Coulomb Blockade and Nonperturbative Ground-State Properties of Ultrasmall Tunnel Junctions

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We present a nonperturbative calculation of the ground-state energy of a normal tunnel junction. The junction with a large conductance shows Coulomb blockade of tunneling provided the external charge Q_x is less than $e/4$. For $Q_x > e/4$, the band is flat and the junction behaves like an Ohmic resistor. We predict a phase transition between insulating and conducting behavior of the junction controlled by an external Ohmic resistance. We plot the corresponding zero-temperature phase diagram and calculate the junction effective resistance.

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Considerable progress in understanding discrete charge-transfer phenomena in ultrasmall tunnel junctions has been achieved in the past several years (see, e.g., Refs. [1,2] for a review). Modern lithographic techniques make it possible to fabricate tunnel junctions with very small capacitances $C \lesssim 10^{-15}$–10^{-16} F and investigate single electron tunneling (SET) effects experimentally. At low temperatures $T < E_c = e^2/2C$, the SET process is strongly influenced by the Coulomb interaction. As a result, at low T and small values of an external charge SET is energetically forbidden (Coulomb blockade of tunneling) and the "Coulomb gap" appears on the dc current-voltage characteristic [1,2]. This effect has been clearly demonstrated experimentally (see, e.g., Refs. [20–28] of the review in [2]).

The Coulomb blockade effects are influenced by quantum fluctuations which correspond to both continuous (induced by an external circuit) and discrete changes of the junction charge. The first type of charge fluctuation, which is particularly important for the experiments with single junctions (e.g., [3]), was investigated in a number of papers [4–7]. The case of a purely Ohmic environment was analyzed in Refs. [4,5]. It was demonstrated that the Coulomb blockade is practically destroyed by charge fluctuations in an external circuit with an Ohmic resistance R_s of order $R_s \gtrsim R_q = \pi/2e^2 \simeq 6.5$ kΩ. On a more general basis, the effect of electromagnetic environment was studied by Nazarov [6] and later by Devoret *et al.* and by Girvin *et al.* [7]. The approach [6,7] allows one to calculate the *I-V* characteristic of a single tunnel junction for an arbitrary external impedance $Z(\omega)$ *perturbatively* in $\alpha_t = R_q/R_t$; R_t is the junction resistance.

In this Letter we present a *nonperturbative* analysis of charge fluctuations and the ground-state properties of a normal tunnel junction. We consider the effect of virtual electron tunneling across the junction on the Coulomb blockade. We calculate the ground-state energy $E_0(Q_x)$ and show that this effect is *qualitatively* different from that of an Ohmic shunt: Even for large values of α_t Coulomb blockade survives provided the external charge Q_x is less than $e/4$, while for $|Q_x| > e/4$ the junction shows Ohmic behavior. We also investigate an additional effect of charge fluctuations in the external circuit. We predict a zero-temperature phase transition between insulating and resistive behavior of a tunnel junction, plot the corresponding phase diagram on the α_s-α_t plane ($\alpha_s = R_q/R_s$), and evaluate the junction effective resistance R_t^{eff}.

We shall consider the grand partition function for a "tunnel junction plus environment" [2],

$$Z = \sum_{m=-\infty}^{\infty} \int d\varphi \int_{\varphi_0}^{\varphi_0 + 4\pi m} D\varphi \int Dq \exp\left[-S_0[\varphi] + i\int d\tau \frac{\dot\varphi q}{2e} - \frac{T}{2}\sum_\omega |\omega| Z(-i\omega) |q_\omega^2| \right], \tag{1}$$

$$S_0[\varphi] = \int d\tau \frac{C}{2}\left(\frac{\dot\varphi}{2e}\right)^2 - \int d\tau \int d\tau' \frac{\alpha_t T^2}{\sin^2(\pi T \tau)} \cos\left(\frac{\varphi(\tau) - \varphi(\tau')}{2}\right), \tag{2}$$

where $0 < \tau < 1/T$, C is the capacitance of a tunnel junction, the phase and the quasicharge variables $\varphi(\tau)$ and $q(\tau)$ are defined by the relations $\dot\varphi(\tau) = 2eV(\tau)$ and $\dot q(\tau) = I(\tau)$, $V(\tau)$ is the voltage across the junction, and $I(\tau)$ is the current in the circuit.

