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The phase-dependent linear conductance of a superconducting quantum point contact

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Abstract

The exact expression for the phase-dependent linear conductance of a weakly damped superconducting quantum point contact is obtained. The calculation is performed by summing up the complete perturbative series in the coupling between the electrodes. The failure of any finite order perturbative expansion in the limit of small voltage and small quasi-particle damping is analyzed in detail. In the low transmission regime this nonperturbative calculation yields a result which is at variance with standard tunnel theory. Our result predicts the correct sign of the quasi-particle pair interference term and exhibits an unusual phase-dependence at low temperatures in qualitative agreement with the available experimental data.

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Since the early stages in the theory of Josephson junctions it has been customary to write the total current through the junction as

$$I = I_J \sin\phi + G_0(1 + \epsilon \cos\phi)V, \tag{1}$$

where the total superconducting phase difference between the electrodes is related to the applied bias voltage by $d\phi/d\tau = 2eV/\hbar = \omega_0$.

Eq. (1) was first derived from a microscopic model by Josephson [1]. An equivalent expression has been widely used to describe superconducting point contacts [2]. The second term in Eq. (1) defines a phase-dependent conductance, $G(\phi) = G_0(1 + \epsilon \cos \phi)$, whose existence was confirmed by a series of experiments during the seventies [3]. However, it soon became apparent that the experimental results for low temperatures seemed to be best fitted by Eq. (1) with a value of the parameter $\epsilon \approx -1$, while tunnel theory predicts $\epsilon = +1$ in the limit $T, V \to 0$ [4]. Furthermore, an experiment measuring the complete phase dependence of the linear conductance in a point contact showed a strong departure of $G(\phi)$ from the simple $\cos \phi$-like form [5], given by tunnel theory. There was at the time a large number of theoretical works trying to explain the discrepancy between tunnel theory and experiments, most of them relying on the introduction of a phenomenological broadening of the Riedel peak (for a review see ref. [4]). However, a completely satisfactory explanation of this issue seems still to be lacking.

On the other hand, there has been in the last few years a renewed interest on the theory of superconducting weak links associated with the increasing technological capability for the fabrication of nano-scale superconducting devices. This opens the possibility of a closer comparison between theoretical predictions and clean experiments even on a nearly atomic scale [6]. It therefore seems appropriate at this point to perform a careful re-examination of the transport properties in superconducting point contacts going beyond the limits of standard tunnel theory. In this direction, one should mention some important theoretical contributions [7,8], clarifying the crucial role played by multiple Andreev-reflections in the explanation of the sub-harmonic structure in superconducting point contacts. This sub-gap structure can be currently analyzed experimentally with increasing resolution [6,9].

As will be shown in this letter, the presence of edge singularities in the spectral densities of the superconductors leads to an enhanced weight of these multiple scattering processes. As a consequence, a nonperturbative calculation is needed to obtain the correct result for the phase-dependent conductance. In a non-biased junction, the summation of the infinite series of multiple scattering events leads to the appearance of bound states inside the superconducting gap, whose existence has been discussed in previous theoretical works [10–12]. In the same way, the presence of bound states will allow us to obtain an exact expression for $G(\phi)$ valid in the limit of small quasiparticle damping.

We consider for simplicity the case of a symmetrical contact. Then, with L and R representing the left and right electrodes, we have $|\Delta_L| = |\Delta_R| = \Delta$ and $\phi = \phi_L - \phi_R$, where Δ is the modulus of the superconducting order parameter, ϕ representing the total phase difference which is supposed to drop abruptly at the interface between both electrodes.

