Virtual Electron Diffusion during Quantum Tunneling of the Electric Charge

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We calculate the rate of the elastic macroscopic quantum tunneling of the electric charge (q-MQT) in a system of two small-area, normal, tunnel junctions in the Coulomb blockade regime. Despite the fact that the intermediate electron state on the central electrode of the system during the tunneling is virtual, the rate of the q-MQT depends crucially on the character of real electron motion through this electrode. Typically this motion is diffusive, so that the tunneling rate is determined by the process of "virtual diffusion" of electrons on the time scale of the inverse Coulomb energy of the system, $\hbar/E_C$.

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Dynamics of small tunnel junctions or multijunction systems in the Coulomb blockade regime[1] (i.e., for small voltages across the system) can be described in terms of macroscopic quantum tunneling of the electric charge (q-MQT).[2] Consider, for instance, a system of two series-connected normal tunnel junctions with small capacitances $C_{1,2}$ and conductances $G_{1,2}$. For small voltages V across the system and low temperatures T the tunneling in either of the two junctions is suppressed, since even a single tunneling event would charge the central electrode and increase the electrostatic energy of the system considerably. The only energy-favorable tunneling is the tunneling through the whole system via a virtual intermediate state with increased electrostatic energy. Such a tunneling arises due to quantum fluctuations of a macroscopic variable, the electric charge Q on the central electrode of the system, and hence can be viewed as a macroscopic quantum process. Because of this tunneling a finite current can flow through the system even in the Coulomb blockade regime. Recently, the q-MQT has been observed[3] in linear arrays of two normal tunnel junctions. Apart from being of fundamental interest, the q-MQT sets an important limitation on the performance accuracy of practical devices based on correlated single-electron tunneling,[1] for instance, the single-electron turnstile device as a fundamental standard of the dc current.[4]

The q-MQT rate in a double-junction system was first calculated[2] in an approach that completely neglects coherence between wave functions of electrons tunneling through different junctions. This approach gives a correct description of the inelastic contribution to the q-MQT, which dominates in the most realistic case when the electron density of states Δ^{-1} on the central electrode is high enough, $\Delta^{-1} \gg E_C^{-1}$, where E_C is the characteristic charging energy of the system (see below). Later it was pointed out[5] that there should also exist an elastic contribution to the q-MQT. However, the current arising due to this tunneling was calculated[5] in an unrealistic model which does not explicitly consider the crucial process of electron propagation inside the central electrode between two tunnel junctions. The purpose of the present Letter is to derive a general expression describing both elastic and inelastic contributions to the q-MQT and calculate accurately the current associated with elastic tunneling.

The Hamiltonian of the double-junction system is (see, e.g., Ref. 1)

$$H = H_0 + H_T, \quad H_0 = H_c + H_1 + H_2 + U, \qquad H_T = H_{T1} + H_{T2}, \tag{1}$$

where H_c and $H_{1,2}$ are the Hamiltonians of, respectively, the central electrode and the external electrodes, and U is the electrostatic charging energy,

$$U = \frac{Q^2}{2C_\Sigma} - \frac{eV}{C_\Sigma}(C_1 n_2 + C_2 n_1), \tag{2a}$$

$$Q = e(n_1 - n_2) + Q_0, \quad C_\Sigma = C_1 + C_2. \tag{2b}$$

Here n_i is the number of electrons that have tunneled through the ith junction and Q_0 describes the potential difference between the central and external electrodes. The terms H_{Ti} describing the tunneling can be expressed via the standard tunneling Hamiltonians:

$$H_{Ti} = H_i^+ + H_i^-, \quad H_i^+ = \sum_{m,n} T_{mn}^{(i)} c_m^\dagger c_n, \qquad H_i^- = (H_i^+)^\dagger. \tag{3}$$

We will consider junctions with small conductances, $G_i \ll R_Q^{-1}$, $R_Q \equiv \pi\hbar/2e^2$, so that we can treat H_{Ti} as a perturbation. Since one act of q-MQT includes two electron tunneling events, the current associated with this tunneling is of the fourth (second nonvanishing) order in H_{Ti}:

$$I = \frac{2e}{\hbar^4}\mathrm{Re}\left\{\int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' [\langle H_1^+(t) H_T(\tau) H_T(\tau') H_T(\tau'')\rangle - \langle H_T(\tau'') H_T(\tau') H_T(\tau) H_1^+(t)\rangle] + \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' [\langle H_T(\tau'') H_T(\tau') H_1^+(t) H_T(\tau)\rangle - \langle H_T(\tau) H_1^+(t) H_T(\tau') H_T(\tau'')\rangle]\right\}, \tag{4}$$

