Microscopic theory of the phase-dependent linear conductance in highly transmissive superconducting quantum point contacts

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Abstract

A microscopic theory for transport properties of a superconducting quantum point contact is presented. According to contact transmission and quasiparticle damping two different physical regimes can be identified. In the limit of small applied voltages and weak damping this theory provides an exact analytical expression for the current through the contact. The phase-dependent linear conductance thus obtained exhibits an unusual behavior at low temperatures which strongly differs from the standard \( \cos \phi \)-like form. It is argued that a realistic highly transmissive contact will be accurately described by our analytical expression.

The field of superconducting point contacts and weak links has been the object of an increasing interest in recent years associated with the advances in the fabrication of nanoscale devices. Illustrative examples of these advances are the development of superconducting quantum point contacts (SQPC) on a nearly atomic scale using break junctions [1] and devices combining superconducting electrodes and microconstrictions in the two-dimensional electron gas of a gated heterostructure [2]. From a theoretical point of view this is an appealing situation due to the presence of quantization effects in the transport properties, which in turn simplifies the analysis considerably allowing a closer comparison with experiments.

In the present communication we report on a recent theoretical approach for the calculation of the transport properties of a SQPC in the limit of a small applied bias voltage. Within this limit, it has been customary to describe the current through a biased superconducting contact or tunnel junction [3, 4] by

\[
I = I_0 \sin \phi + G_0 (1 + \varepsilon \cos \phi) V,
\]

where the first term corresponds to the nondissipative tunneling of Cooper pairs while the second one to the tunneling of quasiparticles. While the \( \sin \phi \) dependence of the supercurrent has been confirmed experimentally, the discrepancy of the phase-dependent linear conductance \( G(\phi) = G_0 (1 + \varepsilon \cos \phi) \) with the experiments has been for a long time a puzzling issue. This discrepancy involves not only the sign of \( \varepsilon \) [4] but also, more importantly, the complete behavior of \( G \) as function of \( \phi \): the experiments [5] indicate a strong departure from a simple \( \cos \phi \) law.

In a recent publication [6], hereafter referred as I, we have discussed the failure of any finite-order perturbative expansion in the coupling between the electrodes for a SQPC in the limit of small voltages and small quasiparticle damping. This implies that a nonperturbative calculation is needed to obtain the correct expression for the current through the SQPC in this regime. In the present paper we shall briefly review the main steps in that calculation leading to an exact analytical expression for the phase-dependent linear conductance (most technical details will be omitted). The range of validity of such expression together with its most relevant experimental consequences will be discussed in detail.

We consider a model SQPC consisting of two BCS superconducting electrodes characterized by complex order parameters \( \Delta_{LR} \exp(i\phi_{LR}) \) coupled by a hopping term of the form

\[
\hat{H}_{LR} = \sum_{\alpha, \beta, \sigma} (t_{\alpha \beta} \epsilon^\dagger_{\alpha \sigma} c^\dagger_{\beta \sigma} + t_{\alpha \beta} \epsilon_{\alpha \sigma} c_{\beta \sigma}),
\]

where \( (\alpha, \beta) \) stand for orbitals on the (left, right) electrodes respectively. For simplicity we restrict our discussion to the
case of a symmetrical contact ($A_L = A_R$) and denote by $\phi$ the total phase difference between the electrodes $\phi_L - \phi_R$. The assumption of a step-like order parameter profile is justified when the contact size is much smaller than the superconducting coherence length [7]. Without loss of generality, the case of a single quantum channel connecting the electrodes will be considered.

Within this model and by means of a gauge transformation, the superconducting phase difference can be taken into account as a phase factor modifying the hopping amplitudes ($t_{LR} \rightarrow t \exp(i\phi)$) [6]. In the presence of a finite bias voltage, $V$, the phase difference varies with time as $\phi(t) = 2eVt/\hbar + \phi_0$.

In order to complete the description of our model it is convenient to introduce two more quantities: the normal transmission coefficient, denoted by $\alpha$ [8] and a quasiparticle energy relaxation rate $\eta$ due to inelastic scattering processes.

The transport properties of this model can be adequately analyzed by means of a nonequilibrium Green functions formalism [7, 9, 10]. The nonequilibrium Green functions obey a Dyson equation that can be formally solved by means of standard perturbative techniques [6] and assuming the coupling Hamiltonian $\hat{H}_{LR}$ as a perturbation.

The calculation of the current for any transmission and voltage range can be a rather involved problem. The difficulty arises essentially from the generation of an infinite series of Andreev reflection processes between the superconducting electrodes as depicted in Fig. 1. The only particularly simple limit is that of large voltages ($V \gg \Delta$), where the series can be truncated at the first step. In this limit the conductance tends to that of a normal contact with an excess current due to single Andreev reflection processes [9, 11].