Let us first consider the case of an isolated junction $[1/Z(\omega) \to 0]$ with an external charge Q_x on it. In this case all nonzero frequency components $q_{\omega\neq 0}$ can be dropped from (1) and the second term in the parentheses of (1) becomes $i\int d\tau (\dot\varphi q/2e) \to 2\pi i Q_x/e$. We shall calculate the ground-state energy $E_0(Q_x)$ for large values of α_t. To evaluate the path integral over $\varphi(\tau)$ in (1) we make use of the fact that for $C \to 0$ there is an instanton trajectory $\tilde\varphi(\tau) = 4\arctan\Omega\tau$ which "connects" states with different m. Substituting this trajectory into (2) we get $\tilde S(\Omega) = 2\alpha_t + \pi\Omega/2E_c$, i.e., an important range of instanton frequencies is $\Omega \lesssim E_c$. Contrary to the case of a superconducting junction [4] (in which small values of Ω do not contribute), non-Gaussian fluctuations with very small Ω play an essential role at $T \to 0$. Because of this the instanton analysis of Ref. [4] cannot be directly applied to the case of a normal junction. The appropriate technique is presented below.

In order to evaluate the contribution of fluctuations around the trajectory $\tilde{\varphi}(\tau)$ we have to calculate the eigenvalues of the operator $\hat{M}_1=\delta^2 S_0/\delta\tilde{\varphi}^2$. For $C\rightarrow 0$ there are two nontrivial zero modes with the eigenfunctions $\varphi_1(\tau)=(8\pi\Omega)^{-1/2}\partial\tilde{\varphi}/\partial\tau$ and $\varphi_2(\tau)=(8\pi/\Omega^3)^{-1/2}\partial\tilde{\varphi}/\partial\Omega$ which correspond to a shift of an instanton in the τ direction and to changes of an instanton size $\sigma=1/\Omega$, respectively. Analogously there are $2N$ nontrivial zero modes of the operator $\hat{M}_N=\delta^2 S_0/\delta\tilde{\varphi}_N^2$, defined on an N-instanton trajectory,

$$\tilde{\varphi}_N(\tau)=\sum_{n=1}^{N}\epsilon_n 4\arctan\Omega_n(\tau-\tau_n),\quad \sum_{n=1}^{N}\epsilon_n=m\,,$$

$\epsilon_n=\pm 1$. Extracting collective coordinates corresponding to these zero modes we present the N-instanton contribution to Z in the form

$$4^N\int d\tau_N\int\frac{d\Omega_N}{\Omega_N}\cdots\int d\tau_1\int\frac{d\Omega_1}{\Omega_1}\left(\frac{\det\hat{M}_0}{\det'\hat{M}_N}\right)^{1/2}\exp\left[-\sum_{n=1}^{N}\tilde{S}(\Omega_n)+\frac{2\pi i m Q_x}{e}\right],\tag{3}$$

where we assume $\tau_N>\tau_{N-1}>\cdots>\tau_1$. The value $\det'\hat{M}_N$ is calculated with the $2N$ zero modes excluded, and $\hat{M}_0=\delta^2 S_0/\delta\varphi^2$ is taken on the trajectory $\varphi(\tau)=0$. As in [4] we define $\delta\hat{M}_N=\hat{M}_0-\hat{M}_N$ and rewrite the ratio of determinants as

$$\frac{\det\hat{M}_0}{\det'\hat{M}_N}=\prod_{n=1}^{N}(\lambda_n^0\lambda_{-n}^0)\exp\left[\sum_{|n|>N}\frac{\phi_n^0\delta\hat{M}_N\phi_n^0}{\lambda_n^0}+O(\delta\hat{M}_N^2)\right],\tag{4}$$

