Environmental effects on Coulomb blockade in a small tunnel junction: A nonperturbative calculation

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A nonperturbative theory of environmental effects on the Coulomb blockade of single-electron tunneling, using the nonequilibrium Green's-function technique and the path-integral method, is presented. A set of self-consistent equations for the current-voltage (I-V) characteristics and the related correlation functions is derived. It is demonstrated that the two existing theories, viz., the microscopic phase correlation theory and the phenomenological quantum Langevin equation approach, are just two special cases of the present self-consistent theory under some particular approximations. [S0163-1829(97)03032-4]

I. INTRODUCTION

The study of Coulomb blockade, a suppression of single-electron tunneling[1,2] (SET) in small capacitance junctions, is attracting much experimental and theoretical interest. Averin and Likharev[1] proposed the semiclassical orthodox theory, according to which the tunneling current is totally suppressed at zero temperature and voltages $V<V_0=e/2C$, where C is the capacitance. It turns out that the Coulomb blockade is most pronounced if the influence of the environment is weak. More recent studies show that for the Coulomb blockade of single-electron tunneling,[2] there are two sources, the leads connecting the junction to the external circuit and the discrete charge transfer (DCT) across the junction, which reduce the effective Coulomb barrier, i.e., partially smear the Coulomb blockade. In the literature, there exists two independent theories of environmental effects on Coulomb blockade. The microscopic phase correlation theory (PCT), which has been developed by several different groups,[3,4] is based on various approximations (without being fully discussed) and a comparison with experiments is not totally satisfactory.[5] In the quantum Langevin equation (QLE) approach,[6,7] one attacks the problem by phenomenonlogically introducing a charge distribution function, to obtain good agreement with the experimental results in the case of a high impedence environment, i.e., the weak-coupling regime where the tunnel junction is weakly coupled to the environment (tunneling resistance $R_T \gg$ quantum resistance R_k). Therefore, we are motivated to analyze the connection and the difference between the PCT and the QLE methods and to develop a theory which embraces the best features of both approaches.

Previously, we have briefly reported[8] on our progress in developing Odintsov's polaron formulation[9] for single-electron tunneling into a self-consistent calculation, where the non-Ohmic effect of the tunneling resistance was considered, and where the range of validity of the Ohmic approximation has been readily identified. Our approach combines (a) the insightful observation of Odintsov[9] on the connection between the polaron model and the quantum-mechanical model for a tunnel junction and (b) the remarkable nonperturbative analysis of Su, Chen, and Ting[10] for the Thornber-Feynman model of a single-electron drifting in a thermal crystal lattice under an applied electric field. Along the same lines, in this paper we extend our previous analysis to include dissipation by means of a self-consistent calculation, which considers not only the discrete charge transfer across the junction, but also the leads connecting the junction to external circuit. Our treatment is based on recent advances in the following two areas: (a) the polaron problem where use has been made of both path integral and closed time-path Green's function formulations;[10] (b) single-electron tunneling by use of the path-integral method.[11–14]

This paper is organized as follows. In Sec. II, we present our model Hamiltonian for the environmental effects on single-electron tunneling. In Sec. III, we derive the self-consistent equations of motion by using the path integral and the closed time-path Green's-function formulation. In Sec. IV, we present our results where we focus on the weak-coupling regime. Our results are summarized in the concluding section.

II. MICROSCOPIC MODELS

In this section, we first review the general microscopic model known in the literature, then we present an equivalent model Hamiltonian, which we will use to develop a nonperturbative approach. The environmental effects on single-electron tunneling have been formulated in a general way from a microscopic theory.[11–14] Starting from a general form of a tunneling Hamiltonian, Ambegaokar *et al.*[12] (AES) derived the action describing single-electron tunneling by a path-integral formulation. Leggett and Caldeira[13] (LC) obtained the action of a Josephson junction coupled to an arbitrary linear circuit with a known frequency-dependent impedance. Based on these works, it has been shown that for a *normal* tunnel junction with tunnel resistance R_T coupled to a linear circuit with impedance $Z(\omega)$, the action in terms of the phase difference φ can be written as[14]

