Coulomb blockade in superconducting quantum point contacts

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Amplitude of the Coulomb blockade oscillations is calculated for a single-mode Josephson junction with arbitrary electron transparency $D$. It is shown that the Coulomb blockade is suppressed in ballistic junctions with $D \to 1$. The suppression is described quantitatively as the Landau-Zener transition in imaginary time.

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Coulomb blockade phenomena in mesoscopic conductors have been actively studied during the past few years [1,2]. They arise from the interplay of discreteness, in units of electron charge $e$, of electric charge $Q$ of a small conductor, and tunneling into the conductor. Coulomb blockade occurs for its existence “localization” of the charge $Q$, the condition that implies that the transparency $D$ of the tunnel barriers isolating the conductor is small, $D \ll 1$. In ballistic junctions with $D \to 1$ the charge can move freely in and out of the conductor and both the charge quantization and associated Coulomb blockade are suppressed. Until now, full quantitative understanding of such a suppression has been worked out only for nearly-ballistic single-mode junctions between two normal conductors [3,4]. It has been shown that for conductors with the quasi-continuous energy spectrum, amplitude of the Coulomb blockade oscillations vanishes as the junction reflection coefficient approaches zero: $R = 1 - D \to 0$. The aim of this work was to study this problem for superconducting junctions, where the situation appears to be different. Coulomb blockade oscillations arise in this case [5] from the formation of Bloch bands in the Josephson potential $U(\varphi)$ periodic in the Josephson phase difference $\varphi$. Since the ballistic junctions also have periodic Josephson potential, one could expect that Coulomb blockade exists even in the ballistic regime. It is shown below that this expectation is incorrect and, similarly to the normal case, the Coulomb blockade is completely suppressed when $R \to 0$. The suppression can be described quantitatively as the Landau-Zener transition in imaginary time.

Coulomb blockade in superconducting junctions can be conveniently discussed as the quantum dynamics of the Josephson phase difference $\varphi$. The standard Hamiltonian for quantum dynamics of $\varphi$ (see e.g., [4,5,6]) consists of the coupling energy $H_c(\varphi)$ of the junction electrodes, which in the case of low-transparency junctions reduces to a simple Josephson potential $U(\varphi)$, and the charging energy $(Q - q)^2/2C$, where $C$ is the junction capacitance, $q$ is the charge injected into the junction from external circuit, and $Q$ is the charge transferred through the junction. Coulomb blockade manifests itself as periodic oscillations of the junction characteristics as a function of the charge $q$ with the period $2e$. These oscillations can take place either in time [3,6,8], when the junction is biased with a dc current $I$, and $q = It$, or as thermodynamic oscillations [7] if one of the junction electrodes is an isolated island and the charge $q$ is induced on the junction capacitance by external gate voltage $V_g$ coupled through a gate capacitance $C_g$: $q = C_g V_g$. In both situations, oscillation amplitude is the same and can be found from the junction free energy $F(q)$.

For a single-mode junction with large transparency, studied in this work, the coupling energy $H_c(\varphi)$ can be represented similarly to the normal case [4] as a sum of the energies $H_{c,R}$ of electrons with momenta $\pm k_F$ moving forward and backward through the junction, and a potential $V$ responsible for scattering between these two directions of propagation. The energy of the forward-moving electrons in a superconductor can be written in the standard matrix form:

$$H_L = \int dx \Psi_L^\dagger(x) \left( -i v_F \partial/\partial x \frac{\Delta(x)}{\Delta^*(x)} i v_F \partial/\partial x \right) \Psi_L(x),$$

$$\Delta(x) = \begin{cases} \Delta, & x < 0, \\ \Delta e^{i \varphi}, & x > 0, \end{cases}$$

where $\Psi_L^\dagger = (\psi_L^\dagger, \psi_{L\uparrow})$ is the creation operator for quasiparticles with momentum $k_F$, and $v_F$ is the Fermi velocity. $H_R$ is given by the same expression with $v_F \to -v_F$. The pair potential $\Delta(x)$ can be written in the step-like form [8] under the assumption that the characteristic junction length $d$ is much smaller than the superconductor coherence length $\hbar v_F/\Delta$.

