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Gert-Ludwig Ingold, Hermann Grabert

Angaben zur Veröffentlichung / Publication details:

Ingold, Gert-Ludwig, and Hermann Grabert. 1991. "Finite-temperature current-voltage characteristics of ultrasmall tunnel junctions." *Europhysics Letters (EPL)* 14 (4): 371–76. <https://doi.org/10.1209/0295-5075/14/4/015>.

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Finite-Temperature Current-Voltage Characteristics of Ultrasmall Tunnel Junctions.

G.-L. INGOLD and H. GRABERT

Fachbereich Physik, Universität Essen - Universitätsstraße 5, D-4300 Essen 1, FRG

Abstract. – The current-voltage characteristics of tunnel junctions are studied in a region where charging effects are important. The influence of the electromagnetic environment on the Coulomb blockade is described in terms of the probability $P(E)$ that a tunnelling electron loses the energy E to the environment. This quantity depends only on the external impedance shunting the junction. Given $P(E)$, the tunnelling current for normal as well as superconducting tunnel junctions can be calculated for finite temperatures and any impedance. It is shown that the density of environmental modes becomes primarily observable in differential current-voltage characteristics.

Coulomb charging effects arising in ultrasmall tunnel junctions have recently attracted a great deal of interest. These phenomena occur if the charging energy $E_c = e^2/2C$ is larger than the thermal energy $k_B T$, where C is the junction capacitance and T the temperature. Some of the theoretically predicted effects [1] have been observed clearly in multijunction circuits [2] and new devices exploiting the Coulomb blockade were fabricated [3]. For single junctions the situation is more complicated. Observations of Coulomb gap structures in point-contact tunnel junctions [4, 5] arise from an effective multijunction circuit, while experiments on single oxide layer tunnel junctions [6] showed a strongly suppressed Coulomb gap. Recently, it became clear that the influence of the electrodynamic environment on single electron tunnelling which was neglected in earlier theoretical treatments is of crucial importance. This problem was addressed by Nazarov [7] on the basis of a many-body Hamiltonian for the junction coupled to an electromagnetic field which propagates in a specified geometry. In an alternative approach developed by Devoret *et al.* [8] the environmental influence is incorporated in the theory through a modified tunnelling Hamiltonian. This theory expresses the effect of the external circuit directly in terms of the environmental impedance $Z(\omega)$. For the case of zero temperature related results were also obtained by Girvin *et al.* [9]. These theories predict that the coupling to the environment leads to a complete wash-out of the Coulomb blockade for the common case of low-impedance environments. However, the Coulomb gap should become visible also for single junctions if the impedance of the electrodynamic environment exceeds the resistance quantum

$R_Q = h/2e^2$. In a set-up where the junction was attached to high-impedance leads [10, 11], a Coulomb gap was recently observed for single normal tunnel junctions by Cleland *et al.* [11]. In this letter we discuss the properties of the function $P(E)$ which contains the relevant information about the coupling of the tunnel junction to its electromagnetic environment. We show that the properties of the environment become mostly apparent in the differential current-voltage characteristics of normal junctions.

The theory by Devoret *et al.* determines the current-voltage characteristic of a normal tunnel junction for tunnelling resistances $R_T \gg R_Q$ and low currents $I \ll e/\tau_c$, where τ_c is the relaxation time of the electromagnetic environment. Under these conditions the tunnelling current is given by

$$I = \frac{1}{eR_T} \int_{-\infty}^{+\infty} dE (eV - E) \frac{1 - \exp[-\beta eV]}{1 - \exp[-\beta(eV - E)]} P(E), \quad (1)$$

where $\beta = 1/k_B T$. In contrast to the standard result, this formula incorporates the influence of the external electrical circuit described through the function

$$P(E) = (2\pi\hbar)^{-1} \int_{-\infty}^{+\infty} dt \exp[J(t) + iEt/\hbar], \quad (2)$$

which gives the probability for a tunnelling electron to loose the energy E to the environment. The dynamical properties of the electrical circuit enter into $P(E)$ through the function

$$J(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{\omega} \frac{\text{Re} Z_t(\omega)}{R_Q} \frac{\exp[-i\omega t] - 1}{1 - \exp[-\beta\hbar\omega]}. \quad (3)$$

$P(E)$ therefore only depends on the temperature and the total impedance

$$Z_t(\omega) = \frac{1}{i\omega C + Z^{-1}(\omega)} \quad (4)$$

of the junction with capacitance C in parallel with the external circuit with impedance $Z(\omega)$. Using these formulae one may determine the I - V characteristic for arbitrary frequency dependence of the external impedance. We note that a related expression for $I(V)$ also holds for the case of a superconducting junction with $\hbar I_0/2e \ll e^2/2C$, where I_0 is the Josephson critical current. Then the occupation probabilities for electronic states have to be replaced by those for Cooper pairs on both sides of the junction which are proportional to δ -functions [12]. From this it is clear that the function $P(E)$ plays a crucial role in describing the influence of the environment on normal as well as superconducting tunnel junctions.