$$S[\varphi]=\int_0^{\hbar\beta}d\tau\left(\frac{C\hbar^2}{8e^2}\,\dot{\varphi}^2-\frac{I}{2e}\,\varphi\right)-\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\alpha_T(\tau-\tau')\cos\left(\frac{\varphi(\tau)-\varphi(\tau')}{2}\right)+\frac{1}{8}\int_0^{\hbar\beta}d\tau\int_0^{\hbar\beta}d\tau'\,\alpha_s(\tau-\tau')[\varphi(\tau)-\varphi(\tau')]^2, \tag{2.1}$$

where $\beta=1/k_BT$, I is the dc bias current, and

$$\alpha_T(t)=\alpha_T\left(\frac{\pi/\hbar\beta}{\sin(\pi t/\hbar\beta)}\right)^2,$$

$$\alpha_T=\hbar/(2\pi e^2R_T)=R_k/(4\pi R_T), \tag{2.2}$$

where $R_k=2\pi e^2/\hbar=25.8\ k\Omega$. Thus α_T is a measure of the dissipative effects due to the junction. In addition, the analytical continuation of the imaginary time kernel $\alpha_s(\tau)$ to real times from the upper (or lower) half plane yields the complex function $\alpha_s^{>(<)}(t)=\alpha_s^R(t)(\pm)i\alpha_s^I(t)$, with

$$\alpha_s^1(\omega)=(\hbar/2e^2)\omega\ \mathrm{Im}Z^{-1}(\omega);$$

$$\alpha_s^R(\omega)=(\hbar/2e^2)\omega\ \coth\frac{\beta\omega}{2}\ \mathrm{Re}Z^{-1}(\omega), \tag{2.3}$$

where $Z(\omega)$ is the impedance of the environment. Thus α_s is a measure of the dissipative effects due to the environment. The AES-LC action (2.1)–(2.3) are rigorous forms for the study of single-electron tunneling. In general one can start from Eqs. (2.1)–(2.3) to obtain the partition function expressed as a path integral over the phase, $Z=\int D\varphi\ \exp[-S(\varphi)/\hbar]$, and then perform various perturbative calculations. To our knowledge, no nonperturbative calculations along these lines have been carried out in the literature.

On the other hand, Odintsov[9] has demonstrated that the polaron model can be used to calculate SET and studied the charging-transfer effects using the Ohmic approximation (which is essentially a perturbation theory in which only the lowest order in R_k/R_T is kept). The work presented here will go beyond Odintsov's perturbation theory in two main aspects. First, we study the environment effects considering not only the charge-transfer effects but also the dissipative effects arising from the leads connecting the junction with a general impedance $Z(\omega)$. Second, we will use sophisticated techniques developed for solving the polaron problem to evaluate SET self-consistently.

Following the idea of Refs. 9, 11, 12, and 14, the polaronic Hamiltonian for the problem of interest can be written as[9,14]

$$H=\frac{p^2}{2m}+eE(t)x+\sum_{n,k=\pm 1} g_{n,k}(b_{n,-k}^{+}+b_{n,k})e^{ikx}+\sum_{n,k=\pm 1}\hbar\omega_{nk}b_{nk}^{+}b_n+\sum_i\left[\frac{p_i^2}{2m_i}+\frac{1}{2}m_i\omega_i^2(x_i-x)^2\right], \tag{2.4}$$

where the first two terms are for an "electron" in an external field E, the third and fourth terms represent the special phonon bath having two wave vectors $k=\pm 1$ but different frequencies ω_n, and interacting nonlinearly with the electron, and the last term describes the linear coupling to the environment (heat bath) the latter being represented by an infinite number of oscillators.

It can be shown that the study of the problem (2.4) is equivalent to the study of an effective action (2.1) if one takes the following three steps.

(i) Variable mapping

$$\left\{\begin{array}{ll} p\leftrightarrow\dfrac{Q}{e}\equiv\dfrac{CV}{e}, & x\leftrightarrow\dfrac{\varphi}{2} \\ \dfrac{1}{2m}\leftrightarrow E_c\equiv\dfrac{e^2}{2C}, & E\rightarrow\dfrac{I}{e}\end{array}\right\}, \tag{2.5}$$

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) The electron-phonon interaction spectral density $[\Sigma_n\ldots\rightarrow\int d\omega\ \rho(\omega)\ldots]$ obeys certain mapping relations with respect to the tunneling resistance R_T. Specifically, following Odintsov,[9] we choose

$$\rho(\omega)g^2(\omega)=\alpha_T\frac{\omega\omega_c^2}{\omega^2+\omega_c^2}, \tag{2.6}$$

where the electron-phonon coupling matrix $g(\omega)$ is k independent and the cutoff frequency ω_c is assumed to be much higher than all of the characteristic frequencies of the problem ($\omega_c\rightarrow\infty$ after integration over ω).

