\tilde{\mathbb{Z}}_1^3$ in $\tilde{\mathbb{Z}}^3$ is infinite.

All of these conditions, that ensure that the backreaction contribution $C_D^{(\Gamma)}$ is well defined without introducing any regularization scheme, impose much more severe ultraviolet restrictions to the choice of fermionic annihilation and creationlike variables than the unitarity requirement (2.8). Besides, it is worth emphasizing that the asymptotic behavior characterized by conditions (3.46) and (3.47) must hold for $\vec{k}$ in a nonempty infinite subset $\tilde{\mathbb{Z}}_1^3$ of the lattice $\mathbb{Z}^3$, while each of the subsets for which one must demand the rest of conditions stated in the cases i and ii above might be empty. At the end of the day, the asymptotic behavior of the characteristic density of states of the Dirac eigenvalues in T^3 determines the specific form of these conditions. Because of this, if we further restricted the choice of annihilation and creationlike variables (e.g., by symmetry considerations) so that they could not depend on the tuple $\vec{k}$ except through the corresponding eigenvalue ω_k, we would conclude that the studied fermionic backreaction would be absolutely convergent if and only if conditions (3.46) and (3.47) are asymptotically satisfied for all $\vec{k} \in \mathbb{Z}^3$ (except, possibly, a finite subset).

Finally, let us comment that one may want to restrict even further the choice of fermionic variables in order to guarantee that the Hamiltonian operator that appears in the Schrödinger equation (3.2) has a well-defined action on the Fock vacuum. As a consequence, the Hamiltonian would then be properly defined in the dense subset of the Fock space $\mathcal{F}_D$ spanned by the n-particle/antiparticle states that have a finite number of fermionic excitations. In that case, the constraint equation (and thus the Schrödinger equations derived from it) would indeed be a rigorously defined equation, at least in what concerns the fermionic d.o.f. Given the normal ordering adopted in the fermionic Hamiltonian, it is clear that only the interacting terms, that annihilate and create infinite pairs of particles and antiparticles, may prevent the image of the vacuum providing a normalizable state in $\mathcal{F}_D$. In fact, this nomalizability holds if and only if the terms that multiply $a_{\vec{k}}^{(x,y)} b_{\vec{k}}^{(x,y)}$ (and their complex conjugates) in the decomposition of $\tilde{H}_D$ as a sum over modes form a square summable sequence. Arguments like those that we have explained show that this happens if and only if one imposes conditions that are similar to the ones displayed in i–ii above, but demanding the stronger requirement of the summability of the sequences

$$\{\omega_k^2 |\theta_{\vec{k}}^{(x,y)}|^2\}_{\vec{k} \in \mathbb{Z}_\uparrow^3}, \qquad \{\omega_k^2 |\vartheta_{\vec{k}}^{(x,y)}|^2\}_{\vec{k} \in \tilde{\mathbb{Z}}_1^3}, \qquad \text{and}$$
$$\{\mathrm{Max}[\omega_k^{-2}, \omega_k^2 |\theta_{\vec{k}}^{(x,y)}|^2]\}_{\vec{k} \in \tilde{\mathbb{Z}}_2^3}. \qquad (3.48)$$

IV. CONCLUSIONS

In this work, we have investigated a possible procedure to avoid some of the typical divergences of quantum field theory in the context of hybrid loop quantum cosmology. Specifically, we have studied in detail the case of a Dirac field minimally coupled to an inflationary cosmology. The Dirac field has been treated as a perturbation, including its zero mode if one exists, and in general additional scalar and tensor perturbations have been permitted. In our perturbative scheme, the action of the system is truncated at second order in all the perturbations. After decomposing the inhomogeneities in suitable modes, defined on the spatial hypersurfaces of the homogeneous model, the resulting relativistic system is subject to the zero mode of the Hamiltonian constraint, that in particular contains all the relevant fermionic contribution to the Hamiltonian, as well as to (an infinite mode collection of) perturbative constraints that are linear in the metric and scalar perturbations. At the considered quadratic perturbative order of our truncation, the time-dependent mode coefficients that describe the fermionic field are automatically gauge invariant with respect to these perturbative constraints. Besides, the rest of the perturbations in the system can be described by means of a set of canonical variables that are formed by the well-known Mukhanov-Sasaki and tensor gauge invariants, and by an Abelianized version of the linear perturbative constraints, together with all their momenta. The hybrid approach for the quantization of this cosmological system is based in a convenient Fock representation for each of the perturbative sectors of the phase space, combined with a less standard quantum gravity-inspired representation of the purely homogeneous d.o.f. (that can be thought to describe an inflationary FLRW cosmology on their own), namely the representation employed in loop quantum cosmology.