To describe the biased point contact we use the following model Hamiltonian

$$\hat{H} = \hat{H}_L + \hat{H}_R + \hat{H}_{LR} + \frac{eV}{2}\left(\hat{N}_L - \hat{N}_R\right), \tag{2}$$

where $\hat{H}_L$ and $\hat{H}_R$ are the BCS Hamiltonians for the uncoupled electrodes, $(\hat{N}_L, \hat{N}_R)$ being the corresponding total number operators, and eV is the applied bias voltage. The term $\hat{H}_{LR}$ coupling both electrodes is assumed to have the following form

$$\hat{H}_{LR} = \sum_{i,j,\sigma}(t_{ij}c^{\dagger}_{i\sigma}c_{j\sigma} + t_{ji}c^{\dagger}_{j\sigma}c_{i\sigma}), \tag{3}$$

where (i, j) stand for orbitals on the (left, right) electrodes respectively. For the present analysis it is convenient to consider first the simplest case in which there is a single channel connecting both electrodes (the multi-channel case will be briefly discussed at the end of the letter). In this case $(i \equiv L, j \equiv R)$ denote the two orbitals connected by the single hopping element $t_{LR} = t$. We perform the standard unitary transformation [15,16], by means of which the system dynamics is governed by the following time-dependent Hamiltonian

$$\hat{H}(\tau) = \hat{H}_L + \hat{H}_R + \sum_{\sigma}(te^{i\phi(\tau)/2}c^{\dagger}_{L\sigma}c_{R\sigma} + te^{-i\phi(\tau)/2}c^{\dagger}_{R\sigma}c_{L\sigma}), \tag{4}$$

where $\phi(\tau) = \phi_0 + 2eV\tau/\hbar$. Within this representation the time-dependent phase only appears in the phase factors multiplying the hopping elements. The transport properties of this system can be analyzed using nonequilibrium Green functions techniques [8,12,18] with the time-dependent coupling term treated as a perturbation. The most relevant quantity in this formalism is the nonequilibrium distribution function $G^{+,-}$, which in a superconducting broken symmetry (Nambu) representation is defined by

$$\hat{G}^{+-}_{i,j}(\tau,\tau') = i \begin{pmatrix} < c^\dagger_{j\uparrow}(\tau') c_{i\uparrow}(\tau) > & < c_{j\downarrow}(\tau') c_{i\uparrow}(\tau) > \\ < c^\dagger_{j\uparrow}(\tau') c^\dagger_{i\downarrow}(\tau) > & < c_{j\downarrow}(\tau') c^\dagger_{i\downarrow}(\tau) > \end{pmatrix} . \tag{5}$$

In terms of these functions the current through the contact can be written as

$$I(\tau) = \frac{2e}{\hbar} \left[\hat{t}(\tau) \hat{G}^{+-}_{RL}(\tau,\tau) - \hat{t}^\dagger(\tau) \hat{G}^{+-}_{LR}(\tau,\tau) \right]_{11} , \tag{6}$$

where $\hat{t}$ is the matrix hopping element in the Nambu representation

$$\hat{t} = \begin{pmatrix} te^{i\phi(\tau)/2} & 0 \\ 0 & -te^{-i\phi(\tau)/2} \end{pmatrix} . \tag{7}$$

Within this perturbative approach the tunnel theory expression for the current (Eq. (1)), can be obtained at the lowest-order in $\hat{H}_{LR}$. The conductance $G_0(1+\epsilon\cos\phi)$ thus obtained becomes a divergent quantity in the limit $V \to 0$ [4]. In order to ensure the existence of a linear regime, a finite energy relaxation rate η must be introduced into this superconducting mean field theory (η represents the damping of the quasi-particle states, which in a real system is always present due to inelastic scattering processes). As we shall see, according to the value of η and the normal transmission coefficient of the junction, α [13], two different regimes can be identified: the weakly damped regime, for which $\eta \ll \alpha\Delta$ and the strongly damped case, where $\eta \gg \alpha\Delta$. In this work we are mostly concerned with the analysis of the first regime, where the most interesting effects appear.