(iii) The electron-heat bath interaction spectral density satisfies the following rule:[3]

$$\frac{\pi}{2}\sum_i m_i\omega_i^2\delta(\omega-\omega_i)=\frac{\hbar\omega}{e^2Z(\omega)}\equiv\alpha_s^I(\omega), \tag{2.7}$$

so that the heat bath can be described by a linear circuit of general impedance $Z(\omega)$. With the use of path-integral techniques, one can show that there is a one-to-one correspondence between the polaron problem (2.4)–(2.7) and the single-electron-tunneling problem (2.1)–(2.3). In other words, we have extended Odintsov's correspondence to incorporate a frequency-dependent environment. In the following sections we study the environmental effects on single-electron tunneling via the polaronic model (2.4)–(2.7).

III. SELF-CONSISTENT EQUATIONS OF MOTION

Since there exists vast literature[9,10] for the study of the polaron problem, the polaronic Hamiltonian (2.4) can be used conveniently to study the environment effects on SET. Here we adopt the closed time-path Green's function method (CTPGF) for the polaron problem as developed by Su, Chen, and Ting,[10] to treat Eqs. (2.4)–(2.7) in such a way as to obtain a set of self-consistent equations for SET.

In the CTPGF framework, the time-dependent Ginzburg-Landau equation for the transport of a macrovariable is a natural consequence of the microdynamics.[10] Also, the CTPGF was shown to be exactly equivalent to the Feynman-Vernon influence-functional approach.[10,15] The basic idea of the CTPGT approach is to derive a steady-state equation, in which the drift motion is directly coupled to the external field as well as to the fluctuation. The nonequilibrium Green's function is then introduced to describe the fluctuation and to derive a set of self-consistent equations. The CTPGF framework of Ref. 10 is directly applicable to the study of Eqs. (2.4)–(2.7), where the only differences are (a) the restriction of k to the values ± 1; (b) special definition for the variables (2.5), and (c) use of the spectral density (2.6) and (2.7).

Following the work of Ref. 10, after some algebra, we obtain from Eqs. (2.4)–(2.7) a set of self-consistent steady-state equations. Specifically, they are as follows.

(i) The momentum balance equation,

$$E=\gamma_s(0)p+4\sum_n g_n^2\int_0^\infty dt\,\sin\left(\frac{pt}{m}\right)\exp[-f_2(t)]\times\{\sin(\omega_n t)\cos[f_1(t)]+\cosh(\beta\omega_n t/2)\cos(\omega_n t)\sin[f_1(t)]\},\tag{3.1}$$

where E is the external field, p is the momentum, and $\gamma_s(\omega)=1/CZ(\omega)$ is a measure of the dissipative effects due to the environment;

(ii) The damping function equation

$$\gamma(\omega)=\gamma_s(\omega)+\frac{4}{m}\sum_n g_n^2\int_0^\infty dt\,\frac{\sin(\omega t)}{\omega}\cos\left(\frac{pt}{m}\right)\times\exp[-f_2(t)]\{\sin(\omega_n t)\cos[f_1(t)]+\cosh(\beta\omega_n t/2)\cos(\omega_n t)\sin[f_1(t)]\},\tag{3.2}$$

where $\gamma(\omega)$ is a measure of the total dissipative effects due to the environment and the DCT effects (the special ''phonon bath'');

(iii) The nonequilibrium Bose distribution equation

$$\omega N(\omega)\gamma(\omega)=\omega N(\omega)\gamma_s(\omega)+\frac{4}{m}\sum_n g_n^2\int_0^\infty dt\,\cos(\omega t)\cos\left(\frac{pt}{m}\right)\times\exp[-f_2(t)]\{-\sin(\omega_n t)\sin[f_1(t)]+\cosh(\beta\omega_n/2)\cos(\omega_n t)\cos[f_1(t)]\},\tag{3.3}$$

where $N(\omega)$ is the nonequilibrium distribution for the charge fluctuation; and

