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NONPERTURBATIVE CALCULATION OF COULOMB BLOCKADE IN A SMALL TUNNEL JUNCTION

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A non-perturbative calculation is performed for Coulomb blockade in a small tunnel junction, by use of the closed-time-path Green's function and Odintsov's polaron formulation. Self consistent forms for the current-voltage (I-V) characteristics, the damping function, the fluctuation function, and the non-equilibrium Bose distribution function, are presented. At T = 0 and in the weak dissipation limit, analytic results are obtained. In particular, we demostrate that the widely used Ohmic approximation (tunneling impedance $Z(\omega) = R_T$) for the effect of dissipation on Coulomb blockade, is satisfactory in the range of $R_T \sim R_k$ to $10R_k$ ($R_k = 25.8$ kΩ).

I. INTRODUCTION

Recent studies show that for the Coulomb blockade of single electron tunneling[1,2], there are two sources, the leads connecting the junction to external circuit and the discrete charge transfer accross the junction, which reduce the effective Coulomb barrier. To date the charge transfer contribution to the smearing of the Coulomb blockade is treated by introducing a constant tunnel Resistance R_T (the Ohmic approximation).[1,2] Due to technical difficulties, these studies have not demonstrated clearly the validity or otherwise of the Ohmic approximation. Therefore, there is a urgent need to analyse the charge transfer process in a more rigorous way. Here we develop Odintsov's polaron formulation[2] for single electron tunneling into a self-consistent calculation, where the non-Ohmic effect of the tunneling resistance is considered, and where the range of validity of the Ohmic approximation can be readily identified. In particular, we will employ the closed time-path Green's function method developed by Su, Chen and Ting. [3]

II.NON-PERTURBATIVE CALCULATION

In this section, we first summarize Odintsov's idea that the polaron model can be used to calculate single electron tunneling (SET). Then we go beyond Odintsov's perturbation theory by using sophisticated techniques developed for solving the polaron problem to evaluateSET non-perturbatively.

The polaronic Hamiltonian, in standard notation can be written as [2,3]

$$H = \frac{p^2}{2m} - eE(t)x + \sum_{n,k} g_{n,k}\left(b^+_{n,-k} + b_{n,k}\right)e^{ikx} + \sum_{n\,k} \hbar\omega_{n,k}\, b^+_{n,k}\, b_{n,k} \qquad (1)$$

In dealing with (1), Odintsov has taken the following three steps: (i) variable mapping

$$\left\{\begin{matrix} p \leftrightarrow \frac{Q}{e} \equiv \frac{CV}{e},\ x \leftrightarrow \frac{\varphi}{2} \\ \frac{1}{2} \leftrightarrow E \equiv \frac{e^2}{2C}\quad E \leftrightarrow \frac{I}{e} \end{matrix}\right\}, \qquad (2)$$

where C is the junction capacitance, Q,φ are the charge and phase on the junction capacitance, and I, V are the dc current and voltage; (ii) there are two kinds of "phonon" modes with the discrete momentum transfer k= ± 1; (iii) the electron-phonon interaction spectral density obeys certain mapping relations with respect to the tunneling resistance R_T . In this way, Odintsov has demonstrated, with the use of path integral techniques, that there is a one-to-one correspondence between the polaron and the single electron tunneling problems.

Next, we use the above idea and adopt the closed time-path Green's function method for the polaron problem as developed by Su, Chen and Ting[3], from which we obtain after some algebra, a set of self-consistent equations for single electron tunneling. Namely, they are the steady state equation

$$I = \frac{V}{R_T} - 4e\alpha_T \int_0^\infty dt \sin\left(eVt/\hbar\right) \left(\frac{\pi/\beta\hbar}{\sinh\left(\pi t/\beta\hbar\right)}\right)^2 \sin\left[f_1(t)\right]\exp\left[-f_2(t)\right] \qquad (3)$$

the damping function equation

$$\gamma(\omega) = \gamma_0\left\{1 - \frac{2}{\pi}\int_0^\infty dt\, \frac{\sin(\omega t)}{\omega}\cos\left(eVt/\hbar\right) \left(\frac{\pi/\beta\hbar}{\sinh\left(\pi t/\beta\hbar\right)}\right)^2 \sin\left[f_1(t)\right]\exp\left[-f_2(t)\right]\right\}, \qquad (4)$$

the fluctuation function equation

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$$f_1(t) = E_c \int \frac{d\omega}{\pi} \frac{\sin^2(\omega t/2)}{\omega^2 + \gamma^2(\omega)} \quad , \tag{5a}$$

$$f_2(t) = E_c \int \frac{d\omega}{2\pi} \frac{\sin^2(\omega t/2)}{(\omega/2)^2} \frac{\omega N(\omega)\gamma(\omega)}{\omega^2 + \gamma^2(\omega)} \quad , \tag{5b}$$

and the non-equilibrium Bose function equation

$$\omega N(\omega)\gamma(\omega) = \gamma_0 \left\{ \frac{\hbar\omega + eV}{2h} \coth \frac{\beta(h\omega + eV)}{2} - E_c + \frac{\hbar\omega - eV}{2h} \coth \frac{\beta(\hbar\omega - eV)}{2} + \frac{2}{\pi}\int_0^\infty dt \cos(eVt/\hbar) \left(\frac{\pi/\beta\hbar}{\sinh(\pi t/\beta\hbar)} \right)^2 \left\{1 - e^{-f_2(t)}\right\} \cos[f_1(t)] \right\} , \tag{6}$$

where $\beta = k_B T$, $\gamma_0 = 1/CR_T$,and $\alpha_T = \hbar/(2\pi e^2 R_T)$.