We have focused our analysis on divergences that may arise in the quantum theory from the standard Fock treatment of the fermionic d.o.f. Actually, we have explored the possibility of avoiding that these infinities appear by taking into consideration the fact that it is the whole phase space of the cosmological system what has to be treated quantum mechanically in a hybrid way, rather than only the fermionic d.o.f., while the FLRW cosmology is maintained as a classical entity. As commented above, this means that each sector of the total phase space is given a qualitatively different quantum representation. This applies in particular to what one may call the homogeneous background sector and the Dirac perturbations. Within this context, it does not seem unnatural to question whether one may separate them in different ways, and thus assign different dynamical roles to each of these sectors. These different alternatives for the splitting can be realized in practice, without affecting the rest of scalar and tensor perturbations, by considering canonical transformations of the fermionic variables that depend on the homogeneous background. When these transformations are completed to be canonical for the entire system (at the considered perturbative order of our truncation), the Hamiltonian that generates the dynamics of the new fermionic variables changes with respect to the original one. We are then tempted to expect that, with an adequate splitting of the joint dynamics of the geometric FLRW d.o.f. and the Dirac field, we may attain a satisfactory control of the divergences that arise from the quantum field theory representation of the fermionic variables in their corresponding Hamiltonian.

In more detail, here we have incorporated the freedom that exists in identifying the Heisenberg dynamics of the fermionic d.o.f., exploiting the different dynamical roles of the homogeneous background and of the fermionic perturbations, by introducing families of annihilation and creationlike variables that are obtained through background-dependent canonical transformations. The specific form of these transformations is *a priori* only restricted by the following physical consideration [and a mild condition on their dependence on the homogeneous d.o.f.: see Eq. (2.9)]. They must define variables that, in the context of quantum field theory in classical curved spacetimes, possess a nontrivial dynamics that is unitarily implementable in Fock space. Besides, the associated Fock vacuum must be invariant under the classical symmetries of the Dirac-FLRW system, and define a standard convention for particles and antiparticles. These families of annihilation and creationlike variables turn out to determine unitarily equivalent Fock representations of the Dirac field. With such a generic collection of different descriptions for the fermionic d.o.f., we have computed the form of the resulting Hamiltonian that generates their dynamics. In particular, we have characterized its asymptotic tail, when it is expressed as an infinite sum in terms of the annihilation and creation coefficients of the spatial eigenmodes of the Dirac operator. This fermionic Hamiltonian has a nontrivial dependence on the resulting homogeneous sector of the cosmological model. In fact, after implementing the hybrid quantization procedure and adopting a kind of Born-Oppenheimer ansatz for the physical quantum states that are annihilated by the zero mode of the entire constraint, one arrives at a fermionic Hamiltonian that is defined by means of expectation values over the homogeneous geometry, and that can be understood to generate a Schrödinger dynamics for the part of the states that encodes the information about the fermionic d.o.f. This Hamiltonian operator, which varies with the specific choice of annihilation and creationlike variables, generalizes the operator that would be obtained in quantum field theory on curved spacetimes, inasmuch as its dependence on the homogeneous background is no longer evaluated on a classical geometry, but replaced with the corresponding expectation values. We have carried out an asymptotic analysis, in the regime of large eigenvalues ω_k of the spatial Dirac operator, of the Heisenberg dynamics associated with this fermionic Hamiltonian, and we have shown that it amounts to a Bogoliubov transformation of the annihilation and creation operators which is unitarily implementable in Fock space. The vacuum state, when evolved with the corresponding unitary operator, can then be seen to provide solutions of the Schrödinger equation with a very specific backreaction term that depends on the geometric expectation values that define the considered dynamics. This backreaction term can serve to measure (in mean value) how much the homogeneous part of the quantum states departs from an exact solution of the unperturbed inflationary model. With the obtained asymptotic information about the Heisenberg dynamics, we have been able to characterize the choices of annihilation and creationlike variables, in the family under consideration, that allow for a finite fermionic backreaction, without the need of introducing any regularization technique or resummations of infinities based on a conditional convergence. Once we have guaranteed that the analyzed backreaction is well defined, we have seen that, with some slightly more stringent conditions on our choice of fermionic variables, we can also ensure that the fermionic Hamiltonian is actually a rigorously defined operator in the dense subset of the Fock space spanned by n-particle/antiparticle states.

