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Transition to Ohmic conduction in ultrasmall tunnel junctions

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The effective dc conductance of an ultrasmall tunnel junction is calculated from the functional-integral description beyond the weak-coupling limit by employing the self-consistent harmonic approximation. With increase in the normal conductance R_N^{-1} , the effective conductance exhibits a crossover from the weak-coupling regime, dominated by thermal activation over the Coulomb gap to the Ohmic behavior in the strong-coupling limit. As the temperature and capacitance approach zero, the results indicate a possibility of a precipitous transition for R_N of the order of \hbar/e^2 .

Recently, several authors^{1,2} have pointed out that the effective conductance of a normal tunnel junction with low capacitance becomes temperature and frequency dependent as a result of quantum voltage fluctuations associated with the electron transfer. Previous calculations of the conductance^{1,2} have been limited to weakly damped junctions, for which the nominal junction resistance R_N (defined by the Ohmic response of a large-capacitance junction) must satisfy the inequality

$$
\frac{R_N}{R_0} \gg \frac{e^2}{k_B T C} \tag{1}
$$

where T is the temperature, C is the capacitance of the junction, and $R_0 = \hbar/e^2 = 4.11$ k Ω . For weakly damped junctions, the calculations^{1,2} predict an activation-type T dependence of the dc conductance:

$$
Y(\omega = 0) = \frac{1}{R_N} \exp\left(-\frac{e^2}{2k_BTC}\right) \tag{2}
$$

Also, the frequency dependence of $\text{Re} Y(\omega)$ is found to exhibit, at low temperatures, a threshold near the charging energy $\hbar \omega \approx e^2/2C$, indicating a photon-assisted tunneling.

The present work attempts to answer the following question: How are the above weak-coupling effects modified as one decreases R_N so that Eq. (1) is satisfied no more? Specifically, we calculate $Y(\omega = 0)$ for a wide range of the parameters $g = \pi R_0 / 2R_N$, and $a = e^2 / 2\pi^2 k_B T C$, well outside the weak-coupling regime. In a strongly damped junction, the charging energy rapidly decays during the electron transfer as a result of the capacitor discharge. Consequently, one expects the dc conductance to depend on g faster than indicated by Eq. (2). This nonlinear dependence of $Y(\omega = 0)$ upon g is borne out by the present calculations. In particular, on increasing the parameter a , the conductance exhibits an interesting trend towards a

precipitous onset at a certain critical value of g, suggestive of a cooperative breakdown of the Coulomb barrier in electron tunneling.

Our calculations start from the Kubo formula for the conductance

$$
\text{Re}Y(\omega) = \frac{1}{\omega} \text{Im} \left[\lim_{i\omega_n \to \omega + i\delta} \int_0^\beta d\,\tau \, e^{i\omega_n \tau} \langle T, I(\tau)I(0) \rangle \right] \tag{3}
$$

where $\omega_n = 2\pi/\beta n$ is the Matsubara frequency and $\beta = (k_B T)^{-1}$. The current-current correlation function is calculated from the generating functional²

$$
Z[\xi] = \text{tr}\left[T_{\tau}\text{exp}\left(-\int_0^{\beta} d\tau [H - I\xi(\tau)]\right)\right],\tag{4}
$$

where H is the Hamiltonian of the junction, including the charging energy and $\xi(\tau)$ is an external potential. Following Ref. 2, the quantity $Z[\xi]$ can be expressed as a path integral over the phase variable $\theta(\tau)$, which is related to the potential difference V across the junction by $\theta = eV/\hbar$. Then the current-current correlation can be expressed also as a path integral²

$$
\langle T_{\tau}I(\tau)I(0)\rangle = \frac{2e^2}{Z[0]} \int D\theta e^{-A[\theta]} \alpha(\tau) \cos[\theta(\tau) - \theta(0)] \tag{5}
$$

where $A[\theta]$ is the effective action of the junction of the form

(5)
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A[\theta]
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$$
A[\theta] = \frac{C\hbar}{2e^2} \int_0^\beta d\tau \dot{\theta}^2(\tau) + 2 \int_0^\beta d\tau \int_0^\beta d\tau' a(\tau - \tau')
$$
\n
$$
\times \sin^2 \left[\frac{\theta(\tau) - \theta(\tau')}{2} \right].
$$
\n(6)