However, the most interesting effects, like the appearance of subharmonic gap structure [11], are found for $V < \Delta$ where the evaluation of the current can only be performed by means of numerical methods [10, 11]. As illustrated in Fig. 1 the number of Andreev reflections taking place inside the gap region increases for decreasing $V$ (this is due to the fact that the energy shift between successive reflections is $2eV$). Only the region around the energy gap gives a significant contribution to Andreev processes, whose amplitude decay as $\Delta/\omega$ inside the continuous part of the spectrum.

In the limit $V \rightarrow 0$ the number of Andreev reflections inside the superconducting gap tends to infinity. As discussed below it is possible to obtain an analytical expression for the current (dissipative and nondissipative parts) within this limit by summing up the complete series of scattering processes inside the gap region. Within our model this is equivalent to the evaluation of the complete perturbative expansion in $t$ (any finite-order calculation would fail to give the correct result in this limit). A well known consequence of this multiple processes is the existence of interface bound states in the point contact spectral density

at $\omega_{3s} = \pm \Delta \sqrt{1 - \alpha^2}$ which carry the whole supercurrent in short constrictions [7, 12].

Let us stress that the above qualitative picture holds for the case of small values of the damping parameter $\eta$. For $\eta$ sufficiently large higher-order Andreev processes are heavily damped and can be neglected. As we show below the separation between the weakly damped (WDR) and strongly damped regimes (SDR) is defined by the condition $\eta \sim 2\Delta$.

Let us now briefly summarize the calculation of the transport properties within our theory in the limit $V \rightarrow 0$. In the general case, all dynamical quantities (spectral and current densities, etc.) can be expanded as a Fourier series of the form

$$A(\omega, V, \phi) = \sum_n A_n(\omega, V) e^{in\phi}.$$  

For analyzing the small voltage regime the Fourier coefficients in Eq. (6) can be expanded as $A_n(\omega, V) \sim A_n^{(0)}(\omega) + A_n^{(1)}(\omega)V$, where $A_n^{(0)} = A_n(\omega, 0)$ and $A_n^{(1)} = (\partial A_n/\partial V)(0, V)$. It must be stressed that such an expansion would be only valid in a voltage interval of the order of $\eta$.

![Fig. 1. Schematic representation of the multiple Andreev reflections inside the gap region taking place in a biased superconducting point contact. Case (a) corresponds to $V = 2\Delta/7$ and (b) to $V = 2\Delta/19$.](image)
around \( V = 0 \). (Notice that a finite \( \eta \) is necessary for the existence of a linear regime.)

In the WDR the coefficients \( A_n^{(n)} \) satisfy a very simple recursive relation within the energy range \( \Delta > |\omega| > \sqrt{1 - \varepsilon \Delta} \) [6]:

\[
A_n^{(n+1)} = e^{\phi(\omega)} A_n^{(n)},
\]

(4)

with \( \phi(\omega) = 2 \arcsin \sqrt{\left( \Delta^2 - \omega^2 \right)/\varepsilon^2} \).

Eq. (4) is the mathematical expression of the physical fact that in this limit (\( V \to 0 \) and \( \eta \ll \varepsilon \Delta \)) all multiple scattering processes contribute equally to the transport and electronic properties. On the other hand, this particular recursive relation is directly related to the existence of the aforementioned bound states in the region \( \Delta > |\omega| > \sqrt{1 - \varepsilon \Delta} \). This can be easily understood by noticing that, provided that a recursive relation like (4) holds, any dynamical quantity \( A(\omega) \) given by Eq. (3) becomes a geometrical series which has a divergent behavior at \( \phi = \phi(\omega) \). This condition is equivalent to the presence of poles in \( A(\omega) \) at \( \omega = \omega_{\text{S}}(\phi) \). Therefore, in this linear regime and in virtue of Eq. (4), calculation of any dynamical quantity reduces to the evaluation of the first coefficients \( A_0^{(0)}(\omega) \) and \( A_1^{(1)}(\omega) \).

In I we describe in detail how this procedure can be applied to the calculation of the current through a superconducting point contact. In this case \( \sum_n A_n^{(0)}(\omega) \exp(n\phi) \) and \( \sum_n A_n^{(1)}(\omega) \exp(n\phi) \) would correspond respectively to the nondissipative and dissipative parts of the total current. The result is then obtained by evaluating the residues of \( A(\omega) \) at \( \omega = \omega_{\text{S}} \) yielding

\[
I_S(\phi) = \frac{e\Delta}{2\hbar} \frac{z \sin \phi}{\sqrt{1 - z \sin^2(\phi/2)}} \tanh \left( \frac{\beta \omega_{\text{S}}}{2} \right),
\]