A remarkable fact about the perturbative expansion in the weakly damped situation is that contributions corresponding to higher order processes turn out to be increasingly divergent in the zero bias limit [14]. In particular, it can be easily demonstrated that contributions to the total current of order t^{2n}, $n \geq 2$, diverge like $\sim t^{2n}/\eta^{n-1}$ (the lowest order contribution diverges as $\sim t^2 \ln\eta$). This result is a direct consequence of the increasing contribution from the superconducting gap edges singularities. Therefore, a correct answer cannot be found in principle by means of a finite order perturbative expansion.

One could draw a formal analogy with the case of a high-density electron gas, where the diagrammatic expansion in the bare Coulomb potential is also increasingly divergent.

As in that case, the solution can be found by "dressing" the perturbative potential, i.e. $\hat{H}_{LR}$. In the present problem the dressed quantities (left-right coupling, propagators) can be exactly obtained in the zero voltage limit by evaluating the complete perturbative series. To this end, we find it convenient to express all quantities in terms of a renormalized left-right coupling element which satisfies the following Dyson equation

$$\hat{T}^{a,r}(\tau,\tau') = \hat{t}(\tau)\delta(\tau-\tau') + \hat{t}(\tau)\hat{g}_R^{a,r}(\tau-\tau_1)\hat{t}^\dagger(\tau_1)\hat{g}_L^{a,r}(\tau_1-\tau_2)\hat{T}^{a,r}(\tau_2,\tau'), \tag{8}$$

where $\hat{g}_L^{a,r}$ and $\hat{g}_R^{a,r}$ represent the (advanced, retarded) Green functions of the uncoupled left and right electrodes respectively (integration over internal times is implicitly assumed). From Eq. (8), the relation between the renormalized coupling $\hat{T}$ and the exact (advanced and retarded) Green functions is easy to obtain. In the same way, the nonequilibrium distribution function $\hat{G}^{+-}$, which is related to $\hat{G}^r$ and $\hat{G}^a$, can be written in terms of $\hat{T}$ [19].

Integral equations like Eq. (8) adopt a simpler form when Fourier transformed with respect to their temporal arguments [8,19]. Defining the Fourier components $\hat{T}_{n,m}(\omega)$ as

$$\hat{T}_{n,m}(\omega) = \int d\tau \int d\tau' e^{-i(n\phi(\tau)-m\phi(\tau'))/2} e^{-i\omega(\tau-\tau')}\hat{T}(\tau,\tau'), \tag{9}$$

the total current can then be expressed in the form $I(\tau) = \sum_m I_m \exp im\phi(\tau)/2$, where the complex coefficients, I_m, do not depend on $\phi(\tau)$ and are given by

$$\begin{aligned} I_m = \frac{2e}{h}\int d\omega \sum_n \Big[& \hat{T}^r_{0,n}\hat{g}_R^{+-}(\omega+n\frac{\omega_0}{2})\hat{T}^{r\dagger}_{n,m}\hat{g}^a_L(\omega+m\frac{\omega_0}{2}) - \hat{g}^r_L(\omega)\hat{T}^r_{0,n}\hat{g}_R^{+-}(\omega+n\frac{\omega_0}{2})\hat{T}^{r\dagger}_{n,m} \\ & +\hat{g}^r_R(\omega)\hat{T}^{a\dagger}_{0,n}\hat{g}_L^{+-}(\omega+n\frac{\omega_0}{2})\hat{T}^a_{n,m} - \hat{T}^{a\dagger}_{0,n}\hat{g}_L^{+-}(\omega+n\frac{\omega_0}{2})\hat{T}^a_{n,m}\hat{g}^a_R(\omega+m\frac{\omega_0}{2})\Big]_{11}. \end{aligned} \tag{10}$$

It can be seen from Eq. (8) that $T_{n,m} = 0$ for even $n-m$ and therefore only even Fourier components of the current are different from zero.