where $\lambda_n^0=\alpha_t|\omega_n|/2\pi+\omega_n^2/8E_c$ and $\varphi_n^0(\tau)=(2T)^{1/2}\cos\omega_n\tau$ are the eigenvalues and the eigenfunctions of the operator $\hat{M}_0$. Disregarding the power-law interinstanton interaction we get

$$\sum_{|n|>N}\frac{\varphi_n^0\delta\hat{M}_N\varphi_n^0}{\lambda_n^0}\simeq 2N\gamma+2\sum_{k=1}^{N}\ln\frac{8\alpha_t E_c}{\pi\Omega_k},\tag{5}$$

with $\gamma\simeq 0.577$ the Euler constant. It is easy to check that higher-order terms in $\delta\hat{M}_N$ can be neglected. To decouple the $2N$ integrations in (3) we denote $d\sigma_n=d\Omega_n/\Omega_n^2$ and introduce new variables $\tau_n^{\pm}=\tau_n\pm\sigma_n/2$. Then summing over all possible instanton configurations and over all winding numbers m we get, for $T\rightarrow 0$,

$$\exp[-E_0(Q_x)/T]$$
$$=\sum_{N=0}^{\infty}\int_0^{1/T}d\tau_N^+\int_0^{\tau_N^+-\tau_c}d\tau_N^-\int_0^{\tau_N^--\tau_c}d\tau_{N-1}^+\cdots\int_0^{\tau_2^--\tau_c}d\tau_1^+\int_0^{\tau_1^+-\tau_c}d\tau_1^-N!\left[4T\Delta\cos\frac{2\pi Q_x}{e}\right]^N,\tag{6}$$

$$\Delta=(8\alpha_t^2E_c/\pi^2)\exp(-2\alpha_t+\gamma)\,,\tag{7}$$

$\tau_c\sim 1/E_c$. Integration over $\tau^{\pm}$ in (6) gives the factor $T^{-2N}/2N!$, and the series (6) is exactly expressed in terms of the probability integral. Then we put $T\rightarrow 0$ and arrive at a final result for the ground-state energy of a normal tunnel junction with large α_t,

$$E_0(Q_x)=\begin{cases}-\Delta\cos(2\pi Q_x/e), & |Q_x|\le e/4\,,\\ 0, & |Q_x|>e/4\,.\end{cases}\tag{8}$$

Equation (8) is one of the main results of the present paper (see Fig. 1). It demonstrates that (i) for $|Q_x|<e/4$ the junction shows the Coulomb blockade even for $\alpha_t\gg 1$ and the effective capacitance $C_{\rm eff}$ (for small Q_x) is renormalized, $C_{\rm eff}\sim(C/\alpha_t^2)\exp(2\alpha_t)$, similarly to the case of a superconducting junction with large α_t [2,4,8], and (ii) for $|Q_x|>e/4$ the band is flat and the junction behaves like an Ohmic resistance, i.e., the discharging process occurs for such values of Q_x.

We see that for $\alpha_t\gg 1$ specific features of the discrete electron tunneling mechanism show up only for $|Q_x|<e/4$, in which case due to an instanton contribution the ground-state energy $E_0(Q_x)$ is less than zero. As a result the charge state $Q=Q_x$ is stable and the Coulomb blockade takes place. On the other hand, for $|Q_x|\ge e/4$ instanton contribution plays no role and a tunnel junction with $\alpha_t\gg 1$ is practically indistinguishable from an Ohmic resistor. More precisely, if the initial charge exceeds $e/4$ the tunneling process occurs and eventually the junction will be discharged up to $|Q|=e/4$. Thus, strictly speaking, there is no ground state in our problem for $|Q_x|>e/4$. The last result differs significantly from that for a superconducting junction which has a stable ground

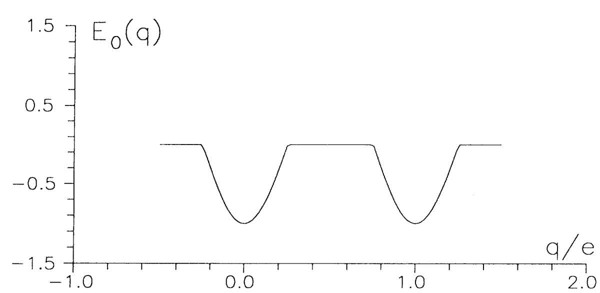

FIG. 1. The ground-state energy $E_0(q)$ of a normal tunnel junction for $\alpha_t\gg 1$.