(iv) The fluctuation function $f(t)=i\{f_1(t)+if_2(t)\}$ equation, where[16]

$$f_1(t)=E_c\int_{-\infty}^{\infty}\frac{d\omega}{\pi\hbar}\,\frac{\gamma(\omega)\sin\omega t}{\omega[\omega^2+\gamma^2(\omega)]},\tag{3.4}$$

$$f_2(t)=E_c\int_{-\infty}^{\infty}\frac{d\omega}{2\pi\hbar}\,\frac{\sin^2(\omega t/2)}{(\omega/2)^2}\,\frac{\omega N(\omega)\gamma(\omega)}{\omega^2+\gamma^2(\omega)}.\tag{3.5}$$

We note that in deriving Eqs. (3.1)–(3.5), the only assumption made is the use of the approximation to truncate the equations obeyed by the Green's functions, where one keeps only the first and the second cumulants with all the higher-order cumulants being assumed negligible.[13] Also, as discussed in Ref. 10, $N(\omega)$ plays the role of a nonequilibrium distribution and Eq. (3.3) can be viewed as reflecting a generalized fluctuation-dissipation theorem; only in the linear-response regime ($p=0$), does (3.3) reduce to the equilibrium Bose distribution $N_0(\omega)=\coth(\beta\omega/2)$.

The self-consistent equations (3.1)–(3.5) give a complete and self-consistent description for the motion of an electron in an external field E and interacting both with a linear heat bath and with ''phonon modes'' having two identical wave vectors $k=\pm 1$ but different frequencies ω_n. In the absence of dissipation in the environment, i.e., when $\gamma_s(\omega)=0$, Eqs. (3.1)–(3.5) parallel Eqs. (5.5), (5.6), (5.11)–(5.13) of Ref. 13, except that here we have taken the summation over $k=\pm 1$ and the $g_n, f_1(t), f_2(t)$ are now all k independent.

Next, we demonstrate that Eqs. (3.1)–(3.3) for SET, based on the CTPGF formalism, can be further simplified. The key point is that as we have taken the summation over k, we can now carry out the sum over n in Eqs. (3.1)–(3.3). We note that a similar procedure is not possible for the actual polaron problem studied in Ref. 10, where one has a sum over an infinite number of k values. Explicitly, by using Eq. (2.6) and the fact that the cutoff frequency ω_c is assumed to be much higher than all of the characteristic frequencies of the problem ($\omega_c\to\infty$ after integration of ω), the summation over n contained in Eqs. (3.1)–(3.3) can be carried out directly, after which we obtain [after first using the mapping given by Eq. (2.5)], respectively,

$$I=V\left(\frac{1}{R_T}+\frac{1}{Z(0)}\right)-4e\alpha_T\int_0^\infty dt\,\sin(eVt/\hbar)\times\left(\frac{\pi/\beta\hbar}{\sinh(\pi t/\beta\hbar)}\right)^2\sin[f_1(t)]\exp[-f_2(t)],\tag{3.6}$$

$$\gamma(\omega)=\gamma_s(\omega)+\gamma_T\left\{1-\frac{2}{\pi}\int_0^\infty dt\,\frac{\sin(\omega t)}{\omega}\cos(eVt/\hbar)\times\left(\frac{\pi/\beta\hbar}{\sinh(\pi t/\beta\hbar)}\right)^2\sin[f_1(t)]\exp[-f_2(t)]\right\},\tag{3.7}$$

$$\omega N(\omega)\gamma(\omega)=\omega N(\omega)\gamma_s(\omega)+\gamma_T\left\{\frac{\hbar\omega+eV}{2\hbar}\coth\left(\frac{\beta(\hbar\omega+eV)}{2}\right)+\frac{\hbar\omega-eV}{2\hbar}\coth\left(\frac{\beta(\hbar\omega-eV)}{2}\right)+E_c-\frac{2}{\pi}\int_0^\infty dt\,\cos\left(\frac{eVt}{\hbar}\right)\cos(\omega t)\times\left(\frac{\pi/\beta\hbar}{\sinh(\pi t/\beta\hbar)}\right)^2\times\{1-\exp[-f_2(t)]\cos[f_1(t)]\}\right\},\tag{3.8}$$

where $\gamma_T=1/CR_T$, and $\alpha_T=R_k/(4\pi R_T)$ is a measure of the dissipative effects due to the DCT effects. Equations (3.4)–(3.8) are the key results of this paper. Before performing a detailed study of these equations in the next section, here we present a few general results which can be derived directly from Eqs. (3.4)–(3.8).