where the time dependence of H_T is determined by H_0, and the average $\langle \cdots \rangle$ is taken over the equilibrium density matrix corresponding to H_0. Collecting the terms in Eq. (4) that describe the q-MQT we get

$$I = e(\gamma^{(+)} - \gamma^{(-)}), \tag{5}$$

$$\gamma^{(+)} = \frac{2}{\hbar^4} \sum_{\substack{p,q=1,2 \\ p\neq q}} \mathrm{Re}\Bigg[\int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' \exp\{-i[E_2(t-\tau)+eV(t-\tau')-E_p(\tau'-\tau'')]/\hbar\} \times \langle H_p^-(\tau'')H_q^-(\tau')H_1^+(t)H_2^+(\tau)\rangle - \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' \exp\{i[E_1(t-\tau)-eV(\tau-\tau')-E_p(\tau'-\tau'')]/\hbar\} \times \langle H_p^-(\tau'')H_q^-(\tau')H_2^+(\tau)H_1^+(t)\rangle \Bigg], \tag{6a}$$

$$\gamma^{(-)} = \frac{2}{\hbar^4} \sum_{\substack{p,q=1,2 \\ p\neq q}} \mathrm{Re}\Bigg[\int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' \exp\{i[E_1(t-\tau)-eV(\tau-\tau'')-E_p(\tau'-\tau'')]/\hbar\} \times \langle H_2^+(\tau)H_1^+(t)H_p^-(\tau')H_q^-(\tau'')\rangle - \int_{-\infty}^{t} d\tau \int_{-\infty}^{\tau} d\tau' \int_{-\infty}^{\tau'} d\tau'' \exp\{-i[E_2(t-\tau)+eV(t-\tau'')+E_p(\tau'-\tau'')]/\hbar\} \times \langle H_1^+(t)H_2^+(\tau)H_p^-(\tau')H_q^-(\tau'')\rangle \Bigg]. \tag{6b}$$

In Eqs. (6) we have written down explicitly the time-dependent phase factors of operators $H_i^{\pm}$ related to the electrostatic energy (2): $E_i \equiv U(n_i+1)-U(n_i)$.

Applying the Wick theorem to the averages in Eqs. (6) we get, for instance,

$$T_{km}^{(1)}T_{k'm}^{*(1)}T_{nl}^{(2)}T_{nl'}^{*(2)}\langle c_l^\dagger c_k c_l c_{k'}^\dagger\rangle \rightarrow -|T_{km}^{(1)}|^2|T_{nl}^{(2)}|^2\langle c_l^\dagger c_l\rangle\langle c_k c_k^\dagger\rangle + T_{km}^{(1)}T_{lm}^{(1)}T_{nk}^{(2)}T_{nl}^{(2)}\langle c_k^\dagger c_k\rangle\langle c_l c_l^\dagger\rangle. \tag{7}$$

(Here and below the indices m,n refer to the energy eigenstates of the external electrodes, while k,l refer to those of the central electrode.)

Those terms in Eqs. (6) which are similar to the first one on the right-hand side of relation (7) are only dependent on the absolute value of the tunneling amplitudes $T^{(i)}$ and thus describe the tunneling process without any coherence between tunneling events in the two junctions. Roughly speaking, it means that two different electrons tunnel in the two junctions: One jumps into the central electrode above its Fermi level, and another one jumps out of the electrode from below the level. Hence, such a tunneling unavoidably involves the creation of an electron-hole excitation on the central electrode, and can be called inelastic. (It seems important to note that this term has nothing to do with inelastic electron scattering in the junction electrodes, which we do not take into account in our model.) In contrast to this inelastic tunneling, elastic tunneling [described by the terms in Eqs. (6) similar to the second one on the right-hand side of relation (7)] does not create such an excitation. In a sense, this implies that the same electron tunnels through both of the junctions. Hence, the rate of elastic tunneling is very sensitive to the electron motion inside the electrode. The information about this motion is contained in the phase factors of the tunneling amplitudes.

Quantitatively, carrying out the transformation (7) in Eqs. (6) we get

$$\gamma^{(\pm)} = \gamma_{\mathrm{in}}^{(\pm)} + \gamma_{\mathrm{el}}^{(\pm)}, \tag{8}$$

$$\gamma_{\mathrm{in}}^{(+)} = \frac{\hbar G_1 G_2}{2\pi e^4} \int d\varepsilon_1 d\varepsilon_2 d\varepsilon_3 d\varepsilon_4 f(\varepsilon_1)[1-f(\varepsilon_2)]f(\varepsilon_3)[1-f(\varepsilon_4)] \times \left[\frac{1}{\varepsilon_2-\varepsilon_1+E_1}+\frac{1}{\varepsilon_4-\varepsilon_3+E_2}\right]^2 \delta(eV+\varepsilon_1-\varepsilon_2+\varepsilon_3-\varepsilon_4), \tag{9}$$