state for $|Q_x|<e/2$ [2,4]. Note that discontinuity of $\partial E_0/\partial Q_x$ at $|Q_x|=e/4$ takes place only for $\alpha_t \gg 1$ while for moderate α_t the energy $E_0(Q_x)$ is smooth and gradually flattens off for $|Q_x| \gtrsim e/4$. For small α_t the tendency to flattening of $E_0(Q_x)$ in the vicinity of the point $Q_x=e/2$ has also been demonstrated in Ref. [8].

Let us emphasize some interesting features of the instanton technique developed here. Contrary to the standard technique in which the size of instantons is small (as compared to the average distance between them) and does not fluctuate, here fluctuations of the instanton size turn out to be important and configurations with large instantons give the main contribution to the partition function. We also point out that the result (8) is insensitive to the specific form of the long-time power-law interaction between instantons which gives an additional factor $\sim at^{-\nu}$ in the preexponent of the expression for Δ, Eq. (7), where we estimate ν as $0 \le \nu \le \frac{1}{2}$. This effect cannot change any of our conclusions and we will not discuss it further below.

Now let us investigate an additional effect of an external circuit. For $\alpha_t \gg 1$ one can split the path integral over $\varphi(\tau)$ (1) into two parts (small fluctuations and instantons). Integration over small fluctuations of $\varphi(\tau)$ near $\varphi=\varphi_0$ leads to the renormalization of the external impedance,

$$\tilde{Z}(-i\omega)=Z(-i\omega)+1/2(C|\omega|+\alpha_t e^2/\pi).$$

An instanton contribution can be evaluated within the framework of the adiabatic approximation in the same spirit as has been done in Ref. [9]. Assuming that the characteristic frequency scale ω_q for the quasicharge variable q is much smaller than the typical instanton frequency Ω^*, one can reproduce the analysis presented above and get

$$Z=\int Dq \exp(-S_{\rm eff}[q]),$$
$$S_{\rm eff}[q]=(T/2)\sum|\omega|\tilde{Z}(-i\omega)|q_\omega^2|+\int d\tau\, E_0(q), \tag{9}$$

where $E_0(q)$ is defined in (8) with $Q_x \to q+pe$, p an integer number. Making use of the result (6) we estimate the typical instanton frequency Ω^* as $\langle\tau^+\rangle \sim \langle\tau^-\rangle \sim 1/\Omega^* \sim 1/\Delta$. Thus the adiabatic form of $S_{\rm eff}$ (8),(9) holds for $\omega_q \ll \Delta$. For $\omega_q > \Delta$ the quasicharge variable introduces a low-frequency cutoff $\Omega \gtrsim \omega_q$ into our problem. In this case we return back to the technique previously developed for a superconducting junction with $\alpha_t \gg 1$ and $E_J \ll E_c$ [4], where ω_q now plays the role of the Josephson coupling energy E_J. Analogously to [4,9] we again derive Eqs. (9) with

$$E_0(q)=-\Delta_1\cos(2\pi q/e),$$
$$\Delta_1=(16\alpha_t E_c/\pi^2)\exp(-2\alpha_t+\gamma), \tag{10}$$

and the corresponding validity condition $E_c \gg \omega_q \gtrsim \Delta \sim \alpha_t\Delta_1$. The crossover between the expressions (10) and (7),(8) takes place at $\omega_q \sim \Delta$. For an interesting range of frequencies $\omega \ll \alpha_t E_c$ we put $\tilde{Z}(-i\omega)=L|\omega|+R_s+R_t$. Then the problem (9),(10) can be mapped onto that of a neutral Coulomb gas of logarithmically interacting charges and treated by the standard renormalization-group (RG) technique (see, e.g., [2,10]). Making use of the results [10], we arrive at the RG equations