First, the structure of Eqs. (3.6) and (3.7) shows that the conductance has a simple form

$$G=\left.\frac{\partial I}{\partial V}\right|_{V=0}=C\gamma(0),\tag{3.9}$$

where $\gamma(\omega)$ is given by Eq. (3.7). The above equation states that for the dc transport, the conductance G is generally a well behavior quantity irrespective of the detailed forms of the fluctuation function $f(t)$. We will comment more about this latter in our discussion.

Second, the charge fluctuation, which is defined as

$$\langle \delta Q(t)\delta Q(t')\rangle = S(t-t') \tag{3.10}$$

can be directly connected to the correlation Green's function. The static charge fluctuation can be obtained in a similar way to that of Ref. 10 as

$$\langle q^2\rangle \equiv S(0) = \frac{\hbar C}{2\pi}\int_{-\infty}^{\infty} d\omega \, \frac{\omega N(\omega)\gamma(\omega)}{\omega^2+\gamma^2(\omega)}. \tag{3.11}$$

Equations (3.9)–(3.11) will prove to be very useful when we discuss the QLE theory in the next section.

IV. RESULTS

In principle, the integral equations (3.4)–(3.8) are numerically solvable, which will result in exact functional forms for $f(t)$, $\gamma(\omega)$, and $N(\omega)$ as well as the I-V characteristics. Here we restrict our discussion to some of the interesting results which are analytically derivable from Eqs. (3.4)–(3.8).

1. Odintsov's Ohmic approximation at $T=0$ and beyond. In the first-order (Ohmic) approximation, the $\gamma(\omega)$ contained in Eqs. (3.4), (3.5) and Eq. (3.8) is frequency independent and is replaced by $\gamma(\omega)=\gamma_0\equiv\gamma_s+\gamma_T=C^{-1}(R_T^{-1}+R_S^{-1})$, and Eqs. (3.4)–(3.8) become uncoupled equations. In this case, in the weak-coupling limit ($\gamma_0\rightarrow 0$), which is equivalent to assuming R_S, $R_T \gg R_k$, Eqs. (3.4) and (3.5) can be evaluated analytically as

$$f_1(t)=E_c t/\hbar, \quad f_2(t)=b_0(2E_c/\hbar)^2 t^2, \tag{4.1}$$

where the fluctuation parameter $b_0=-0.5\alpha_0 \ln(6.23\alpha_0)$, with $\alpha_0=\hbar\gamma_0/(4\pi E_c)$.

In Ref. 9, Odintsov used Eq. (4.1) to study the steady-state equations (3.6) and (3.7), where many interesting analytical results for the charge-transfer effects on single-electron tunneling have been reached. For example, the linear conductance (3.9) is obtained by first substituting Eq.(4.1) into Eq. (3.7) and then taking the $\omega\rightarrow 0$ limit to get the $\gamma(0)$. It is easy to show that at $T=0$, the result is

$$G_0=\frac{1}{R_T}\,\mathrm{erfc}\,\frac{1}{4\sqrt{b_0}}. \tag{4.2}$$

Equation (4.2) implies that in the weak-coupling limit ($\alpha_T\rightarrow 0$) G_0 tends to zero as a function of $\alpha_T^{3/2}e^{-1/\alpha_T}$. On the other hand, in the above calculation, the use of Eq. (4.1) in Eqs. (3.6) and (3.7) is of a higher order in γ_0, and is obviously not consistent with the assumption of the Ohmic approximation. In the following, we present a more rigorous calculation.