where $f(\varepsilon)$ is Fermi distribution function [the backward tunneling rate $\gamma_{\mathrm{in}}^{(-)}$ is given by Eq. (9) with $V \rightarrow -V$, $E_i \rightarrow E_i + eV$]. At zero temperature Eq. (9) reduces to Eq. (32) of Ref. 2. For small voltages, $eV \ll E_i$, the inelastic contribution to the tunnel current can be found explicitly for nonvanishing but low temperatures ($T \ll E_i$):

$$I_{\mathrm{in}} = e(\gamma_{\mathrm{in}}^{(+)} - \gamma_{\mathrm{in}}^{(-)}) = \frac{\hbar G_1 G_2}{12\pi e^3}\left[\frac{1}{E_1}+\frac{1}{E_2}\right]^2 [(eV)^2+(2\pi T)^2]V. \tag{10}$$

The elastic tunneling rate $\gamma_{\rm el}^{(+)}$ is

$$\gamma_{\rm el}^{(+)} = \frac{2\pi}{\hbar} \sum_{m,n,k,l} T_{km}^{(1)} T_{lm}^{*(1)} T_{nk}^{(2)} T_{nl}^{*(2)} f(\varepsilon_m)[1-f(\varepsilon_n)] F(\varepsilon_l,\varepsilon_m,\varepsilon_n) F(\varepsilon_k,\varepsilon_m,\varepsilon_n) \delta(\varepsilon_m - \varepsilon_n + eV) , \tag{11a}$$

$$F(\varepsilon,\varepsilon_m,\varepsilon_n) = \frac{1-f(\varepsilon)}{E_1+\varepsilon-\varepsilon_m} - \frac{f(\varepsilon)}{E_2-\varepsilon+\varepsilon_n} \tag{11b}$$

[the backward tunneling rate $\gamma_{\rm el}^{(-)}$ is given by Eqs. (11) with $V \to -V$, $E_i \to E_i + eV$, and $\varepsilon_m \leftrightarrow \varepsilon_n$]. As will become clear below, the elastic tunneling rate is smaller than the inelastic one by a factor of Δ/E_C. Thus, the elastic tunneling can be essential only for $eV \ll E_i$, when the inelastic tunneling should be weak at sufficiently low temperatures [see Eq. (10)]. In this region the elastic current, $I_{\rm el} = e(\gamma_{\rm el}^{(+)} - \gamma_{\rm el}^{(-)})$, depends linearly on the voltage, and it is sufficient to calculate the corresponding conductance $G_{\rm el} \equiv (dI_{\rm el}/dV)|_{V=0}$. In order to take into account the phases of the tunneling amplitudes it is convenient to write down the amplitudes in the coordinate representation,

$$T_{km} = \int d^3y \int d^3z \, T(y,z) \psi_k^*(y) \psi_m(z) . \tag{12}$$

Substituting (12) into (11) we get for the elastic conductance

$$G_{\rm el} = \frac{2\pi e^2}{\hbar} \int d\varepsilon \int d\varepsilon' F(\varepsilon) F(\varepsilon') R(\varepsilon,\varepsilon') , \tag{13a}$$

$$R(\varepsilon,\varepsilon') = \int d^3z_1 d^3z_2 d^3z_3 d^3z_4 d^3y_1 d^3y_2 d^3y_3 d^3y_4 T^{(1)}(y_1,z_1) T^{(2)}(y_3,z_3) T^{*(1)}(y_2,z_2) T^{*(2)}(y_4,z_4)$$
$$\times K_0(z_2,z_1) K_0(z_3,z_4) K_\varepsilon(y_1,y_3) K_{\varepsilon'}(y_4,y_2) . \tag{13b}$$

where the points z_j and y_j are located in the external electrodes and the central electrode, respectively; $F(\varepsilon) \equiv F(\varepsilon,0,0)$, and

$$K_\varepsilon(x,x') \equiv \sum_q \psi_q^*(x) \psi_q(x') \delta(\varepsilon - \varepsilon_q) .$$

Acting along the same lines as in Ref. 6, one can show that in the quasiclassical approximation[7,8] $R(\varepsilon,\varepsilon')$ is

$$R(\varepsilon,\varepsilon') = R(\varepsilon-\varepsilon') = \frac{\hbar}{8\pi^3 e^4 \nu} \int d^2x_{1,2} d^2n_{1,2} g_1(x_1,\mathbf{n}_1) g_2(x_2,\mathbf{n}_2) \int dt \exp[i(\varepsilon-\varepsilon')t/\hbar] P(x_1,\mathbf{n}_1,0;x_2,\mathbf{n}_2,|t|) . \tag{14}$$