$$d\tilde{\Delta}/d(\ln\omega_c)=\tilde{\Delta}(4\alpha_0-1), \quad d\alpha_0/d(\ln\omega_c)=0, \tag{11}$$

where $\tilde{\Delta}=\Delta_1/\omega_c$, $\omega_c=\min(E_c, 1/\alpha_0 Le^2)$, and $\alpha_0=R_q/(R_s+R_t)$. Equations (11) show that $\tilde{\Delta}$ scales out to zero with decreasing ω_c if $\alpha_0>\frac{1}{4}$ and grows if $\alpha_0<\frac{1}{4}$. It means that for $\alpha_0>\frac{1}{4}$ the potential $E_0(q)$ (10) does not play any role and can be dropped. In this case fluctuations of the charge in the external circuit completely destroy the correlation between SET events (and thus the Coulomb blockade) and the tunnel junction effectively behaves like an Ohmic resistance $R \simeq R_t$. On the other hand, for $\alpha_0<\frac{1}{4}$ the Coulomb blockade is *not* destroyed by the charge fluctuations in the external leads. For simplicity let us assume that the inductance L is small and $\omega_c \sim E_c$. Then using the expression for Δ_1 (10) we rewrite the first RG equation (11) for $\alpha_0<\frac{1}{4}$ and $\alpha_t \gg 1$ as

$$d\alpha_t/d(\ln\omega_c)=(\tfrac{1}{2}-2\alpha_0)(1+1/2\alpha_t). \tag{12}$$

In the limiting case $\alpha_s=\alpha_0=0$, Eq. (12) practically coincides with the RG equation derived by Guinea and Schön [8] for a superconducting junction with $E_J \ll E_c$ and $\alpha_t \gg 1$ by means of a different technique. Equation (12) shows that the effective (dimensionless) conductance of a tunnel junction α_t decreases during the scaling procedure for $\alpha_0<\frac{1}{4}$. If we start renormalization at $\omega_c \sim E_c$, stop it at $\omega_c=\omega^*$, and then put $\omega^*=T$ we immediately recover the effective linear resistance $R_t^{\rm eff}(T)$ at $\alpha_0<\frac{1}{4}$. For $R_q \lesssim R_t^{\rm eff} \lesssim R_t$ we get

$$R_t^{\rm eff} \simeq R_t\left[1+\frac{1-4\alpha_0}{2\alpha_t}\ln\frac{t}{E_c}+\frac{1}{2\alpha_t}\ln\left(1+\frac{1-4\alpha_0}{2\alpha_t}\ln\frac{T}{E_c}\right)\right]^{-1}. \tag{13}$$

For lower temperatures two competing processes—thermal activation and quantum tunneling of the charge in the potential $E_0(q)$ (8)—contribute to the junction conductance. For $\alpha_0<\frac{1}{4}$ both processes yield a zero junction conductance $1/R_t^{\rm eff} \to 0$ at $T \to 0$. Combining this result with the scaling equation for $\alpha_t \ll 1$ and small L, $d\alpha_t/d(\ln\omega_c)=\alpha_t/2\alpha_s$, which also demonstrates that α_t decreases with ω_c and $R_t^{\rm eff} \propto T^{-1/2\alpha_s}$ [the exact expression for $R_t^{\rm eff}(T)$ for $\alpha_t \ll 1$ is given in Refs. [2,4]], we can conclude that at $T \to 0$ the tunnel junction shows insulating *linear* response for all α_t provided α_s is small enough (phase I in Fig. 2). For $\alpha_t \gg 1$ the phase transition between insulating and resistive (R) phases takes place at $\alpha_s=1/(4-1/\alpha_t)$. The position of the phase boundary for small α_t is a subject for further investigations.