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The function $\alpha(\tau)$ is given by²

$$
\alpha(\tau) = \frac{1}{2\pi} \left(\frac{R_0}{R_N} \right) \frac{(\pi k_B T/\hbar)^2}{\sin^2(\pi k_B T \tau/\hbar)} \tag{7}
$$

According to Eqs. (3) and (5), the calculation of the conductance involves the phase correlator, defined as a non-Gaussian path integral

$$
\Gamma(\tau) = \frac{1}{Z[0]} \int D\theta e^{-A[\theta]} \cos[\theta(\tau) - \theta(0)] \quad . \tag{8}
$$

$$
A_0[\theta] = \frac{C\hbar}{2e^2} \int_0^\beta d\tau \dot{\theta}^2(\tau) + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' a(\tau - \tau')[\theta(\tau')]^2 \tag{11}
$$

The function $K(\tau-\tau')$ plays a role of the variational parameter which is determined from Eq. (9) by requiring that $\delta F_t = 0$ when $K \rightarrow K + \delta K$. This yields a self-consistent equation for K:

$$
K(\tau - \tau') = \exp[-\frac{1}{2}D(\tau - \tau')] \tag{12}
$$

where

$$
D(\tau - \tau') = \frac{1}{Z_0} \int D\theta e^{-A_0[\theta]} [\theta(\tau) - \theta(\tau')]^2
$$
 (13)

According to Eq. (8), the phase correlator $\Gamma(\tau)$, evaluated within the SCHA, is given by the Gaussian path integral

$$
[\Gamma(\tau)]_{\text{SCHA}} = \Gamma_0(\tau) = \frac{1}{Z_0} \int D\theta e^{-A_0[\theta]} \cos[\theta(\tau) - \theta(0)] = K(\tau) \tag{14}
$$

The explicit solution of Eqs. (12) and (13) is done by expanding $\theta(\tau)$ into a Fourier series³

$$
\theta(\tau) = \sum_{n = -\infty}^{\infty} \theta_n e^{-i\omega_n \tau} \tag{15}
$$

Then the path integral (13) reduces to a multiple Gaussian integration over the coefficients θ_n . An integral equation for $\Gamma_0(\tau)$ is obtained in the form

$$
\Gamma_0(\tau) = \exp\left(\frac{-e^2 \beta}{2\pi^2 C} \sum_{n=1}^{\infty} \frac{1 - \cos(\omega_n \tau)}{n^2 + (e^2 \beta^2 / 2\pi^2 C) \int_0^{\beta} d\tau a(\tau) \Gamma_0(\tau) [1 - \cos(\omega_n \tau)]}\right) \tag{16}
$$

Introducing the dimensionless parameters $a = e^2 \beta / 2\pi^2 C$ and $g = \pi R_0 / 2R_N$, changing the variable τ to $x = (2\pi/\beta) \tau$, and using Eq. (7) for $\alpha(\tau)$ we obtain from Eq. (16)

$$
\Gamma_0(x) = \exp\left[-a \sum_{n=1}^{\infty} \frac{1 - \cos(nx)}{n^2 + ag \int_0^{\pi} \Gamma_0(x) \frac{1 - \cos(nx)}{1 - \cos x} dx}\right].
$$
\n(17)

This equation has been solved numerically for $\Gamma_0(x)$ by the method of successive approximations. This method exhibits, in the present case, a good convergence, allowing us to limit the number of iterations to 10. On the other hand, the Fourier series in the exponent of Eq. (17) shows a slow convergence, especially when the parameters a and g are large. Hence, the number of terms in the series was taken $n = 10³$, in which case the overall accuracy of $\Gamma_0(x)$ was of the order of 1%.

In order to test whether some sort of critica1 behavior takes place, as a result of the non-Gaussian nature of the effective action $A[\theta]$, we calculate the effective conductance at $\omega = 0$, which according to Eqs. (3)-(14) is given by

$$
Y_{\text{SCHA}}(\omega = 0) = \frac{1}{\pi R_N} \int_0^{\pi} dx \, \Gamma_0(x) \tag{18}
$$

the dimensionless conductance Y_{SCHA} defined as

$$
Y_{\text{SCHA}} = \frac{\pi^2 R_0}{2} Y_{\text{SCHA}}(\omega = 0) = g \int_0^{\pi} dx \, \Gamma_0(x) \tag{19}
$$

as a function of the coupling constant g for three values of the parameter a.

