Influence of the electrodynamic environment on electron tunneling at finite traversal time

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The influence of the electrodynamic environment on the I - V characteristics of a normal tunnel junction is investigated beyond the framework of perturbation theory and the tunneling Hamiltonian method. It is possible to get a complete answer using semiclassical methods. The physical background of the effect is discussed, and the case of a strong Coulomb blockade is considered as an example.

In recent years, progress in ultrasmall-tunnel-junction fabrication has made possible the observation of Coulomb effects in these systems.¹ It was shown both theoretically^{2,3} and experimentally^{4,5} that the single normal junction responds to the electrodynamic environment; to the external electrical circuit connected to the junction, for example. This response is due to inelastic tunneling, that is, when the tunneling electron emits or absorbs electromagnetic excitations propagating in the environment. A typical frequency scale for these processes is defined by the maximum energy loss which is possible during the tunneling, i.e., $\max(eV, T)$. Here V is the voltage applied to the junction and T is the temperature. The crucial value is the effective frequency-dependent impedance that the electron experiences when tunneling. It consists of the intrinsic capacitance of the junction and the external circuit impedance.

If the effective impedance at the typical frequency scale is of the order of the quantum value $R_Q = 2\pi/e^2(\hbar = 1)$, there is a strong suppression of the tunneling rate in comparison with the high-voltage and/or high-temperature Ohm's law.^{1,3,5} If not, there are only small deviations due to the environment.^{4,6}

There also is another typical scale for tunneling: the inverse traversal time of the underbarrier motion⁷ (for a review see Ref. 8). One may have some doubts about the relevant scale. The usual treatments of tunneling based on the tunneling Hamiltonian method assume this traversal time to be infinitely short: the theory should be modified in order to take into account a finite traversal time. We will do this by simple physical reasoning using a method which is similar to those used in Refs. 9 and 10.

Let us consider two metals divided by a potential barrier assumed to be smooth enough so that the semiclassical description of electron motion is valid. If a time-dependent voltage is applied to the junction, there will be a uniform electrical field inside the barrier. If the barrier is thick enough and its transparency is low, the main contribution to the tunnel current comes from electrons with momenta perpendicular to the barrier surface and hence we can consider it only a one-dimensional problem. The Schrödinger equation for the time-dependent electron wave function inside the barrier has the form

$$i \frac{\partial \psi}{\partial t} = \left[\frac{[-i\partial_x - (e/c)A(t)]^2}{2m} + U(x) \right] \psi(x, t). \quad (1)$$

Here the x axis is perpendicular to the barrier surface and the electromagnetic field is included using the vector potential A . Suppose we have in the left-hand metal the incoming wave with energy $E + E_F$. We seek solutions of the form

$$\psi(x, t) = \exp(-iE_F t) \exp\left[-\int_0^x dx' m v(x')\right] \times \exp[-i\theta(x, t)]. \quad (2)$$

Here $x=0$ is a left turning point for the energy E_F , and $v(x) = 2[U(x) - E_F m^{-1}]^{-1/2}$. In the semiclassical WKB approximation we get a simple equation for θ ,

$$i \frac{\partial \theta}{\partial t} v(x)^{-1} = \frac{e}{c} A(t) + \frac{\partial \theta}{\partial x}, \quad (3)$$

with the boundary condition

$$\theta(0, t) = Et.$$

The value of θ at the right turning point $\theta(L, t)$ defines the amplitudes of waves transmitted with different energies into the right-hand metal. A similar consideration has been done in Ref. 11.

Now our goal is to take into account thermal and quantum fluctuations of the electromagnetic field. We will consider only fluctuations of the space scale that are larger than the barrier width. The reason for such a restriction is that the electromagnetic excitation propagates much faster than the electron moves. Hence they produce a uniform electric field in the place where the electron is tunneling, and we can use the previous results in our analysis. We can write the electromagnetic field operator in the form

$$\frac{L}{c} \hat{A}(t) = \sum_n \rho_n [\hat{b}_n \exp(i\omega_n t) + \hat{b}_n^\dagger \exp(-i\omega_n t)] + Vt. \quad (4)$$

Here we introduce a system of boson states and the appropriate creation and annihilation operators in order to describe the electrodynamic properties of the junction environment.¹² Solving Eq. (3) we obtain

$$\theta(L, t) = \theta_1 + \theta_2 + \sum_n \theta_n, \quad (5)$$

where

$$\begin{aligned}\theta_1 &= iE\tau + Et \quad [\tau = \int_0^L dx v(x)^{-1}], \\ \theta_2 &= -eVt - ieV\tau_1 \quad [\tau_1 = \int_0^L dx v(x)^{-1} x L^{-1}], \\ \theta_n &= e\rho_n [\hat{b}_n \exp(i\omega_n t) g(\omega_n) + \hat{b}_n^\dagger \exp(-i\omega_n t) g(-\omega_n)] \\ \{g(\omega) &= L^{-1} \int_0^L dx \exp[\omega \int_x^L dx' v(x')^{-1}]\}.\end{aligned}$$