Finally, let us briefly discuss the I-V curve of the system at $T=0$. We switch the voltage source V_x in series with the impedance $Z(\omega)$ and calculate the current in the circuit I or, equivalently, the nonlinear resistance of the junction $R_t^{\text{eff}}(V_x)=V_x/I-R_s$. For $\alpha_t \ll 1$ this calculation has been carried out in Refs. [2,4,7]. In the limit $\alpha_t \gg 1$, there are several different regimes. For $eV_x<2\pi\Delta$ and $\alpha_0<\frac{1}{4}$ the quasicharge q cannot move classically and the effective resistance $R_t^{\text{eff}}(V_x)$ is very large for small V_x. This is the Coulomb blockade regime. In this regime $R_t^{\text{eff}}(V_x)$ is finite only due to quantum fluctuations of q. For $eV_x>2\pi\Delta$ and $\alpha_s \ll 1$ the classical dynamics of q in the periodic potential $E_0(q)$ (8) is described by a simple equation $R_0\dot{q}+\partial E_0/\partial q=V_x$, which yields

$$I=\frac{V_x}{R_s+R_t}\left\{\frac{1}{2}+\frac{2}{\pi}\left[1-\left(\frac{2\pi\Delta}{eV_x}\right)^2\right]^{-1/2}\arctan\left(\frac{1+2\pi\Delta/eV_x}{1-2\pi\Delta/eV_x}\right)^{1/2}\right\}^{-1}. \tag{14}$$

This is the SET oscillation regime. The result (14) is valid provided the frequency of SET oscillations I/e is smaller than Δ, i.e., for $eV_x \lesssim \Delta/\alpha_s$. For larger values of V_x the resistance $R_t^{\text{eff}}(V_x)$ can be evaluated from Eq. (12) provided we put $\omega^*=eV_x/[1+R_s/R_t^{\text{eff}}(V_x)]$. For $\alpha_0<\frac{1}{4}$ and $[\alpha_t\exp(-2\alpha_t)]^{1/(1-4\alpha_0)} \lesssim \alpha_s eV_x/E_c \lesssim 1$, with logarithmic accuracy we get

$$R_t^{\text{eff}} \simeq R_t\left(1+\frac{1-4\alpha_0}{2\alpha_t}\ln\frac{\alpha_s eV_x}{\alpha_t E_c}\right)^{-1}. \tag{15}$$

In this regime coherent SET oscillations are washed out. For larger values $eV_x \gtrsim \min(E_c,\alpha_s E_c)$, instanton effects are not important and the physical difference between discrete and continuous charge-transfer mechanisms practically disappears. In this limit the I-V curve is described by the theory [5] for all α_s and α_t.

In conclusion, we present a nonperturbative analysis of quantum fluctuations of the charge in normal tunnel junctions. We calculate the ground-state energy of the junction and demonstrate that the Coulomb blockade of electron tunneling is not destroyed even for $\alpha_t \gg 1$ but restricted to the values of an external charge $|Q_x|<e/4$ (for $\alpha_t \to 0$ the analogous condition reads $|Q_x|<e/2$ [1]). For $|Q_x|>e/4$ and $\alpha_t \gg 1$ the junction behavior is Ohmic. We show that quantum fluctuations of the charge in the external circuit essentially influence SET effects and predict a zero-temperature phase transition between insulating and resistive phases which correspond, respectively, to high and low external impedances $Z(\omega \to 0)$. We present a nonperturbative calculation of the junction resistance R_t^{eff} for a wide range of parameters of the system. Finally, we would like to note that tunnel junctions with moderate α_t (e.g., $\alpha_t \approx 2$–3) appear to be most appropriate for experimental investigation of the effects discussed here since for very large α_t technical problems with getting to exponentially low temperatures $T/E_c \propto \exp(-2\alpha_t)$ can make quantum effects practically unobservable.

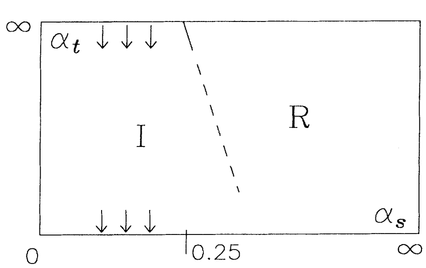

FIG. 2. The phase diagram of a normal tunnel junction at $T=0$. It consists of insulating (I) and resistive (R) phases. RG flow lines for α_t are indicated by arrows.

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