For the sake of comparison, we also show, as dashed curves, the conductance \overline{Y}_H calculated in the harmonic approximation, which is based on the Gaussian choice for the action (6) :

$$
A_H[\theta] = \frac{Ch}{2e^2} \int_0^{\beta} d\tau \theta^2(\tau)
$$

+ $\frac{1}{2} \int_0^{\beta} d\tau \int_0^{\beta} d\tau' a(\tau - \tau')[\theta(\tau) - \theta(\tau')^2]$ (20)

where $\Gamma_0(x)$ is the solution of Eq. (17). In Fig. 1, we plot Y_H is then given by Eqs. (18) and (19), with $\Gamma_0(\tau)$ re-

In what follows, we employ the self-consistent harmonic approximation (SCHA) to evaluate $\Gamma(\tau)$. This approximation can be derived from the variational principle^{3,4}

$$
F \le F_0 + \frac{1}{\beta Z_0} \int D\theta e^{-A_0[\theta]} (A - A_0) = F_t , \qquad (9)
$$

where

$$
Z_0 = e^{-\beta F_0} = \int D\theta e^{-A_0[\theta]} \tag{10}
$$

The trial action $A_0[*θ*]$ is chosen in the form

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FIG. 1. Dimensionless dc conductance \overline{Y} of a tunnel junction plotted as a function of the coupling constant $g = \pi \hbar/2e^2R_N$, where R_N is the nominal resistance of the junction. The parameter $a = e^2/2\pi^2 k_B T C$, where C is the capacitance. The full lines represent \overline{Y}_{SCHA} given by Eq. (19); the dashed lines give the conductance \overline{Y}_H , based on the harmonic approximation of Eq. (20).

placed by

$$
\Gamma_H(\tau) = \frac{1}{Z_h} \int D\theta e^{-A_H[\theta]} \cos[\theta(\tau) - \theta(0)] \quad . \tag{21}
$$

We see that the values of \overline{Y}_{SCHA} are always smaller than those for \overline{Y}_H , indicating that the harmonic approximation overestimates the role of dissipation in the suppres-
sion of the phase fluctuations. The difference \overline{Y}_H $-\bar{Y}_{SCHA}$ becomes more pronounced as the parameter a increases, showing the increasing role of the non-Gaussian phase fluctuations. We note that the "weak-coupling" conductance \overline{Y}_{wc} , calculated from Eq. (2), yields straight lines (not shown in Fig. 1) with the slopes 0.8, 0.06, and 0.006 for $a = 1$, 10, and 100, respectively. For very large values of g, both the \overline{Y}_H and \overline{Y}_{SCHA} curves tend to exhibit, for all values of a, the same asymptotic "strong-coupling"

slope, equal to π . The most interesting feature of the SCHA calculations is the existence of the crossover between these weak-coupling and the strong-coupling regimes, which takes place, for large values of a , over a narrow region near some critical value of the coupling constant g_c . The values of g_c increase with the parameter a, but tend to saturate towards $g_c \approx 3$. This indicates that, for large values of a, the weak-coupling approximation breaks down when $g \geq 3$, which is consistent with the criterion $R_N/R_0 \gg 1$. The latter weak-coupling condition can be also written as $R_N C \gg \hbar/E_c$, where E_c is the charging energy (Coulomb gap). This implies that, in a weakly coupled junction, the time constant for the capacitor discharge is large enough so as not to smear the Coulomb gap.

Extrapolating the SCHA results to $a \rightarrow \infty$, one expects that in this limit the \bar{Y}_{SCHA} curve develops a precipitous onset, marking a transition from an insulating to conducting regime at some critical value of g_c . In this context, it is useful to remark that as $\beta = 1/k_B T$ goes to infinity, the action (6) is equivalent to a one-dimensional xy model with long-range interactions along the τ axis given by the kernel $a(\tau) \propto \tau^{-2}$. According to the renormalization-group analysis of Fisher, Ma, and Nickel⁵ the interaction decaying as τ^{-2} has a borderline range for the possibility of hav ing a phase transition in a one-dimensional system. Although true phase transition with broken symmetry $(\langle \theta \rangle \neq 0)$ is not expected in the problem of a tunnel junction, the present calculations indicate the possibility of a critical behavior in the phase correlation function.

It should be interesting to apply the functional integration method to granular metals consisting of arrays of ultrasmall tunnel junctions.⁶ The crossover from activated to Ohmic conduction found in the present work for a single junction may also contribute to the metal-insulator transition in granular films.⁷

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