Using properties of boson operators it is possible to show that the tunneling amplitude from the state with energy E in the left-hand metal to the state with energy E' in the right-hand metal is proportional to

$$\int_{-\infty}^{+\infty} dt \exp[-i\theta(L, t) + iE't]$$

so that the probability of tunneling is

$$\begin{aligned}W_{LR}(E, E') &\sim \int_{-\infty}^{+\infty} d(t_1 - t_2) \langle \exp[i\theta^\dagger(t_1)] \exp[-i\theta(t_2)] \rangle \\ &\sim \exp(2E\tau - 2eV\tau_1) P_{LR}(E' - E + eV).\end{aligned}\quad (6)$$

The angular brackets are a notation for averaging over boson states. We can express average exponents of boson operators through exponents of its average quadratic forms and get for P_{RL}

$$P_{LR}(E) = \int_{-\infty}^{+\infty} dt \exp(\langle \theta^\dagger(t) \theta(0) \rangle - \{\langle [\theta^\dagger(0)]^2 \rangle + \langle [\theta(0)]^2 \rangle\} / 2 - iEt). \quad (7)$$

The average quadratic forms of θ operators can be expressed in terms of boson filling factors $N(\omega)$:

$$\begin{aligned}\langle \theta^\dagger(t) \theta(0) \rangle &= \sum_n e^2 \rho_n^2 \{g^2(\omega_n) N(\omega_n) \exp(i\omega_n t) + g^2(-\omega_n) [1 + N(\omega_n)] \exp(i\omega_n t)\} \\ \{\langle [\theta^\dagger(0)]^2 \rangle + \langle [\theta(0)]^2 \rangle\} / 2 &= - \sum_n e^2 \rho_n^2 g(\omega_n) g(-\omega_n) [1 + N(\omega_n)].\end{aligned}$$

Let us go to the limit of a continuous boson spectrum. The coefficients ρ_n can be expressed in terms of a response function in this limit (see, e.g., Ref. 12)

$$\sum_n \rho_n^2 \rightarrow \int \frac{d\omega}{\omega\pi} \text{Re} Z(\omega).$$

To verify this, one may calculate field fluctuation in two ways: first, with the aid of Eq. (4); second, with the aid of the fluctuation-dissipation theorem. Substituting, we obtain

$$P_{LR}(E) = \int_{-\infty}^{+\infty} dt \exp[Q(t) + F_1(T) + F_2 + iEt], \quad (8)$$

$$\begin{aligned}Q(t) &= \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} \frac{\text{Re} Z(\omega)}{2R_Q} \left[\coth \left(\frac{\omega}{T} \right) - 1 \right] \\ &\quad \times [g^2(\omega) e^{i\omega t} - 1],\end{aligned}\quad (8a)$$

$$\begin{aligned}F_1 &= \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} \frac{\text{Re} Z(\omega)}{2R_Q} \left[\coth \left(\frac{\omega}{T} \right) - 1 \right] \\ &\quad \times [1 - g(\omega) g(-\omega)],\end{aligned}\quad (8b)$$

$$F_2 = \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} \frac{\text{Re} Z(\omega)}{2R_Q} [1 - g(\omega) g(-\omega)]. \quad (8c)$$

Here we introduce the effective impedance that the tunneling electron experiences. Its dependence on the frequency scale can be determined either by the external circuit and the intrinsic junction capacitance, or by the electrodynamic properties of the nearest junction environment.^{2,6}

For $\omega \gg 1/\tau$, $g(\omega)$ grows as $\exp(\omega\tau)$. This means that the integrals $Q(t)$, $F_2(T)$ converge below the crossover temperature between quantum- and thermally-activated tunneling.¹³ As to the integral F_2 , it diverges formally,

but as it is a constant, it can be included in the coefficient of proportionality in (6). This integral determines the renormalization of the tunneling probability due to electromagnetic field zero fluctuations. It can be evaluated beyond the framework of the semiclassical approach used here as has been done in Ref. 14. In Ref. 14, modes with high frequency—of the order of the barrier height—were taken into account and also the change in the imaginary-time trajectory was evaluated.

