Adiabatic dynamics of superconducting quantum point contacts

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Starting from the quasiclassical equations for nonequilibrium Green's functions we derive a simple kinetic equation that governs the ac Josephson effect in a superconducting quantum point contact at small bias voltages. In contrast to existing approaches the kinetic equation is valid for voltages with arbitrary time dependence. We use this equation to calculate frequency-dependent linear conductance, and dc *I-V* characteristics with and without microwave radiation for resistively shunted quantum point contacts. A novel feature of the *I-V* characteristics is the excess current $2I_c/\pi$ appearing at small voltages. An important by-product of our derivation is the analytical proof that the microscopic expression for the current coincides at arbitrary voltages with the expression that follows from the Bogolyubov–de Gennes equations, if one uses appropriate amplitudes of Andreev reflection, which contain information about the microscopic structure of the superconductors.

Point contacts between normal metals have simple Ohmic *I-V* characteristics regardless of their electron transparency D. In contrast to this, *I-V* characteristics of the superconducting point contacts may be highly nonlinear even in the simplest situation of short constriction between two ideal BCS superconductors, and exhibit a nontrivial dependence on D. The origin of this complexity is the oscillating Josephson current, which makes electron motion in the contact essentially inelastic.[1,2] Recently, there has been considerable progress in calculation of both dc and ac (Refs. 3–5) components of current in such contacts. However, the results were limited to the situation when the contact is biased with a constant (in time) voltage supplied by an ideal source with vanishing impedance.

It is of interest to generalize the theory of electron transport in superconducting point contacts to the case of finite impedance of the voltage source as well as to time-dependent voltages. This generalization is particularly important in view of the fact that most experimental realizations of superconducting quantum point contacts[6,7] are based on the superconductor/semiconductor heterojunctions, which typically have relatively large impedance. Below we develop such a generalization, which is valid for small bias voltages $V \ll \Delta/e$, where Δ is the superconductor energy gap in the electrodes.

We consider a ballistic quantum point contact with characteristic dimensions much smaller than both the elastic scattering length and coherence length of the superconducting electrodes. dc supercurrent in such a contact is known to be carried by the two discrete energy states with energies $\epsilon_\pm = \pm\Delta\cos\varphi/2$ inside the energy gap,[8–10] where φ is the Josephson phase difference across the contact. These states are spatially localized in the contact region because of the Andreev reflection. At low voltages $V \ll \Delta/e$, the dynamics of these states is slow on the frequency scale given by the energy gap, $\dot{\varphi} = 2\ \mathrm{eV}/\hbar \ll \Delta/\hbar$, and one could expect the ac Josephson effect in this regime to be described in terms of the same two quasistationary states. However, in contrast to the stationary regime ($V \equiv 0$) when the occupation of these states is given simply by the equilibrium Fermi-Dirac probabilities, in the nonstationary situation the occupation of these states is quite nontrivial.

We first discuss our final result, the kinetic equation that governs the evolution of occupation probabilities $p_\pm$ of the levels $\epsilon_\pm$. (The systematic development leading to this equation is presented in the last part of the paper.) Because of the normalization condition $\Sigma_\pm p_\pm = 1$, it is convenient to write the kinetic equation in terms of the difference of the two probabilities, $p(\varphi(t)) \equiv p_- - p_+$. Kinetic equation for $p(\varphi)$ is

$$\dot{p}(\varphi(t)) = \gamma(\epsilon)[n(\epsilon) - p(\varphi(t))], \tag{1}$$

where $n(\epsilon) = \tanh(\epsilon/2T)$ is the equilibrium value of $p(\epsilon(\varphi))$; $\gamma(\epsilon)$ is the rate of quasiparticle exchange between the bulk electrodes and discreet levels in the constriction, and $\epsilon = \epsilon(\varphi) \equiv \Delta\cos\varphi/2$. The rate γ is roughly proportional to the subgap density of states in the superconducting electrodes; it vanishes in the ideal BCS case; if the gap is slightly smeared by finite electron-phonon interaction, γ is given by the following expression:[11,12]

$$\gamma(\epsilon) = \alpha \int d\epsilon' \frac{\Theta(\epsilon'^2 - \Delta^2)}{\sqrt{\epsilon'^2 - \Delta^2}} \frac{(\epsilon - \epsilon')^3 \cosh(\epsilon/2T)}{\sinh[(\epsilon - \epsilon')/2T]\cosh(\epsilon'/2T)}. \tag{2}$$