Eqs. (3)-(6) are the key results of this paper. In the first order (Ohmic) approximation, (4) is replaced by $\gamma(\omega) = \gamma_0$, and (3)-(6) become uncoupled equations. In this case, in the weak coupling limit ($\gamma_0 \to 0$), (5) can be evaluated analytically as

$$f_1(t) = E_c t/\hbar , \quad f_2(t) = b_0 t^2 \quad , \tag{7}$$

where the fluctuation parameter $b_0 = -0.5\alpha_T \ln(6.23\alpha_T)$. In Ref. 2, (7) is then used to study the steady state equation (3), which is of higher order in γ_0 and which is obviously not consistent with the assumption of Ohmic approximation. On the other hand, our equations. (3)-(6) can be solved self-consistently. Also, we would like to mention that from (3) and (4), the linear conductance can be easily derived as

$$G = \frac{\partial I}{\partial V}\bigg|_{V=0} = C\gamma(0) \quad . \tag{8}$$

III. ANALYTICAL RESULTS

In the T = 0 and $\gamma_0 \to 0$ limit, (3)-(6) can be solved analytically in the following way. First, based on the knowledge of (7), we postulate

$$f_1(t) = at, \quad f_2(t) = bt^2 \quad . \tag{9}$$

Next, using (9), after some algebra we obtain from (4) and (6), respectively,

$$\gamma(\omega) = \gamma_0 \left\{1 - \operatorname{erf}\frac{a}{2\sqrt{b}}\right\} + O(\omega^2) \tag{10}$$

$$\omega N(\omega)\gamma(\omega) \approx \gamma_0 \left\{ \omega + a\left[\operatorname{erfc}\frac{a}{2\sqrt{b}} - \frac{2}{a}\sqrt{\frac{b}{\pi}}\, e^{-\frac{a^2}{4b}}\right]\right\} . \tag{11}$$

Substituting (10) and (11) into (5), and expressing the subsequent result in the form of (9), we obtain

$$a = E_C/\hbar \quad , \quad b = b_0 - \frac{\alpha_T}{2}\ln\frac{16b}{\pi} + \frac{\alpha_T}{16b} \quad . \tag{12}$$

The above non-perturbative results (12) can be used to assess the validity or otherwise of the Ohmic approximation. This can be observed in Fig. 1, where we plot (12) in a form of b/b_0 vs. α_T . As can be seen from the figure, the Ohmic approximation is satisfactory only in the region of $\alpha_T \sim 5\mathrm{x}10^{-3}$ - $5\mathrm{x}10^{-2}$ ($R_T \sim R_k$ - $10R_k$), where the value of b is very close to the Ohmic value b_0. Also for $\alpha_T \le 5\mathrm{x}10^{-3}$, the fluctuation parameter b deviates from b_0 exponentially, which implies that in the $\alpha_T \to 0$ limit, the use of (7) is not correct.

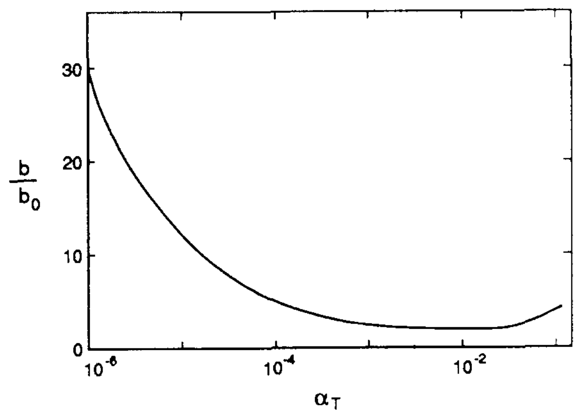

Figure 1 Fluctuation parameter b vs. damping parameter α_T as calculated by (12).

In conclusion, we have presented a non-perturbative microscopically formulated equations (3)-(6) for Coulomb blockade in a single small tunnel junction. Our analytical solution (12) in the T = 0 and weak coupling limit indicates that the Ohmic approximation is satisfactory only in the region of $R_T \sim R_k$ to $10R_k$, and numerical work, based on our self-consistent equations, is needed in the $\alpha_T \to 0$ limit.

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REFERENCES

1. For reviews, see Z.Phys.B**85**,No.3,(1991).
2. A. Odintsov, Sov. Phys. JETP 67,1265(1988).
3. Z. B. Su, L. Y. Chen, and C. S. Ting, Phys.Rev.B<u>38</u> 3866(1988).