Below we limit ourselves to the case of adiabatic phase dynamics assuming that all energies, including characteristic charging energy $E_C = (2e)^2/2C$ and temperature $T$ are much smaller than $\Delta$. The adiabatic condition $E_C, T \ll \Delta$ allows us to make several simplification in the junction Hamiltonian. First, since in this case quasiparticles are not excited in the junction electrodes, the charge $Q$ is carried only by Cooper pairs. This means that $Q$ can be expressed directly in terms of the Josephson phase difference $\varphi$: $Q = -2e \partial \varphi/\partial \varphi$. Even more importantly, the energy spectrum of electrons moving in the contact can be determined in this regime treating $\varphi$
as stationary. The Hamiltonian $H_L + H_R$ is reduced then to a sum of the quasiparticle energies $\varepsilon_k(\varphi)$ of the occupied states, and the total junction Hamiltonian can be written as

$$H = \frac{1}{2C}(\frac{2e}{i}\frac{\partial}{\partial \varphi} - q)^2 + \sum \varepsilon_k(\varphi) + V. \quad (2)$$

The spectrum of eigenenergies $\varepsilon_k(\varphi)$ is found by solving the Bogolyubov-de Gennes (BdG) equations with the pair potential $\Delta(x)$ [4]. It consists of the continuum of states at energies outside the gap, $|\varepsilon| > \Delta$, and two discrete states in the gap:

$$\varepsilon^\pm(\varphi) = \mp \Delta \cos \varphi/2, \quad \Psi^\pm(x) = \sqrt{\xi/2} \left(1 \mp e^{-i\varphi/2}\right)e^{\pm ik_Fx - \xi|x|}, \quad (3)$$

where $\xi = (\Delta/hv_F) \sin \varphi/2$. In all these expressions $\varphi \in [0, 2\pi]$, and they should be continued periodically in $\varphi$ beyond this interval. In the regime of classical phase dynamics, only the subgap states [3] contribute to both the dc Josephson current [11,12] and the ac current at low voltages [13], and one could expect that only they are relevant for quantum phase dynamics. In fact, as we will see below, the continuous part of the spectrum plays important role in determining the effective potential for the evolution of $\varphi$.

The subgap states merge with the continuum when $\varphi = 0 \bmod(2\pi)$. Equation (4) shows that as $\varphi$ varies from 0 to $2\pi$ the state with momentum $k_F$ moves across the energy gap from the lower half of the continuum, $\varepsilon < -\Delta$, to the upper half, $\varepsilon > \Delta$, while the $-k_F$ state moves in the opposite direction. The states in the continuum also shift up or down in a similar fashion. To see this we calculate the variation of the density of states $\rho(\varepsilon)$ with evolution of $\varphi$ using the Friedel sum rule (see, e.g., [14,15]):

$$\frac{\partial \rho(\varepsilon)}{\partial \varphi} = \frac{i}{2\pi} \frac{\partial^2}{\partial \varphi \partial \varepsilon} \ln \det(S(\varepsilon)), \quad (4)$$

where $S(\varepsilon)$ is the scattering matrix for scattering off the discontinuity of the pair potential $\Delta(x)$ [4]. Straightforward solution of the BdG equations shows that for $+k_F$ states

$$S(\varepsilon) = \frac{1}{e^{i\varphi} - a^2} \begin{pmatrix} |a| & (1 - e^{i\varphi})/(1 - a^2) & (1 - a^2) \end{pmatrix} \begin{pmatrix} 1 - a^2 & |a| & (1 - e^{i\varphi})/(1 - a^2) \end{pmatrix}, \quad (5)$$

where $a(\varepsilon) = \text{sign}(\varepsilon)(|\varepsilon| - (\varepsilon^2 - \Delta^2)^{1/2})/\Delta$ is the amplitude of Andreev reflection from a superconductor. Scattering matrix for momentum $-k_F$ is obtained from (3) by replacing $\varphi$ with $-\varphi$.