Here α is a constant determined by the parameters of electron-phonon interaction. To the kinetic equation (1) we should add a "boundary condition" which states that the level occupation reaches equilibrium as soon as the levels hit the gap edges, $\epsilon = \pm\Delta$ (Fig. 1), that is,

$$p(\varphi) = (-1)^m n(\Delta) \quad \text{for} \quad \varphi = 2\pi m, \tag{3}$$

where $m = 0, \pm 1, \ldots$.(3) We can take into account small reflection coefficient $\mathscr{R}$ of the point contact, $\mathscr{R} \ll 1$, by including in the kinetic equation the Zener transitions between the two levels that occur at the point $\varphi = \pi \mathrm{mod}(2\pi)$ with the probability λ.[5] For vanishing external resistance the transition probability is $\lambda = \exp\{-2\pi\mathscr{R}\Delta/\hbar|\dot{\varphi}|\}$, where $\dot{\varphi}$ is taken

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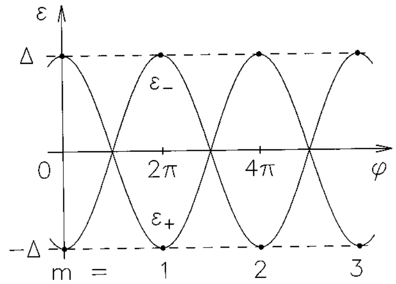

FIG. 1. Energies $\epsilon_{\pm}$ of the two Andreev-bound levels in a short constriction between two superconductors as functions of the Josephson phase difference φ. Solid dots represent "thermalization points" where occupation of the 2 level always reaches equilibrium. The diagram illustrates sign conventions for the kinetic equation (1) and the boundary condition (3).

at the transition point. Account of the Zener transitions is achieved by imposing one more boundary condition on $p(\varphi)$:

$$p[\varphi+0\,\mathrm{sgn}(\dot{\varphi})]=(2\lambda-1)p[\varphi-0\,\mathrm{sgn}(\dot{\varphi})] \qquad (4)$$

for $\varphi=\pi \bmod (2\pi)$. The function $p(\varphi(t))$ given by Eqs. (1)–(4) determines the current $I(t)$ in the point contact:

$$I(t)=(\pi\Delta/eR_N)\sin[\varphi(t)/2]\,p(\varphi(t)), \qquad (5)$$

where $R_N=\pi\hbar/Ne^2$ is the normal-state resistance of the contact, and N is the number of transverse modes that are all assumed to be identical.

Equations (1)–(5) allow us to describe the dynamics of the point contact under arbitrary bias conditions. As a first example, we consider the *linear response* of the voltage-biased point contact to small oscillations of the Josephson phase difference around some stationary point φ_0, i.e., $\varphi(t)=\varphi_0+\varphi_\omega e^{-i\omega t}$, $|\varphi_\omega|\ll 1$. Equations (1) and (5) with this $\varphi(t)$ give that the current oscillates around the stationary value:[13]

$$I_s(\varphi_0)=(\pi\Delta/eR_N)\sin(\varphi_0/2)\tanh(\epsilon_0/2T), \qquad (6)$$

so that $I=I_s+I_\omega e^{-i\omega t}$, and the frequency-dependent linear conductance is

$$Y(\omega)=\frac{I_\omega}{V_\omega}=\frac{2eiI_\omega}{\hbar\omega\varphi_\omega}=\frac{2\pi\Delta}{\hbar\omega R_N}\left[\frac{\Delta}{4T}\,\frac{\sin^2(\varphi_0/2)}{\cosh^2(\epsilon_0/2T)}\,\frac{\gamma(\epsilon_0)}{\omega+i\gamma(\epsilon_0)}+\frac{i}{2}\cos\frac{\varphi_0}{2}\tanh\left(\frac{\epsilon_0}{2T}\right)\right], \qquad (7)$$

where $\epsilon_0=\epsilon(\varphi_0)$. This equation generalizes the corresponding expression obtained by Zaitsev[1] for large temperatures $T\gg\Delta$. [Note that Eq. (7), as well as the kinetic equation (1), gives only the leading terms in small relaxation rate γ.]