For the following analysis it is useful to divide the total current into dissipative and nondissipative contributions. The supercurrent part, given by $I_S = -2\sum_{m>0}\mathrm{Im}(I_m)\sin[m\phi(\tau)]$, tends to a finite value in the limit $V \rightarrow 0$. On the other hand, the dissipative part is given by $I_D = I_0 + 2\sum_{m>0}\mathrm{Re}(I_m)\cos[m\phi(\tau)]$, and goes to zero as $I_D \sim G(\phi)V$, $G(\phi)$ being the zero voltage conductance. The linear term can be straightforwardly derived from Eq. (10) by expanding the Fermi functions appearing in $\hat{g}^{+-}_{L,R}$ [17] up to first order in V and evaluating the remaining factors at zero voltage.

In this limit the Fourier components satisfy $\hat{T}_{n,m} = \hat{T}_{0,m-n} \equiv \hat{T}_{m-n}$, and can be shown to obey the simple recursive relations

$$\begin{aligned} \hat{T}_{n+2}(\omega) &= z(w)\hat{T}_n(\omega) \\ \hat{T}_{-n-2}(\omega) &= z(\omega)\hat{T}_{-n}(\omega) \qquad (n \geq 1), \end{aligned} \tag{11}$$

where $z(\omega)$ is a scalar complex function. In the weakly damped regime and within the energy interval $\Delta > |\omega| > \Delta\sqrt{1-\alpha}$ this function reduces to a phase factor $z(\omega) = \exp i\varphi(\omega)$, where

$$\varphi(\omega) = \arcsin\left(\frac{2}{\alpha\Delta^2}\sqrt{\Delta^2 - \omega^2}\sqrt{\omega^2 - (1-\alpha)\Delta^2}\right). \tag{12}$$

This clearly shows that in the weakly damped regime and within this energy interval all multiple scattering processes become equally important. Therefore, all Fourier components contribute to the renormalized coupling in this region, giving rise to singularities which can be shown to be associated with the existence of interface bound states. In fact, the renormalized coupling in this energy region can be easily obtained from Eqs. (11) and (12), giving

$$\sum_n \hat{T}_n(\omega)e^{in\phi/2} = \frac{\hat{T}_1(\omega)e^{i\phi/2}e^{i(\varphi+\phi)}}{1 - e^{i(\varphi+\phi)}} + \frac{\hat{T}_{-1}(\omega)e^{-i\phi/2}e^{i(\varphi-\phi)}}{1 - e^{i(\varphi-\phi)}}, \tag{13}$$

which exhibits singularities at $\varphi(\omega) = \pm\phi$. From Eq. (12) it follows that these singularities correspond to simple poles at $\omega_S = \pm\Delta\sqrt{1 - \alpha\sin^2(\phi/2)}$. These are the interface bound states inside the gap of a superconducting point contact, as derived by different authors [10–12].

In the same way, the complete harmonic series must be evaluated in order to obtain the contributions to both the dissipative and nondissipative parts of the current coming from the energy range $\Delta > |\omega| > \Delta\sqrt{1-\alpha}$. Again, these infinite summations can be easily performed making use of the recursive relations of Eq. (11). It is then found that the integrand for both parts of the current becomes singular at $\omega = \pm\omega_S$. The contribution of these poles yields

$$I_S(\phi) = \frac{e\Delta}{2\hbar}\frac{\alpha\sin\phi}{\sqrt{1-\alpha\sin^2(\phi/2)}}\tanh(\frac{\beta\omega_S}{2}) \tag{14}$$

and

$$I_D(\phi) = \frac{2e^2}{h}\frac{\pi}{16\eta}\left[\frac{\Delta\alpha\sin\phi}{\sqrt{1-\alpha\sin^2(\phi/2)}}\mathrm{sech}(\frac{\beta\omega_S}{2})\right]^2\beta V. \tag{15}$$

In Eq. (14) the previously known result for the zero bias supercurrent is recovered [10–12]. The expression for the dissipative current given above is the main result of this letter. The linear conductance thus obtained can be seen to depend on η as $\sim 1/\eta$, i.e. proportional to a relaxation time. This result seems more physically sound than that of tunnel theory which predicts a dependence $\sim \ln\eta$. Notice that in the low barrier transparency regime Eq. (15) depends on the transmission coefficient as α^2 which means that Andreev reflection processes dominates over single quasiparticle tunneling in the zero voltage limit.