From eq. (4) we get

$$\frac{i}{2\pi} \int_0^{2\pi} d\varphi \frac{\partial}{\partial \varphi} \ln \det(S(\varepsilon)) = \begin{cases} 1, & |\varepsilon| > \Delta, \\ 0, & |\varepsilon| = \Delta. \end{cases} \quad (6)$$

Combined with eq. (4), this equation means that when $\varphi$ increases from 0 to $2\pi$, $+k_F$ states in the continuum move up in energy, so that precisely one state is removed from the lower half of the continuum, $\varepsilon \leq -\Delta$, and is added to the upper half, $\varepsilon \geq \Delta$. Together with the shift of the subgap states this means that the whole spectrum of $+k_F$ states shifts by one state up in energy. The spectrum of $-k_F$ states shifts by one state down. The change in energies in this process is infinitesimal for all states besides the two states (3) which move across the gap and change their energy by $2\Delta$.

**FIG. 1.** Two branches of the Josephson potential in a ballistic junction with transparency $D = 1$: one that corresponds to the equilibrium occupation of Andreev states at $\varphi = 0$ ($s = 1$), and another with equilibrium at $\varphi = 2\pi$ ($s = -1$).

Such a motion of the energy spectrum determines the effective potential for the dynamics of $\varphi$ in the Hamiltonian (4). At $\varphi = 0$, when there are no states in the gap, the equilibrium occupation of the eigenstates implies that at $T < \Delta$ all the states with $\varepsilon \leq -\Delta$ are filled, while those with $\varepsilon \geq \Delta$ are empty. Since the adiabatic variation of $\varphi$ does not induce transitions between different quasiparticle states, the shift of the energy spectrum with these occupation probabilities gives rise to the following aperiodic potential for $\varphi$ (Fig. 1):

$$U(\varphi) = \sum \varepsilon_k(\varphi) = \Delta(2m + \varepsilon_{s+1}/2) \cos \varphi/2, \quad (7)$$

$m \equiv \text{int}(|\varepsilon|/2\pi).$

The rise of the potential (4) with $\varphi$ means that the phase can increase beyond the points $\varphi = 0 \bmod(2\pi)$ only at the expense of creating quasiparticles in the junction electrodes. In the case of classical Josephson dynamics, this process generates real quasiparticles and creates dissipative component of the Josephson current [13]. The energy relaxation restores then the $2\pi$-periodicity of all the junction characteristics. It should be noted that the potential (4) for quantum phase dynamics can not be obtained if one takes into account only the subgap states [14]. It is also worth mentioning that the mechanism of
the spectrum shift creating the potential (7) is very similar to the mechanism of the chiral anomaly in the 1D quantum electrodynamics – see, e.g., [17].

An important consequence of aperiodicity of the potential (6) is complete suppression of the Coulomb blockade oscillations in ballistic junctions. Since the Coulomb blockade in superconducting junctions results from the characteristic range of the potential obviously suppresses the Coulomb blockade. However, the periodic nature of the potential and Coulomb blockade are restored by finite reflection in the junction. Indeed the aperiodicity of the potential (6) is the result of the transfer of one occupied $+k_F$ states from the energy range $\varepsilon \leq -\Delta$ to $\varepsilon \geq \Delta$ and one empty $-k_F$ state in the opposite direction as phase evolves from 0 to $2\pi$. The backscattering term $V$ in the Hamiltonian (2) couples $\pm k_F$ states and prevents such a transfer. One can see this by looking at the two subgap states (3) which in absence of backscattering cross the gap range in the course of $\varphi$ evolution: the occupied $\psi^+$ state which moves from $\varepsilon \leq -\Delta$ to $\varepsilon \geq \Delta$, and the empty $\psi^-$ state moving from $\varepsilon \geq \Delta$ to $\varepsilon \leq -\Delta$. At $\varphi = \pi$, the energies of these states coincide and $V$ couples them effectively. If this coupling is sufficiently strong, the occupied state which starts off at $\varphi = 0$ as $\psi^+$ turns into $\psi^-$ after passing the point $\varphi \simeq \pi$ and moves back into the energy range $\varepsilon \leq -\Delta$. Similarly, the empty state starting at $\varphi = 0$ as $\psi^-$ turns into $\psi^+$ and goes back to $\varepsilon \geq \Delta$. This means that at $\varphi = 2\pi$ all states with $\varepsilon \leq -\Delta$ remain occupied while those with $\varepsilon \geq \Delta$ remain empty, as at $\varphi = 0$. In this way the backscattering couples the branch (6) of the Josephson potential with no quasiparticles at $\varphi = 0$ to the one with no quasiparticles at $\varphi = 2\pi$ (the same as (7) but shifted along the $\varphi$ axis by $2\pi$ – see Fig. 1), thus creating the periodic low-energy branch of the potential.