We also can define the linear response to small dc voltage, $V\ll\hbar\gamma/e$. In this case the phase increases indefinitely, $\varphi(t)=\varphi_0+2\ \mathrm{eV}t/\hbar$, but deviation of the occupation probability p from equilibrium is still small. For such an evolution of φ, Eqs. (1) and (5) give

$$I(t)=I_s[\varphi(t)]+\frac{V}{R_N}\,\frac{\pi\Delta^2}{2\hbar\gamma(\epsilon)T}\,\frac{\sin^2[\varphi(t)/2]}{\cosh^2(\epsilon/2T)}, \qquad (8)$$

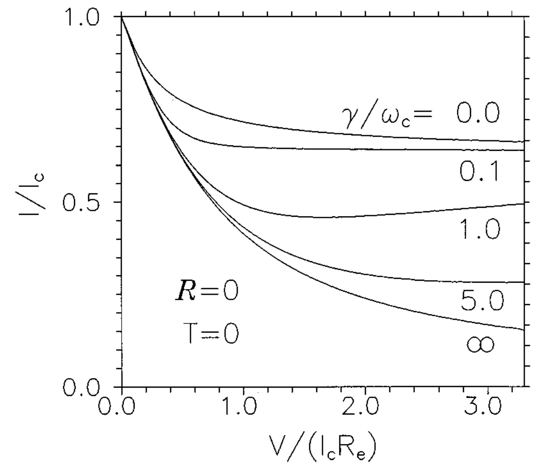

FIG. 2. dc *I*-*V* characteristics of the resistively shunted ballistic superconducting quantum point contact for various ratios of external Ohmic resistance R_e and relaxation rate γ at zero temperature; $\omega_c\equiv 2eI_cR_e/\hbar$.

where $\epsilon=\epsilon[\varphi(t)]$. This equation is the generalization of the recent result[14] to energy-dependent relaxation rate $\gamma(\epsilon)$. We see that both types of linear response are sensitive functions of $\gamma(\epsilon)$ and therefore they may be used to measure the subgap density of states in the superconductors.

As another application of the kinetic equation (1) we consider *resistively shunted* superconducting quantum point contact biased by an external current I_e (see inset in Fig. 3). For such a bias condition, the evolution equation for φ reads

$$\hbar\dot{\varphi}(t)/2eR_e=I_e-I[\varphi(t)], \qquad (9)$$

where current $I[\varphi(t)]$ should be calculated from Eqs. (1)–(5) self-consistently with $\varphi(t)$, and R_e is the shunting Ohmic resistance, which adiabatic approximation requires to be small: $R_e\ll R_N$. We limit ourselves to low temperatures $T\ll\Delta$.

For very small external resistances $R_e/R_N\ll\{(\hbar\gamma/\Delta),\mathscr{R}\}$, the rate of φ evolution is small and the current $I(\varphi)$ is given by the stationary relation (6). Applying this relation in Eq. (9), we conclude that the dc I-V characteristic of the point contact is given by the same relation as in the standard resistively shunted junction (RSJ) model (see, e.g., Ref. 15, Sec. 4.2). In the opposite limit of relatively large external resistances $R_e/R_N\gg\{(\hbar\gamma/\Delta),\mathscr{R}\}$, the *I*-*V* characteristic is given by the following relations:

$$V=\frac{(I_e^2-I_c^2)^{1/2}}{R_e}\,\frac{\pi}{4\ \arctan\sqrt{(I_e+I_c)/(I_e-I_c)}},\quad I=I_e-V/R_e. \qquad (10)$$

The main qualitative difference between expression (10) and the quasistationary RSJ *I*-*V* characteristics is the excess current: $I\rightarrow 2/\pi I_c$ for $V\gg I_cR_e$ in Eq. (10), whereas the current vanishes at large voltages in the quasistationary case. Note that Eq. (10) and Figs. 2 and 3 give the *I*-*V* characteristics in the form (i.e., without the linear term V/R_e) that is directly applicable to typical bias conditions of point contacts that are not shunted intentionally. Under these conditions there is no shunting resistance at zero frequency, but there is finite impedance of the biasing leads in series with the contact at