It is also worth commenting that Eq. (15) can be derived in a different way, by relating the linear conductance to the equilibrium current fluctuations via the fluctuation- dissipation theorem, giving further support for the validity of this expression. This will be the subject of a forthcoming publication.

Our theory yields a phase-dependent linear conductance which strongly deviates from the tunnel theory result of Eq. (1). In the limit of low barrier transparency, Eq. (15) predicts $G(\phi) \sim 1-\cos(2\phi)$ instead of $G(\phi) \sim 1+\epsilon\cos\phi$ of standard tunnel theory. Therefore, the linear conductance in Eq. (1) can never be recovered in the weakly damped regime. On the other hand, with increasing values of η multiple scattering processes are progressively damped (the function $z(\omega)$ is no longer a phase factor decaying exponentially with η); eventually, when $\eta \gg \alpha\Delta$ only the lowest-order processes contribute to the current and Eq. (1) is recovered. This explains the discrepancy between tunnel theory and the experiments (usually referred to as the "$\cos\phi$ problem"), because the experimental conditions should correspond to the weakly damped case in order that the Josephson effects could be observed [20].

Another interesting limiting case of Eq. (15) corresponds to the ballistic, i.e. $\alpha \to 1$, regime. In this case and for large temperatures $G(\phi)$ behaves approximately as $(1 - \cos\phi)$, in agreement with the result given by Zaitsev [18]. However, the most unusual phase-dependence of $G(\phi)$ appears for high values of the transmission and low temperatures ($k_B T < \Delta$). This is illustrated in Fig. 1, where $G(\phi)$ is plotted for two different temperatures and increasing values of the transmission. The only experiment where the full phase dependence of $G(\phi)$ was measured is, to our knowledge, that of ref. [5]. Their measured $G(\phi)$ strongly deviates from a $\cos\phi$-like form, being almost negligible for small values of ϕ and exhibiting a large increase around $\phi \sim \pi/2$. As can be observed in Fig. 1, this behavior is in qualitative agreement with our results at any given temperature for sufficiently large transmission. However, a detailed comparison should require a more exhaustive experimental study of $G(\phi)$ for different barrier transparencies and temperature regimes. We believe that these measurements are now becoming feasible with recent advances in the fabrication of nanoscale superconducting contacts.

The multi-channel generalization of our results is formally straightforward. For a general contact geometry it would lead to a superposition of contributions like those of Eqs. (14) and (15) for each transverse mode, which can in principle have different transmission probabilities. We do not expect that this effective averaging process would alter in a significant way the phase dependence of Eqs. (14) and (15).

In conclusion, it has been shown that a nonperturbative calculation is needed for obtaining the total current through a weakly damped superconducting point contact in the linear regime. Using a simple model Hamiltonian we are able to obtain exactly the phase-dependent linear conductance. The resulting expression is in good agreement with the available experimental data and we believe it can provide a motivation for more detailed experimental studies.