In the following we will discuss some general properties of $P(E)$ which are related to the fact that it describes the probability that a tunnelling electron exchanges the energy E with the environment. Firstly, by disregarding the coupling to an external circuit, that is for $Z(\omega) = 0$, one has $P(E) = \delta(E)$ and thus does not account for the possibility to excite an external mode. When this is inserted into (1) one recovers the usual ohmic I - V characteristic with tunnelling resistance R_T . For arbitrary impedance and temperature of the environment

$P(E)$ is positive and normalized, *i.e.* $\int_{-\infty}^{+\infty} dE P(E) = 1$, and it satisfies the sum rule $\int_{-\infty}^{+\infty} dE E P(E) = e^2/2C$. Using these properties, one can show that for large voltages and

arbitrary impedance the I - V curve of a normal junction is ohmic with resistance R_T but shifted in voltage by $e/2C$. This is a manifestation of the Coulomb blockade at large voltages. Further, $P(E)$ obeys the detailed balance symmetry, $P(E) = \exp[\beta E]P(-E)$. For zero temperature $P(E) = 0$ for $E < 0$ since the tunnelling electron cannot absorb energy from the environment.

Clearly, $P(E)$ cannot be evaluated analytically except for simple cases and one has to resort to numerical methods. There are at least two possibilities to compute $P(E)$ numerically. One may use formulae (2)-(4) directly. Given $Z_t(\omega)$ one calculates $\partial J(t)/\partial t$, from where one goes back to the frequency domain to obtain $P(E)$. This method involves two often slowly converging Fourier integrals and one standard integration. Of course, it is more reasonable to evaluate $P(E)$ directly without going to the time domain. To this end, we derive an integral equation for $P(E)$. When addressing this problem one has to treat the asymptotic behaviour of the correlation function $J(t)$ carefully. We assume that the total impedance $Z_t(\omega)$ has an ohmic component, *i.e.* $\text{Re} Z_t(\omega = 0) \neq 0$ which is the case for realistic electromagnetic environments. In the experimentally relevant case of a finite circuit temperature, we split off the leading asymptotic behaviour of $J(t)$ for large t

$$J(t) = -D|t| + J_1(t), \quad (5)$$

where $D = (\pi/\beta\hbar)(\text{Re} Z_t(0)/R_Q)$. Equation (5) defines $J_1(t)$ which then approaches a constant value for $t \rightarrow \infty$. By differentiating $\exp[J_1(t)]$ with respect to time and formal reintegration under the condition $\exp[J_1(0)] = 1$, we arrive at

$$\exp[J_1(t)] - 1 = -i \int_0^t dt' \int_{-\infty}^{+\infty} d\omega k(\omega) \exp[-i\omega t'] \exp[J_1(t)], \quad (6)$$

where the function

$$k(\omega) = \bar{k}(\omega) - \frac{1}{\beta\hbar\omega} \frac{\text{Re} Z_t(0)}{R_Q}, \quad (7)$$

with

$$\bar{k}(\omega) = \frac{1}{1 - \exp[-\beta\hbar\omega]} \frac{\text{Re} Z_t(\omega)}{R_Q}, \quad (8)$$

contains the dependence on the external impedance and temperature. From (3) we see that $\bar{k}(\omega)$ is proportional to the Fourier transform of the time derivative of $J(t)$. In view of (2), we have

$$\frac{1}{2\pi\hbar} \int_0^\infty dt \exp\left[\frac{i}{\hbar}Et\right] \exp[J(t)] = \frac{1}{2}P(E) + \frac{i}{2\pi} \int_{-\infty}^{+\infty} du \frac{P(E-u)}{u}, \quad (9)$$

where the integral on the r.h.s. is to be taken as a Cauchy principal-value integral. We now use (9) with (5) to rewrite (6) in terms of $P(E)$. Taking the real part, we get after some rearrangements the integral equation

$$P(E) = I(E) + \int_{-\infty}^{+\infty} d\omega K(E, \omega) P(E - \hbar\omega). \quad (10)$$