(5)

and

\[
G(\phi) = \frac{2e^2}{\hbar} \frac{\pi}{16\eta} \left[ \frac{\Delta z \sin \phi}{\sqrt{1 - z \sin^2(\phi/2)}} \sech \left( \frac{\beta \omega_{\text{S}}}{2} \right) \right]^2, \quad (6)
\]

Fig. 2. Transition between the weakly and strongly damped regimes. The ratio between the exact numerical conductance and: (a) the analytical expression of Eq. (6) and (b) the tunnel theory \( O(\eta^2) \) conductance, is plotted against \( \eta/\Delta \). The values of \( z \) considered are: (i) 0.15, (ii) 0.48, (iii) 0.64, (iv) 0.78, (v) 0.88, (vi) 0.95 and (vii) 0.99.

\[
G(\phi) = \frac{2e^2}{\hbar} \frac{\pi}{16\eta} \left[ \frac{\Delta z \sin \phi}{\sqrt{1 - z \sin^2(\phi/2)}} \sech \left( \frac{\beta \omega_{\text{S}}}{2} \right) \right]^2, \quad (6)
\]

where \( \beta = 1/k_B T \). Eq. (5) for the supercurrent has been previously derived using different approaches in Ref. [7, 12]. The expression of Eq. (6) for \( G(\phi) \) is our main new result. It is interesting to point out the existence of an analogy between our expression for \( G(\phi) \) and the conductance of a normal mesoscopic loop threaded by a magnetic flux [13]. The reason for this analogy lies in the fact that in both systems the current is mainly carried by two phase-dependent discrete levels.

One of the most striking consequences of Eq. (6) is that when \( z \to 0 \) the tunnel theory conductance \( G(\phi) = G_0(1 + \varepsilon \cos \phi) \) is not recovered. In fact, the tunnel theory result becomes only valid in the SDR. It is therefore worth to analyze in detail the transition from the WDR to the SDR.

In the SDR the recursive relation (4) no longer holds. On the contrary, higher harmonics are very quickly damped. For \( \eta \) sufficiently large (i.e. \( \eta \gg \varepsilon \Delta \)) the series (3) can be truncated after the first harmonic. Thus, when \( z \ll 1 \) and \( \eta \gg \varepsilon \Delta \) a perturbative calculation to the lowest order in the coupling \( t \) becomes a good approximation.

Figs. 2(a) and (b) illustrate the transition from the WDR to the SDR and allow to establish more precisely the range.
of validity of our expression for $G(\phi)$. In Fig. 2(a) the ratio between the exact conductance to the analytical expression of Eq. (6) is plotted as a function of $\eta$ for increasing values of the transmission coefficient (the exact linear conductance is obtained by the numerical evaluation of the harmonic series associated to the dissipative current). As can be observed, this ratio tends to unity for $\eta$ sufficiently small, within a range $\eta < \eta A$ in agreement with the criterion for the definition of the WDR previously discussed. Notice that when approaching perfect transmission the range of validity of the WDR approximation becomes $\eta \sim A$.

On the other hand, the validity of standard tunnel theory for the SDR is illustrated in Fig. 2(b), where the ratio between the exact numerical conductance and the $O(\epsilon^2)$ expression is represented as a function of $\eta$. From this figure it is clear that tunnel theory becomes valid only for sufficiently small transmissions such that $\eta / A \gg 1$. We can therefore conclude that a realistic highly transmissive point contact, in which $\eta$ can be assumed to be a small fraction of $A$, will be always described better by our WDR result [14].

The more unusual and interesting experimental consequences of Eq. (6) would arise when measuring the complete phase dependence of the linear conductance at low temperatures. An experiment of this kind was performed by Rifkin and Deaver [5] using an experimental setup in which the point contact was connected to a superconducting ring (this allows to control the phase by varying the magnetic flux through the ring). In Fig. 3 the experimental data of Rifkin and Deaver for $G(\phi)$ is represented together with our theoretical results for some selected values of the parameters $\alpha$ and temperature. In both cases $G(\phi)$ exhibits a clear asymmetry with respect to $\phi = \pi/2$ in contrast to the expected $\cos(\phi)$-like form of standard tunnel theory.

In conclusion, we have obtained an exact analytical expression for the phase-dependent linear conductance valid for the WDR. This expression predicts an unusual phase dependence (with a strong departure from a simple $\cos(\phi)$-like form) specially for low temperatures and large transmissions, in agreement with the available experimental data. Further experimental investigation of this quantity taking advantage of the recently developed nanoscale SQPCs would be desirable.

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References

[8] The normal transmission coefficient is given in our model by $\eta = 4(2\epsilon/W)^2/(1 + (2\epsilon/W)^2)^2$, where $W$ is the electrodes half-bandwidth. See for instance J. Ferrer, A. Martin-Rodero and F. Flores, Phys. Rev. B 38 (1988) 10113.