The relevance of our characterization of the families of fermionic annihilation and creationlike variables that prevent divergences within the hybrid framework of loop quantum cosmology can be seen twofold. On the one hand, we have shown that, for an infinite number of modes, the canonical transformation that defines the fermionic variables must display a very specific asymptotic dependence on the homogeneous geometry, as well as on the mass of the Dirac field [see Eqs. (2.8) and (3.46)]. This dependence in the ultraviolet regime of large ω_k actually implies a severe restriction, in the quantum theory, about which part of the dynamical d.o.f. of the system must be treated as geometric, and which part contains the information about the genuine fermionic excitations. On the other hand, it is clear that a specific characterization of the physically admissible annihilation and creationlike variables leads to a restriction on the choice of fermionic vacuum, among the infinitely many that are available (even when restricting all considerations to choices selected by the unitarity of the classical dynamics). In fact, the already mentioned, specific dependence on the homogeneous background of the transformations that define the fermionic variables has the effect of reducing the asymptotic order of the interaction terms in the corresponding fermionic Hamiltonian. One could think that a further restriction of the choice of fermionic variables, and therefore of their vacuum, is possible if one investigates even deeper the asymptotic tail of the Hamiltonian and tries to eliminate completely its interacting contribution. If this procedure were viable, the variables determined in this way for the description of the fermionic d.o.f. would then diagonalize the resulting Hamiltonian, at least in the ultraviolet sector, and therefore might be thought to be optimally adapted to the quantum dynamics of the entire cosmological system.

Furthermore, the specification of suitable variables for the quantum description of the fermionic d.o.f. can, at least in certain regimes of physical interest, shed light on the influence that the dynamics of this type of matter might have on the quantum evolution of the homogeneous background geometry. In this work, such effects can be found, first, in the redefinition of the scale factor and its momentum that is required in order that they remain canonical with respect to the introduced fermionic variables. Besides, at least at the level of expectation values, a genuinely quantum backreaction of the fermionic d.o.f. on the behavior of the partial wave function that describes this homogeneous geometry is contained in the function $C_D^{(\Gamma)}$, inasmuch as it measures, in mean value, how much the homogeneous background differs from a quantum solution of the nonperturbed cosmology. These effects can be given precise formulas [see Eqs. (2.10), (2.11) and (3.44)] which, if shown to be well-defined quantities as $C_D^{(\Gamma)}$ has been seen to be here, can serve as a starting point for the quantitative determination of modifications that the presence of fermionic matter may introduce in the dynamics of the background geometry, with respect to the purely homogeneous scenario found in standard linearized cosmology (even when this is described within the context of loop quantum cosmology). These modifications would likely, in turn, leave some imprint in the evolution of the primordial perturbations of scalar and tensor type. Following techniques like those explored recently in Ref. [46], one may investigate the consequences and physical relevance that these modifications may have on the power spectrum of the cosmological perturbations, as well as on possible non-Gaussianities. Actually, it should be possible to perform an analysis similar to the one conducted in this work in order to specify a privileged family of variables for the description of scalar and tensor perturbations in quantum cosmology, such that their quantum Hamiltonian and backreaction effects display well-behaved properties. If that were the case, it might even be possible to investigate the interplay between their associated backreaction functions [analogous to $C_D^{(\Gamma)}$] [27], the fermionic contribution, and the quantum evolution of the background geometry.

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