Here, the inhomogeneity

$$I(E) = \frac{1}{\pi\hbar} \frac{D}{D^2 + E^2/\hbar^2} \quad (11)$$

corresponds to the $P(E)$ for a purely ohmic environment in the limit of vanishing junction capacitance and high temperatures. The integral kernel $K(E, \omega)$ is given by

$$K(E, \omega) = \frac{E/\hbar}{D^2 + E^2/\hbar^2} k(\omega) + \frac{D}{D^2 + E^2/\hbar^2} \kappa(\omega), \quad (12)$$

where $\kappa(\omega)$ is the Hilbert transform of $k(\omega)$ which may be written as

$$\kappa(\omega) = i\bar{k}(\omega) - i\omega\hat{J}(-i\omega)/\pi. \quad (13)$$

Here, $\hat{J}(z)$ is the Laplace transform of $J(t)$. It can be shown [13] that the fluctuation-dissipation theorem implies the relation

$$\hat{J}(z) = \frac{\pi}{R_Q \hbar \beta z} \left[-\frac{Z_t(-iz)}{z} + 2 \sum_{n=1}^{\infty} \frac{z Z_t(-iz) - \nu_n Z_t(-i\nu_n)}{\nu_n^2 - z^2} \right] - i \frac{\pi}{2R_Q} \frac{Z_t(-iz)}{z} \quad (14)$$

between $\hat{J}(z)$ and the impedance $Z_t(\omega)$. Now (13) and (14) combine to yield

$$\kappa(\omega) = -\frac{1}{1 - \exp[-\beta\hbar\omega]} \frac{\text{Im} Z_t(\omega)}{R_Q} - \frac{2}{\hbar\beta} \sum_{n=1}^{\infty} \frac{\nu_n}{\nu_n^2 + \omega^2} \frac{Z_t(-i\nu_n)}{R_Q}. \quad (15)$$

For simple cases the sum in (15) may be expressed in closed form. Let us consider an external circuit described by a resistance R in series with an inductance L . This impedance was used by Cleland *et al.* [11] to model their experimental set-up. The total impedance now reads

$$\frac{Z_t(\omega)}{R_Q} = \alpha \frac{1 + iQ^2\omega/\omega_c}{1 + i\omega/\omega_c - Q^2(\omega/\omega_c)^2}. \quad (16)$$

Here, $\alpha = R/R_Q$ is the damping strength, $\omega_c = 1/RC$ the inverse relaxation time, and $Q = \omega_c/\omega_s$ the quality factor with the resonance frequency of the undamped circuit $\omega_s = (LC)^{-1/2}$. The sum in (15) can be done and we get

$$\begin{aligned} \kappa_{LR}(\omega) = & -\frac{\text{Im} Z_t(\omega)}{R_Q} \left(\frac{1}{2} + \frac{1}{\beta\hbar\omega} \right) + \frac{1}{\pi} \frac{\text{Re} Z_t(\omega)}{R_Q} \text{Re} \psi \left(1 + i \frac{\beta\hbar\omega}{2\pi} \right) \\ & + \frac{\alpha/\pi}{\sqrt{1-4Q^2}} \left[\frac{Q^2}{\lambda_+ - 1 + Q^2(\omega/\omega_c)^2} \psi \left(1 + \frac{\beta\hbar\omega_c}{2\pi} \lambda_+ \right) - \frac{Q^2}{\lambda_- - 1 + Q^2(\omega/\omega_c)^2} \psi \left(1 + \frac{\beta\hbar\omega_c}{2\pi} \lambda_- \right) \right], \quad (17) \end{aligned}$$

where $\psi(x)$ is the logarithmic derivative of the Γ -function and $\lambda_{\pm} = (1 \pm \sqrt{1-4Q^2})/2Q^2$. In the limit $Q \rightarrow 0$ (17) also includes the case of an environment consisting of a purely ohmic resistor.

For the impedance (16) it is now straightforward to evaluate the function $P(E)$ numerically by virtue of the integral equation (10). We solved the integral equation by simple iteration starting with the inhomogeneity $I(E)$ as first trial function. For $0.1 < Q < 100$ and $0.01 < k_B T/E_c < 1$ we used about 4000 node points and convergence was usually reached in about 10 steps. The solution was then stable with a relative error below 10^{-4} .

Using the numerical results one may calculate the current-voltage characteristic from (1). By differentiating the integrand in (1) one may also calculate derivatives of the I - V characteristic. Some sample numerical results are shown in fig. 1 and 2. The effect of a