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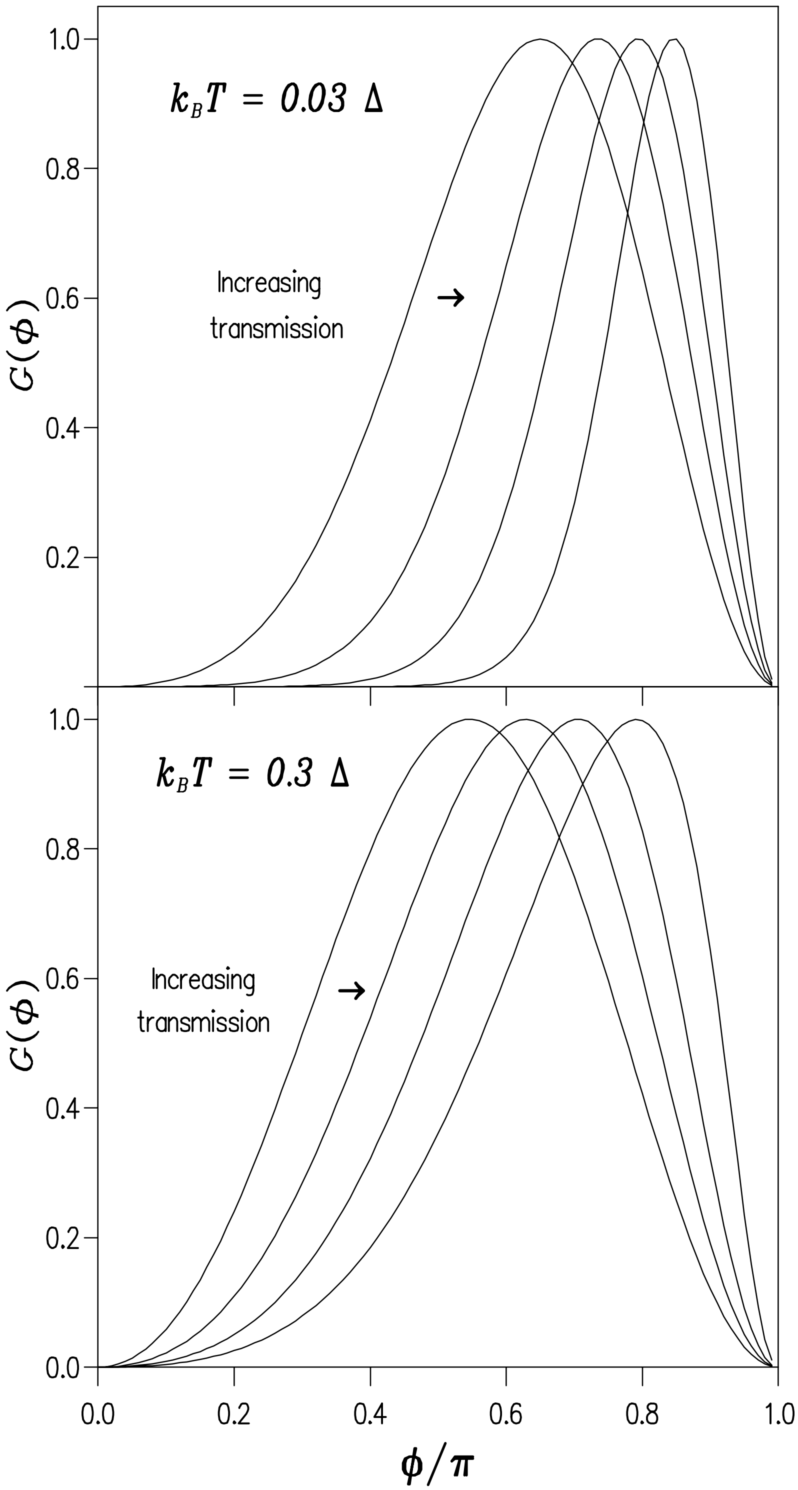
[20] The actual observation of the Josephson effects is usually hindered by thermal fluctuations and it is therefore necessary to have large enough barrier transparencies or sufficiently low temperatures.

FIGURES

FIG. 1. Phase dependence of the linear conductance given by Eq. (15) for two different temperatures and increasing values of the normal transmission coefficient ($G(\phi)$ is normalized to its maximum value).



$k_B T$ = 0.03 Δ
Increasing transmission
$k_B T$ = 0.3 Δ
Increasing transmission
G(φ)
G(φ)
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
φ/π