In the $T=0$ and $\gamma_0\rightarrow 0$ limit, Eqs. (3.4)–(3.8) can be solved analytically in the following way. First, based on the knowledge of Eq. (4.1), we postulate

$$f_1(t)=at, \quad f_2(t)=b(2E_c/\hbar)^2 t^2, \tag{4.3}$$

where a and b are to be determined. Next, using Eq. (4.3), after some algebra we obtain from Eqs. (3.7) and (3.8), respectively,

$$\gamma(\omega)=\gamma_s(0)+\gamma_T\left\{1-\mathrm{erf}\,\frac{a}{2\sqrt{b}}\right\}+0(\omega^2), \tag{4.4}$$

$$\omega N(\omega)\gamma_T(\omega)=\gamma_T\left\{\omega+a\left[\mathrm{erfc}\,\frac{a}{2\sqrt{b}}-\frac{2}{a}\sqrt{\frac{b}{\pi}}\,e^{-a^2/4b}\right]\right\} + O(\omega). \tag{4.5}$$

It is clear from the structure of the integrands in Eqs. (3.4) and (3.5) that higher powers of ω give negligible contributions. Substituting Eqs. (4.4) and (4.5) into Eqs. (3.4) and (3.5), and expressing the subsequent result in the form of Eq. (4.3), we obtain

$$a=E_C/\hbar, \quad b=b_0-\frac{\alpha_T}{2}\ln\frac{16b}{\pi}+\frac{\alpha_T}{16b}, \tag{4.6}$$

where the fluctuation parameter $b_0=-0.5\alpha_0\ln(6.23\alpha_0)$, with $\alpha_0=\hbar\gamma_0/(4\pi E_c)$ and $\gamma_0\equiv\gamma_s+\gamma_T=C^{-1}(R_T^{-1}+R_S^{-1})$. We note that the structure of Eqs. (3.4) and (3.5) shows that in essence Eq. (4.3) is a short-time form of Eqs. (3.4) and (3.5). Also, we note that in the Ohmic approximation, the $\gamma(\omega)$ contained in Eqs. (3.4), (3.5), and (3.8) are replaced by $\gamma(\omega)=\gamma_0$, and Eqs. (3.4)–(3.8) become uncoupled equations. This is the case studied by Odintsov,[10] where Eqs. (3.4) and (3.5) take the form of Eq. (4.3) with $b=b_0$. Our self-consistent results (4.3) and (4.4) combined with Eqs. (3.7) and (3.10) can be easily used to show that the Ohmic approximation underestimates the smearing of the Coulomb blockade due to the DCT effects particularly in the $\alpha_T\rightarrow 0$ limit. This is illustrated in Fig. 1, where we plot Eq. (4.4). As can be seen from the figure, the Ohmic approximation is satisfactory only in the range of $\alpha_T\sim 0.005-0.05$ ($R_T/R_k\sim 1-10$, $R_k=25.8$ kΩ), where the value of b is very close to the Ohmic value b_0. However, for $\alpha_T<0.005$, b deviates from b_0 exponentially and the Ohmic approximation of Ref. 10 is no longer valid.

With the self-consistently determined $f_1(t)$ and $f_2(t)$ of Eq. (4.3), one can easily evaluate the linear conductance G of Eq. (3.9) by using Eq. (3.7), and the result is

$$G_{\rm sc}=\frac{1}{R_T}\,\mathrm{erfc}\,\frac{1}{4\sqrt{b}}. \tag{4.7}$$

Since $b>b_0$, from Eqs. (4.2) and (4.7) in general one has $G_{\rm sc}>G_0$. Again, this implies that the Ohmic approximation underestimates the smearing of the Coulomb blockade due to the charge fluctuations, particularly in the $\alpha_T\rightarrow 0$ limit. In fact, Eq. (4.6) implies that in the weak-coupling limit ($\alpha_T\rightarrow 0$) $G_{\rm sc}$ tends to zero as a function of $\alpha_T^{5/4}e^{-1/\sqrt{\alpha_T}}$.

2. I-V characteristics: PCT and QLE. The I-V characteristics can be studied conveniently in our formalism by rewriting Eq. (3.6) as

$$I=V\left(\frac{1}{R_T}+\frac{1}{Z(0)}\right)-4e\alpha_T\int_0^\infty dt\ \sin(eVt/\hbar)\left(\frac{\pi/\beta\hbar}{\sinh(\pi t/\beta\hbar)}\right)^2\ \sin[f_1(t)]\exp[-f_2(t)]$$
$$=V\left(\frac{1}{R_T}+\frac{1}{Z(0)}\right)+\frac{1}{eR_T}\int_0^\infty dE\ E\ \coth(\beta E/2)\ \frac{1}{\pi\hbar}\int_0^\infty dt\ e^{-f_2(t)}\ \sin[f_1(t)]\left[\sin\frac{(eV+E)t}{\hbar}-\sin\frac{(E-eV)t}{\hbar}\right]$$
$$=\frac{V}{Z(0)}+\frac{1}{eR_T}\int_{-\infty}^\infty dE\ P(E)\left\{\frac{eV-E}{1-e^{-\beta(eV-E)}}+\frac{eV+E}{1-e^{\beta(eV+E)}}\right\}, \tag{4.8}$$