Quantitatively, the backscattering term in the Hamiltonian (2) is $V = \int dx U(x) \rho(x)$, where $U(x)$ is the potential profile along the junction and

$$\rho(x) = \sum_{L,R} \Psi^L_{L,R} \sigma_3 \Psi_{L,R} + (\Psi^L_{R,L} \sigma_3 \Psi_{L,R} e^{2ikFx} + h.c.)$$

is the operator of electron density. Here and below $\sigma$’s denote the Pauli matrices. To evaluate the backscattering term $V$ in the basis of the subgap states (3) we use the fact that the characteristic range of the potential $U(x)$ is defined by the junction length $d$ which was assumed to be much smaller than the coherence length $\hbar v_F/\Delta$. We find then that the only nonvanishing matrix elements are those that couple the two branches of the potential:

$$\langle \Psi^- | V | \Psi^+ \rangle = ir\Delta \sin \varphi/2,$$

where $r = -U(2k_F)/\hbar v_F$ is the reflection amplitude of the junction (6), and $U(2k_F)$ is the Fourier component of the potential $U(x)$. At small $r$, the backscattering term (8) is relevant only in the vicinity of $\varphi = \pi$, where it reduces to $ir\Delta$. Then, the junction Hamiltonian (6) for $\varphi \in [0, 2\pi]$ takes the following form in the basis of two branches of the potential:

$$H = \frac{1}{2C} \left( \frac{2e}{i} \frac{\partial}{\partial \varphi} - q \right)^2 + \Delta (i r \sigma_+ - i r^* \sigma_- - \sigma_3 \cos \varphi/2).$$

(9)

![Figure 2](image)

**FIG. 2.** The probability amplitude $w (\varphi)$ for the Josephson phase difference $\varphi$ to stay in the low-energy branch of the Josephson potential in junctions with small reflection coefficient $R \ll 1$.

The width of the Bloch bands and associated with it amplitude of the Coulomb blockade oscillations depend on the probability amplitude $w$ of staying on the low-energy periodic branch of the potential in the Hamiltonian (6). This amplitude is controlled by the usual Landau-Zener transition, the same as in the case of classical phase dynamics [3]. The only difference with the classical case is that now the transition should take place in the course of $\varphi$ motion under the potential barrier, i.e. in “imaginary time”. Indeed, in the quasiclassical approximation, the stationary Schrödinger equation with the Hamiltonian (6) and energy $\varepsilon \simeq -\Delta$ describing the evolution of $\varphi$ near the level-crossing point $\varphi \simeq \pi$ is:

$$2(\varepsilon C/\Delta)^{1/2} \partial \psi_s/\partial x = -sx \psi_s/2 + \sqrt{R}\psi_{-s},$$

(10)

where $x \equiv \varphi - \pi$, and $s = \pm 1$ is the potential branch index (Fig. 1). In eq. (10) we removed the phase $\Theta$ of the coupling terms in the Hamiltonian (6) by the simple unitary transformation $\psi_s \rightarrow e^{i\Theta/s} \psi_s$. Equations (10) are the imaginary-time version of the equations describing the regular Landau-Zener transitions, and their solution is provided by the parabolic cylinder functions. From the asymptotes of these functions [19] we find that the probability amplitude $w$ for the state $s = 1$ starting at $x \rightarrow -\infty$ to reach the state $s = -1$ at $x \rightarrow \infty$ is:

$$w = \frac{1}{\Gamma(\lambda)} \left( \frac{2\pi}{\lambda} \right)^{1/2} \left( \frac{\lambda}{\varepsilon} \right)^{\lambda} , \quad \lambda \equiv (R/2)(\Delta/E_C)^{1/2}.$$

(11)
The amplitude $w$ is plotted in Fig. 2. It tends to 1 at $R \gg (E_C/\Delta)^{1/2}$, while $w \approx (2\pi\lambda)^{1/2}$ at $R \ll (E_C/\Delta)^{1/2}$. Since the amplitude of the Coulomb blockade oscillations is proportional to $w$, eq. (11) shows that similarly to the normal junctions, in the superconducting case these oscillations vanish as $R^{1/2}$ at $R \to 0$.