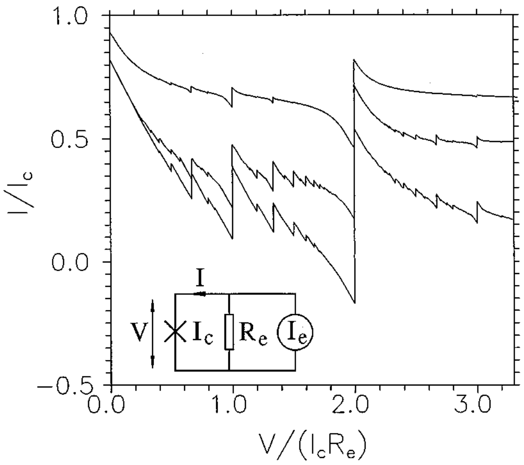

FIG. 3. Effect of microwave radiation with the amplitude $A=2I_c$ and frequency $\Omega=2\omega_c$ on the dc I-V characteristics of the resistively shunted superconducting point contact. The contact parameters are the same as in Fig. 2. From top to bottom, the curves correspond to $\gamma/\omega_c=0,1,\infty$.

frequencies of the Josephson oscillations. It is known that this situation can be reduced to the RSJ model by simple subtraction of the dc current through the resistor (see, e.g., Ref. 15, Sec. 12.4).

Figure 2 shows how I-V characteristics evolve from the quasistationary RSJ form into Eq. (10) with increasing external resistance. The curves were calculated numerically from Eq. (9) assuming no reflection in the point contact ($\mathscr{R}=0$), and also assuming that γ is a phenomenological constant independent of energy. In the case when this transition is driven not by finite relaxation rate γ but by finite reflection $\mathscr{R}$ the curves look qualitatively very similar.

Figure 3 shows dc I-V characteristics of the point contact under microwave irradiation, $I_e(t)=I_0+A\cos(\Omega t)$, which exhibit the usual Shapiro steps at voltages $V_{k,m}=(k/m)\hbar\Omega/2e$. We see that the height of the subharmonic steps ($m\neq 1$) that are the hallmark of the presence of higher harmonics in $I(\varphi)$ depends strongly on the value of external resistance. It increases for small external resistance due to the current discontinuity at $\varphi=\pi \bmod 2\pi$.

Now we briefly outline the major steps leading to our basic kinetic equation (1). We start with the quasiclassical equation for nonequilibrium Green's functions of the superconductors (for a general introduction to this technique see, e.g., Ref. 16). The Green's functions can be represented as $G^{(0)}+G$, where G is a space-dependent nonequilibrium addition to the equilibrium part $G^{(0)}$ that is constant inside each electrode. For short constrictions, equations for the retarded and advanced parts of G read[11,1]

$$iv_F\frac{\partial G_{R,A}}{\partial z}=[H_{R,A},G_{R,A}],\quad H_{R,A}=(\delta_{R,A}+i\gamma_{el})G^{(0)}_{R,A},\tag{11}$$

where $\delta_{R,A}\equiv[(\epsilon\pm i\gamma_1)^2-(\Delta\pm i\gamma_2)^2]^{1/2}$; $\gamma_{1,2}$ and $\gamma_{\rm el}$ are, respectively, inelastic and elastic scattering rates, v_F is the Fermi velocity, and coordinate z measures the distance from the point contact ($z=0$) into the electrodes ($z\rightarrow\pm\infty$). All functions in Eq. (11) are matrices in the electron-hole space; for instance, $G^{(0)}_{R,A}(\epsilon,\epsilon')=\{[(\epsilon\pm i\gamma_1)\sigma_z+(\Delta\pm i\gamma_2)i\sigma_y]/\delta_{R,A}\}\delta(\epsilon-\epsilon')$, with σ's here and below denoting Pauli matrices.

The functions G should decay inside the electrodes (at $z\rightarrow\infty$). If we perform "rotation" in the electron-hole space diagonalizing $G^{(0)}_{R,A}$,

$$G^{(0)}_{R,A}(\epsilon,\epsilon')\rightarrow U_{R,A}(\epsilon)G^{(0)}_{R,A}(\epsilon,\epsilon')U^{-1}_{R,A}(\epsilon')=\pm\sigma_z\delta(\epsilon-\epsilon'),$$

$$U_{R,A}=(1+a_{R,A}\sigma_x)/\sqrt{1-a^2_{R,A}},\tag{12}$$

where $a_{R,A}\equiv(\epsilon\pm i\gamma_1-\delta_{R,A})/(\Delta\pm i\gamma_2)$; Eq. (11) shows then explicitly that solutions decaying inside the electrodes should have the following matrix form:

$$G^{(1,2)}_R=U_R^{-1}u^{(1,2)}_R\sigma_\pm U_R,\quad G^{(1,2)}_A=U_A^{-1}u^{(1,2)}_A\sigma_\mp U_A,\tag{13}$$

where $\sigma_\pm=\sigma_x\pm i\sigma_y$, and $G^{(1,2)}$ denote the function in the first ($z<0$) and the second ($z>0$) electrode, respectively.