Here ν is the density of states per unit volume of the central electrode, and $P(x_1,\mathbf{n}_1,0;x_2,\mathbf{n}_2,t)$ is the quasiclassical probability to find an electron at time $t>0$ at the point x_2 with the momentum $p_F\mathbf{n}_2$ (where p_F is the absolute value of the momentum on the Fermi surface, and $\mathbf{n}_i$ is its direction) if at time $t=0$ it was in the state $(x_1,\mathbf{n}_1)$. The quasiclassical probabilities $g_i(x_i,\mathbf{n}_i)$ for the electron to tunnel from the ith external electrode to the state $(x_i,\mathbf{n}_i)$ are normalized in such a way that the junction conductances per unit area $g_i(x_i)$ and their total conductances G_i are

$$g_i(x_i) = \int d^2n_i \, g_i(x_i,\mathbf{n}_i), \quad G_i = \int d^2x_i \, g_i(x_i) . \tag{15}$$

The integration d^2x_i in Eqs. (14) and (15) is carried out over the ith junction area.

Equations (13a) and (14) are the main result of our work. They describe the rate of elastic charge MQT in the double-junction system in terms of the classical electron motion through the central electrode of the system. The only fact that reminds us of the virtual character of electron motion in the tunneling process is that the tunneling rate depends on the characteristics of classical motion on the time scale $E_C/\hbar$. Thus, $E_C/\hbar$ plays the role of the time which the virtual electron can spend to propagate from one junction to another.

The rate of the elastic tunneling and the corresponding conductance $G_{\rm el}$ depend, in general, on the geometry of the junctions. If the characteristic dimensions L of the central electrode is larger than the electron elastic mean free path l ($L \gg l$), one can use the usual diffusion equation to describe the electron motion inside the electrode. In this case the probability P in Eq. (14) does not depend on $\mathbf{n}_i$, so that

$$R(\varepsilon) = \int d^2x_{1,2} g_1(x_1) g_2(x_2) \int dt \, e^{i\varepsilon t/\hbar} P(x_1,0;x_2,|t|) . \tag{16}$$

If the characteristic tunneling time $\hbar/E_C$ is much larger than the classical time L^2/D of diffusion through the electrode (where D is diffusion coefficient, i.e., $E_C \gg E_{\rm th} \equiv \hbar D/L^2$), the probability P is constant on the essentially large time scale, $P=1/V$, where V is the volume of the electrode. It follows from Eqs. (13a) and (16) that, in such a case, irrespective of the shape of the central electrode,

$$G_{\rm el} = \frac{\hbar G_1 G_2 \Delta}{4\pi e^2} \left(\frac{1}{E_1} + \frac{1}{E_2} \right) . \tag{17}$$

In the opposite limit, $E_i \gg E_{\rm th}$, the conductance $G_{\rm el}$

depends on the specific form of the central electrode and nonuniformity of conductances $g_i(x_i)$ along the junction areas. Solving the diffusion equation for the simplest case of a rectangular electrode and $g_i(x_i)=\text{const}$, we get for low temperatures $(T \ll E_{\text{th}})$

$$G_{\text{el}} = \frac{\hbar^2 G_1 G_2 \Delta}{16e^2} \left(\frac{1}{E_1} + \frac{1}{E_2} \right)^2 \frac{\pi^{1/2} D}{L^2}, \tag{18}$$

where L is the length of the electrode (the distance between parallel planes of the junctions). At larger temperatures, $E_i \gg T \gg E_{\text{th}}$, the elastic conductance rapidly decreases and becomes exponentially small:

$$G_{\text{el}} \simeq \exp\{-(4\pi T/E_{\text{th}})^{1/2}\}. \tag{19}$$

Equation (19) implies that there should exist a temperature region where the total linear conductance of the system, $G_{\text{el}}+G_{\text{in}}$, also decreases with temperature.

When the central electrode of the junctions is comparable to electron elastic mean free path, the probability P depends essentially on momentum direction $\mathbf{n}_i$, so that the $\mathbf{n}_i$ dependence of the tunneling probabilities $g_i(x_i, \mathbf{n}_i)$ becomes of importance. In order to find $P(t)$ [(14)] in this case one should solve a kinetic equation for the specific shape of the electrode with the specific boundary conditions describing the surface scattering. In the most realistic case when the surface scattering is diffusive and $E_C \ll E_{\text{th}}$ $(E_{\text{th}} = \hbar v_F/L)$, the elastic conductance is again given by Eq. (17).

In conclusion, we have analyzed the charge transport through a metal particle in the Coulomb blockade regime where the tunneling electron can charge the particle only virtually. The inelastic and elastic processes contribute to the current. The elastic tunneling dominates only at very small voltages and temperatures. Despite the virtual origin of this elastic tunneling it can be described in terms of the real electron motion inside the particle.

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