In the same manner we are able to calculate the probability of tunneling from the right to the left:

$$W_{RL}(E, E') \sim \exp(2E\tau - 2eV\tau_1) P_{RL}(E' - E + eV). \quad (9)$$

It is possible to show that these probabilities obey the detailed balance symmetry so that

$$\frac{e^{2E\tau} P_{LR}(E' - E)}{e^{2E'\tau} P_{LR}(E - E')} = \exp \left(\frac{E - E'}{T} \right). \quad (10)$$

The tunneling current is given by the usual formula

$$\begin{aligned}I(V) &\sim \int dE dE' \{f_L(E) [1 - f_R(E')] W_{LR}(E, E')\} \\ &\quad - \{f_R(E) [1 - f_L(E')] W_{RL}(E, E')\}.\end{aligned}\quad (11)$$

Here $f_{L,R}(E)$ are electron filling factors in the left and right electrodes, respectively, at a certain energy. From (6) and (9)–(11), we obtain finally the expression for the current-voltage characteristics:

$$\begin{aligned}I(V) &= \frac{G_0(T)}{2\tau} \exp(-2eV\tau_1) \\ &\quad \times \int \frac{d\omega}{2\pi} \frac{1 - \exp(-eV/T)}{1 - \exp(\omega/T)} P_{LR}(\omega + eV).\end{aligned}\quad (12)$$

Here the factor $\exp(F_2)$ is included in G_0 , and the

current-voltage characteristics should be compared with that in the absence of interaction with the environment:¹³

$$I(V) = \frac{G_0(T)}{2\tau} \exp(-2eV\tau_1) [1 - \exp(2eV\tau)] \left(G_0(T) = G_0(0) \frac{2\pi\tau T}{\sin(2\pi\tau T)} \right). \quad (13)$$

The last form reminds us that the barrier transparency depends exponentially on energy at the scale $E - E_F \sim 1/\tau$. If the voltage at this scale drops across the junction, it may be considered as an effective barrier suppression by the voltage.

In the limit of infinitely short traversal time $\tau \rightarrow 0$, $g(\omega) \rightarrow 0$ and Eq. (12) becomes the expression for the current-voltage curve of the normal tunnel junction affected by the environment [see, e.g., Eqs. (3) and (5) of Ref. 10], Eq. (13) converts to Ohm's law.

What changes when τ becomes finite? First, the effective impedance is renormalized [see (8a) and (8b)], second, $I(V)$ becomes strongly nonlinear at the scale $eV \sim \tau$ due to the barrier suppression. It allows us to formulate two simple conclusions:

(i) If the typical frequency scales (such as eV , T , energy scale related to Coulomb suppression of the tunneling rate, and peculiar frequencies of the impedance) are much less than the inverse traversal time, the influence of traversal time effects is negligibly small.

(ii) If these scales are comparable, we should take into account these effects, but it also means that the barrier-suppression effect is strong and the current-voltage curve is strongly nonlinear as a consequence.

In experiments,¹⁵ a significant tunneling rate suppression at small voltages has been observed and has been interpreted as the manifestation of Coulomb effects. This interpretation was based on a hypothesis which implied that the charging energy can be estimated from the distance through which the electromagnetic field propagates during the traversal time. This work suggests that the hypothesis is wrong, because the time which corresponds to an energy uncertainty of the order of the estimated energy is much greater than the traversal time. It means that the field has a larger time for propagation and the hypothesis has an inner contradiction.

As an example, we consider the case of strong Coulomb blockade due to intrinsic junction capacitance. In this case the real part of impedance is simply $\pi C_T^{-1} \delta(\omega)$, and for the probability to have an energy loss E when tunneling from the left to the right we get

$$P_{LR}(E) = \exp \left[-\frac{(E - E_Q)^2}{4TE_Q} - E\tau \right] 2(E_Q T / \pi)^{1/2}. \quad (14)$$

At $\tau \ll E_Q = e^2/2C_T$ this probability has a peak at energy E_Q which is needed for charging of the tunnel capacitor,¹

FIG. 1. Temperature-dependent shift of the Coulomb gap. The temperature decreases from the left-hand-side curve to the right-hand-side one, $2T\tau = 1, 0.8, 0.6, 0.4, 0.2, 0$ for different curves. The Coulomb energy is significantly larger than inverse traversal time, $E_Q\tau = 10$.

and the current-voltage curve exhibits a Coulomb gap at $eV < E_Q$. If the temperature is comparable with the inverse traversal time, the peak position shifts to $E_Q \times (1 - 2T\tau)$. Also, if $E_Q\tau \gg 1$, the well-shaped Coulomb gap is visible at this energy. The gap voltage must be equal to the typical energy loss and consequently the temperature-dependent shift of the Coulomb gap energy is predicted.

This shift is illustrated in Fig. 1. A set of current-voltage curves at different temperatures is presented here. The parameter $E_Q\tau$ is chosen big enough so that the curves are strongly nonlinear at the scale of E_Q and the gap is visible at $T \sim 1/\tau$. At zero temperature (right-hand-side curve) there is a sharp jump in differential conductivity. When the temperature increases (i) the jump becomes smoother and (ii) the whole curve shifts in accordance with (14). At the crossover temperature $T_0 = (2\tau)^{-1}$ (left-hand-side curve) the gap becomes zero.

The traversal time for usual oxide or vacuum barriers between metals is of the order of 10^{-15} sec and as a rule is less than the relevant time scale. It is not so for artificial, wide tunnel barriers formed by doping or by applying the gate voltage in GaAs systems. For these barriers the traversal time may be of the order of 10^{-12} and its finiteness is likely to be important.

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