The total Green's functions should be continuous at the point contact ($z=0$). Imposing this condition and taking into account that there is a voltage drop V between the two electrodes of the point contact we can determine the functions $u^{(1,2)}_{R,A}$ in Eq. (13). At small voltages $V\rightarrow 0$, we get then for the total Green's functions $\bar{G}_{R,A}=G_{R,A}+G^{(0)}_{R,A}$ at $z=0$:

$$\bar{G}_{R,A}(\epsilon,t)=\int\frac{d\epsilon'}{2\pi}\bar{G}_{R,A}\left(\epsilon+\frac{\epsilon'}{2},\epsilon-\frac{\epsilon'}{2}\right)e^{i\epsilon' t}$$

$$=\frac{i}{2\pi}\frac{\sigma_z\cos[\varphi/2-\arccos(\epsilon/\Delta)]+i\sigma_y}{\sin[\varphi/2-\arccos(\epsilon/\Delta)\pm i0]},\tag{14}$$

where $\bar{G}_{R,A}$ depend on time t via the time dependence of the Josephson phase difference φ, $\varphi=2\ {\rm eV}\ t/\hbar+\varphi_0$. In Eq. (14) we neglected the relaxation rates $\gamma_{1,2}$ assuming that they are small. This is a legitimate approximation since, as usual, the effect of small energy relaxation on the occupation probabilities (i.e., on G_K) is much more important than the effect on the density of states. For $\bar{G}_{R,A}$ given by Eq. (14), the latter effect would be a small broadening of the Andreev-bound level.

One can check directly from Eq. (14) that this equation agrees with the stationary Green's functions calculated first by Kulik and Omel'yanchuk.[13] In particular, in the subgap range $|\epsilon|<\Delta$ it corresponds precisely to one of the two Andreev-bound discrete energy levels: ${\rm Re}\bar{G}_{R,A}\propto\delta[\epsilon-\Delta\ {\rm sgn}(\sin\varphi/2)\cos\varphi/2]$. Since the evolution equation (11) and, consequently, Eq. (14) refer to electrons moving in the positive z direction ($p_z>0$) this is the level that carries current in one direction. The evolution equation for electrons with $p_z<0$ differs only by the sign in front of v_F. In this case we get that $\bar{G}_{R,A}$ corresponds to the energy level at $\epsilon=-\Delta\ {\rm sgn}(\sin\varphi/2)\cos\varphi/2$.

To find the current $I(t)$ in the point contact we need to calculate the Keldysh component G_K of the Green's function:[11,1]

$$I(t)=\frac{\pi}{2R_N}\int d\epsilon{\rm Sp}\{\sigma_z(\bar{G}^{(p_z>0)}_K(\epsilon,t)-\bar{G}^{(p_z<0)}_K(\epsilon,t)\}.$$

The equation for G_K is

$$iv_F\,\partial G_K/\partial z = H_R G_K + H_K G_A - G_R H_K - G_K H_A\,, \quad (15)$$

where $H_K = H_R n - n H_A$, $H_{R,A}$ are defined in Eq. (11), and n is the equilibrium quasiparticle distribution, $n(\epsilon,\epsilon') = \tanh(\epsilon/2T)\,\delta(\epsilon-\epsilon')$. This equation shows that G_K can be written as[3] $G_K = G_R n - n G_A + G_H$, where G_H is the part that satisfies the homogeneous equation

$$iv_F\,\partial G_H/\partial z = H_R G_H - G_H H_A\,. \quad (16)$$

Following the same steps that led to Eq. (131) we get that G_H should have the following matrix form:

$$G_H^{(1,2)} = U_R^{-1} u_H^{(1,2)} (1 \pm \sigma_z) U_A\,. \quad (17)$$

Imposing again the continuity condition at $z=0$, we calculate $u_H^{(1,2)}$ and then find the current at arbitrary voltages: $I(t) = \sum_k I_k e^{i2keVt/\hbar}$, where

$$I_k = \frac{1}{eR_N}\left\{ eV\delta_{k0} - \int d\epsilon\, \tanh\left(\frac{\epsilon}{2T}\right)[1-|a_R(\epsilon)|^2] \times \sum_{n=0}^{\infty} \prod_{m=1}^{n} |a_R(\epsilon+meV)|^2 \prod_{m=n+1}^{n+2k} a_R(\epsilon+meV) \right\}. \quad (18)$$

Equation (18) has the same form as the corresponding expression that follows from calculations based on the Bogolyubov–de Gennes equations.[5] The only difference is that the function $a_R(\epsilon)$, which has the meaning of generalized Andreev reflection amplitude, now contains full information about the microscopic properties of the superconducting electrodes, and is, in general, different from its "ideal" BCS value. In the particular case considered here it includes finite-energy relaxation rates $\gamma_{1,2}$. For small γ's, the part of Eq. (18) related to the dc current ($k=0$) reduces to the so-called BTK expression for the current.[2] To the best of our knowledge, this is the first explicit proof that the widely used BTK approach is equivalent to the microscopic theory of electron transport in short ballistic constrictions.

Finally, to obtain the kinetic equation (1) we consider the Green's function $\bar{G}_K$ in the limit $V\to 0$, when it is given by the following expression:

$$\bar{G}_K(\epsilon,t) = \frac{\Delta}{2}\left|\sin\frac{\varphi}{2}\right| \delta(\epsilon - \Delta\,\mathrm{sgn}(\sin\varphi/2\,\cos\varphi/2) N(\epsilon,t),$$

where

$$N(\epsilon,t) = n(\epsilon) + \int_\epsilon^\Delta d\epsilon'\, \frac{\partial n}{\partial \epsilon'}\, \exp\left\{ -\int_\epsilon^{\epsilon'} \frac{d\epsilon''\hbar\gamma(\epsilon'')}{\mathrm{eV}\sqrt{\Delta^2-\epsilon''^2}} \right\}. \quad (19)$$

Here $\hbar\gamma \equiv 2[\gamma_1 - (\epsilon/\Delta)\gamma_2]$, so that γ is given by Eq. (2).

Comparison of this expression for G_K with the subgap density of states that follows from Eq. (14) shows directly that $N(\epsilon,t)$ has the meaning of quasiparticle distribution, so that $[1-N(\epsilon,t)]/2$ can be interpreted as an occupation probability of one of the two Andreev-bound levels inside the gap. Equation (19) with this interpretation immediately gives the kinetic equation (1) and the boundary condition (3). Indeed, taking into account the definition of p in the kinetic equation we see that it is related to N as follows: $p = N\,\mathrm{sgn}(\sin\varphi/2)$. This relation together with Eq. (19) give the boundary condition (3). Furthermore, differentiating Eq. (19) with respect to energy and making use of the relation between energy and phase, $\epsilon = \mathrm{sgn}(\sin\varphi/2)\Delta\,\cos\varphi/2$, we finally arrive at Eq. (1). Although we have assumed so far that the voltage V is constant in time, it is obvious that the evolution equation (1) in the differential form is valid for arbitrary time dependence of the voltage, as long as the voltage itself and the rate of its variations are small.

As a last remark we should mention that thermalization of the occupation probability p due to the boundary condition (3) is instantaneous only on the long time scale set by the period of the Josephson oscillation. A crude estimate of the energy interval $\delta\epsilon$ near the gap edge that determines p is $(\Delta e^2 V^2)^{1/3}$, so that the corresponding time scale of thermalization is $\delta t \simeq \hbar/\delta\epsilon$. In the relevant limit $eV/\Delta \to 0$, δt is much less than the period of the Josephson oscillations.

In conclusion, we developed an adiabatic theory of the ac Josephson effect in short constrictions between two superconductors. The theory is based on the simple kinetic equation for the nonequilibrium occupation probabilities of the two Andreev-bound states localized in the constriction. The kinetic equation is rigorously derived from the microscopic equations for quasiclassical Green's functions of the constriction, and can be applied to situations with arbitrary time dependence of the bias voltage.

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