Rapid Communications

The Rapid Communications section is intended for the accelerated publication of important new results. Manuscripts submitted to this section are given priority in handling in the editorial office and in production. A Rapid Communication may be no longer than 3½ printed pages and must be accompanied by an abstract. Page proofs are sent to authors, but, because of the rapid publication schedule, publication is not delayed for receipt of corrections unless requested by the author.

Transition to Ohmic conduction in ultrasmall tunnel junctions

R. Brown and E. Šimánek Department of Physics, University of California, Riverside, California 92521 (Received 21 April 1986)

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

$$\frac{R_N}{R_0} \gg \frac{e^2}{k_B T C} , \qquad (1)$$

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

$$Y(\omega=0) = \frac{1}{R_N} \exp\left[-\frac{e^2}{2k_B T C}\right] .$$
 (2)

Also, the frequency dependence of $\operatorname{Re} Y(\omega)$ is found to exhibit, at low temperatures, a threshold near the charging energy $\hbar \omega = e^2/2C$, 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 $a = e^2/2\pi^2k_BTC$, 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

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

$$Z[\xi] = \operatorname{tr}\left[T_{\tau} \exp\left(-\int_{0}^{\beta} d\tau [H - I\xi(\tau)]\right)\right], \qquad (4)$$

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

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

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

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

2958

R. BROWN AND E. ŠIMÁNEK

(11)

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

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

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

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

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

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 $K \to K + \delta K$. This yields a self-consistent equation for K:

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

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

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

$$\Gamma_{0}(\tau) = \exp\left[\frac{-e^{2}\beta}{2\pi^{2}C}\sum_{n=1}^{\infty}\frac{1-\cos(\omega_{n}\tau)}{n^{2}+(e^{2}\beta^{2}/2\pi^{2}C)\int_{0}^{\beta}d\tau\,\alpha(\tau)\Gamma_{0}(\tau)[1-\cos(\omega_{n}\tau)]}\right].$$
(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)

$$\Gamma_0(x) = \exp\left[-a \sum_{n=1}^{\infty} \frac{1 - \cos(nx)}{n^2 + ag \int_0^{\pi} \Gamma_0(x) \frac{1 - \cos(nx)}{1 - \cos x} dx}\right].$$
(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 $n = 10^3$, in which case the overall accuracy of $\Gamma_0(x)$ was of the order of 1%.

In order to test whether some sort of critical 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

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

where $\Gamma_0(x)$ is the solution of Eq. (17). In Fig. 1, we plot

the dimensionless conductance Y_{SCHA} defined as

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

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):

$$A_{H}[\theta] = \frac{C\hbar}{2e^{2}} \int_{0}^{\beta} d\tau \dot{\theta}^{2}(\tau) + \frac{1}{2} \int_{0}^{\beta} d\tau \int_{0}^{\beta} d\tau' \alpha(\tau - \tau') [\theta(\tau) - \theta(\tau')^{2}] . \quad (20)$$

 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}

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

where

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

The trial action $A_0[\theta]$ is chosen in the form

RAPID COMMUNICATIONS



FIG. 1. Dimensionless dc conductance \overline{Y} of a tunnel junction plotted as a function of the coupling constant $g = \pi \hbar/2e^2 R_N$, 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

$$\Gamma_{H}(\tau) = \frac{1}{Z_{h}} \int D \,\theta e^{-A_{H}[\theta]} \cos[\theta(\tau) - \theta(0)] \quad (21)$$

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 suppression of the phase fluctuations. The difference \overline{Y}_H $-\overline{Y}_{SCHA}$ 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 $a \to \infty$, one expects that in this limit the \overline{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 $\alpha(\tau) \propto \tau^{-2}$. 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 having 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

The authors would like to thank Professor F. Cummings for discussion and advice in the initial stages of this work.

- ¹T. L. Ho, Phys. Rev. Lett. 51, 2060 (1983).
- ²E. Ben-Jacob, E. Mottola, and G. Schon, Phys. Rev. Lett. **51**, 2064 (1983).
- ³R. P. Feynman, Statistical Mechanics (Benjamin, New York, 1972), Chap. 3.
- ⁴E. Šimánek and K. Stein, Physica A **129**, 40 (1984).
- ⁵M. E. Fisher, Shang-keng Ma, and B. G. Nickel, Phys. Rev. Lett. **29**, 917 (1972).
- ⁶A. Kawabata, J. Phys. Soc. Jpn. **43**, 1491 (1977).
- ⁷G. Deutscher, B. Bandyopadhay, T. Chui, P. Lindenfeld, W. L. McLean, and T. Worthington, Phys. Rev. Lett. **44**, 1150 (1980).