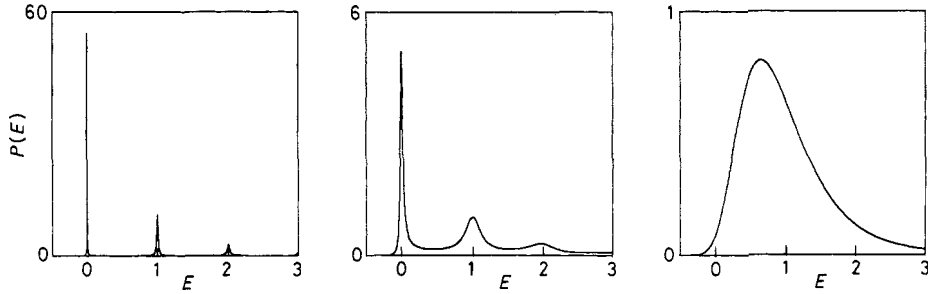


Fig. 1. - The function $P(E)$ giving the probability that a tunnelling particle loses the energy E to the environment is depicted for an LCR -circuit formed by the junction capacitance C and the external leads of inductance L and resistance R . The energy is measured in units of $\hbar\omega_s$ where $\omega_s = 1/\sqrt{LC}$ is the resonance frequency. The diagrams show results for $\hbar\omega_s = E_c$ and low temperatures $k_B T = 0.05E_c$. Further, from left to right $Q = 50, 5, 0.25$, where $Q = \sqrt{L/C}/R$ is the quality factor of the LCR -circuit.

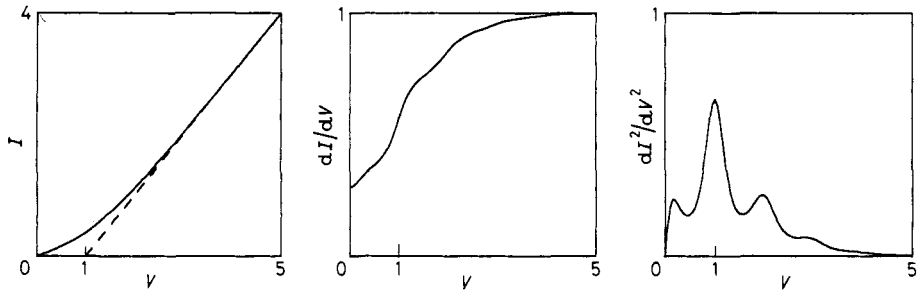


Fig. 2. - The I - V characteristic and its first and second derivatives are shown for a normal metal tunnel junction with the function $P(E)$ of fig. 1 for $Q = 5$. Currents are measured in units of $e/2CR_T$ and voltages in units of $e/2C$. The dashed line indicates the characteristic for ideal Coulomb blockade.

resonance in the environmental spectrum on electron tunnelling is examined in fig. 1. For a narrow resonance [$Q = 50$] $P(E)$ shows a sequence of peaks at integer multiples of the environmental mode energy $\hbar\omega_s$. These peaks describe the absorption and emission of one or more energy quanta $\hbar\omega_s$ by the tunnelling electron. Since fig. 1 gives results for the low temperature $k_B T = 0.05E_c$, the peaks corresponding to the absorption of energy are strongly suppressed. The limiting case of an LC -circuit [$Q = \infty$] is treated analytically in ref. [8, 14]. Figure 1 shows that with decreasing quality factor Q the resonance structure is washed out and for $Q = 0.25$ the spectrum is already close to the purely resistive case. In fig. 2 the I - V characteristic and its first and second derivatives with respect to voltage are presented. The spectral density of the environment becomes primarily observable in derivatives of the I - V characteristic. Near resonances dI/dV vs. V displays steplike structures. This is due to the fact that an electron can only transfer the energy $n\hbar\omega_s$ to the environment if the voltage exceeds $n\hbar\omega_s/e$. Correspondingly, d^2I/dV^2 vs. V shows a peak structure which reproduces the resonance structure of $P(E)$. For $T = 0$ one has $d^2I/dV^2 = (e/R_T)P(eV)$. Finite-temperature corrections to this relation arise primarily for voltages below $k_B T/e$ which is the reason why the quasi-elastic peak of $P(E)$ is suppressed in the d^2I/dV^2 vs. V diagram of fig. 2.

These results show that measurements of differential I - V characteristics should be particularly useful in gaining information about the effect of the external circuit on tunnel junctions. We note that a $P(E)$ extracted from the d^2I/dV^2 vs. V curve of a Josephson

junction driven normal by means of an applied magnetic field should be consistent with the measured I - V characteristic in the superconducting case where $I = (\pi\hbar I_0^2/4e)P(2eV)$ at $T = 0$ [12]. Hence, measurements with the same set-up in the normal and the superconducting state of the junction electrodes should allow for a decisive test of the theoretical model employed here.

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The authors would like to thank M. H. DEVORET, D. ESTEVE, H. POTHIER and C. URBINA for a very inspiring collaboration on single charge tunnelling and are grateful to J. CLARKE, A. N. CLELAND, J. M. MARTINIS and YU. V. NAZAROV for sharing their expertise with us. We also acknowledge helpful conversations with D. B. HAVILAND and L. S. KUZ'MIN. This work was supported by the Deutsche Forschungsgemeinschaft through Sonderforschungsbereich 237.

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