The low-energy periodic branch of the potential in the Hamiltonian (1) coincides with the classical stationary Josephson potential which for arbitrary junction transparency $D$ is (1,2): $U(\varphi) = -\Delta [1 - D \sin^2(\varphi/2)]^{1/2}$. For $D$ larger than the small ratio $E_C/\Delta$, the characteristic magnitude of the potential $U(\varphi)$ is larger than $E_C$, and one can find the first few eigenenergies $\varepsilon_n$ for $\varphi$ motion in this potential using the quasiclassical wavefunctions $\psi_n$ corresponding to the oscillator wavefunctions in the vicinity of the potential minima at $\varphi = 0, 2\pi$ and matching them to the oscillator wavefunctions in the vicinity of these points. Taking into account that the wavefunctions should be periodic: $\psi(\varphi + 2\pi) = \psi(\varphi)$, we find that each oscillator eigenenergy acquires a small correction $-\delta_n$: 

$$\varepsilon_n = \hbar\omega_p(n + 1/2) - \delta_n,$$

where

$$\delta_0 = \Delta bDw \left(\frac{E_C}{2\pi^2\Delta D}\right)^{1/4} e^{-a\sqrt{\Delta D/E_C}} \cos \frac{\pi q'}{e}, \quad (12)$$

$$\delta_n = (-1)^n \delta_0 \frac{b^{2n}}{n!} \left(\frac{\Delta D}{2E_C}\right)^{n/2}.$$ 

Here $\omega_p = (E_C\Delta D/2\hbar)^{1/2}$ is the frequency of small oscillations around the potential minima, and $q' = q - e\Theta/\pi$ is the induced charge shifted by the phase of the backscattering coupling. The numerical factors $a$ and $b$ in eq. (12) can be expressed in terms of elliptic integrals of the first and third kind (3), and are plotted as functions of the transparency $D$ in Fig. 3. At $D \ll 1$, $a = 2\sqrt{2}$ and $b = 4$, while at $D \to 1$: $a = 8(\sqrt{2} - 1) + R\ln\sqrt{R}$, $b = 8(\sqrt{2} - 1)$. The width $\delta_n$ of the Bloch bands decreases gradually with increasing $D$ at intermediate $D$'s because of the exponential factor in eq. (12) reflecting the increase of the Josephson potential, and then rapidly goes to zero at $D \to 1$ together with the probability amplitude $w$ (1).

Summing the corrections $\delta_n$ (12) over $n$, we can find the $q$-dependent part of the junction free energy at finite temperatures ($T \ll \Delta$) on the order of $\hbar\omega_p$:

$$F(q) = -\delta_0(q) (1 - e^{-\hbar\omega_p/T}) \exp\{-b^2 \left(\frac{\Delta D}{2E_C}\right)^{1/2} e^{-\hbar\omega_p/T}\}.$$ 

(13)

The free energy (13) determines the amplitude of the Coulomb blockade oscillations, for instance, oscillations of the voltage across the junction: $V(q) = dF(q)/dq$. It should be possible to observe the $D$-dependence of the amplitude of the Coulomb blockade oscillations (13) experimentally either in the controllable atomic point contacts (2) or in the semiconductor/superconductor heterostructures (21).

In summary, we have studied the Coulomb blockade oscillations in single-mode Josephson junctions with arbitrary electron transparency $D$ in the adiabatic limit $E_C \ll \Delta$. It was shown that the amplitude of these oscillations decreases steadily with increasing $D$ at intermediate $D$'s and then is rapidly suppressed (on the scale $(E_C/\Delta)^{1/2}$) at $D \approx 1$. The rapid suppression is described quantitatively by the amplitude (11) of the Landau-Zener transition between two branches of the Josephson potential.

FIG. 3. Exponent $a$ and the preexponential factor $b$ in the amplitude of the Coulomb blockade oscillations (12) in a single-mode Josephson junction as functions of the junction transparency $D$.

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