where $f(t)=i\{f_1(t)+if_2(t)\}$ is defined by Eqs. (3.4) and (3.5), and

$$P(E)=\frac{1}{2\pi\hbar}\int_{-\infty}^\infty dt\ e^{-f(t)+iEt/\hbar}. \tag{4.9}$$

Using our analytical results (4.3)–(4.6) or numerically solving the $f(t)$ through Eqs. (3.4)–(3.8) in a general way, Eq. (4.8) gives a self-consistent description of the I-V characteristics. Another advantage of the present approach is that the existing theories of environmental effects on single-electron tunneling, viz., the phase correlation theory and the quantum Langevin theory, can both be rederived from the general expressions (4.8) and (4.9) under certain approximations, which we discuss in the following.

A. Linear heat bath approximation: The phase correlation theory

In the low impedence regime, the tunnel junction is strongly coupled to the leads, and the linear heat bath (which models the leads) dominates the charge-transfer effects, i.e., $\gamma_T(\omega)\ll\gamma_S(\omega)$. In this case, it is a good approximation to write Eq. (3.7) as

$$\gamma(\omega)\approx\gamma_S(\omega)=1/CZ(\omega). \tag{4.10}$$

Here we discuss an interesting situation where, in addition to Eq. (4.10), one adopts the equilibrium approximation,

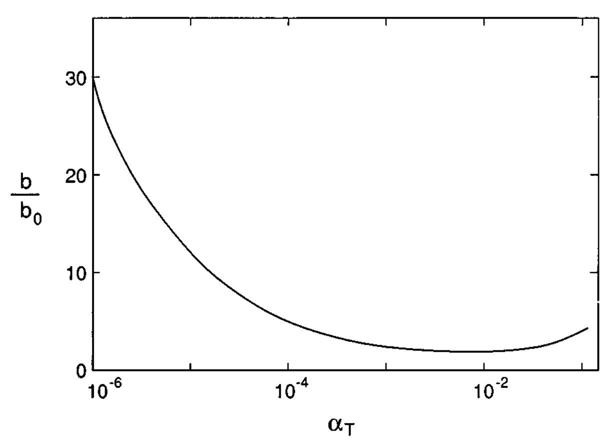

FIG. 1. Fluctuation parameter b (in units of the corresponding value b_0 for the Ohmic model), as calculated by the self-consistent result (4.4), as a function of the damping parameter α_T, at $T=0$ and in the weak-coupling region.

$$N(\omega)\approx N_0(\omega)\equiv\coth\frac{\beta\hbar\omega}{2}. \tag{4.11}$$

Using Eqs. (4.10) and (4.11), the fluctuation functions (3.4) and (3.5) become

$$f_1(t)=E_c\int\frac{d\omega}{\pi\hbar}\frac{\gamma_s(\omega)\sin\omega t}{\omega[\omega^2+\gamma_s^2(\omega)]}, \tag{4.12}$$

$$f_2(t)=E_c\int\frac{d\omega}{2\pi\hbar}\frac{\sin^2(\omega t/2)}{(\omega/2)^2}\frac{\omega N_0(\omega)\gamma_s(\omega)}{\omega^2+\gamma_s^2(\omega)}. \tag{4.13}$$

It is interesting to note that, from Eqs. (4.12) and (4.13), $f(t)$ is independent of R_T, and it follows that the $\gamma(\omega)$ of Eq. (3.7) consists of a term independent of R_T and a term linear in $1/R_T$. It is clear from Eq. (3.9) that the conductance G exhibits the same behavior. Also we note that Eq. (4.8) supplemented by Eqs. (4.9)–(4.13) and use of the detailed balance relation $P(-E)=e^{-\beta E}P(E)$, is now exactly the same as the result of the phase correlation theory.[2–5] Our derivation of Eq. (4.8) from the self-consistent equations (3.4)–(3.8), clearly demonstrates that the main approximations used in obtaining the standard phase correlation theory are (i) neglect of the charge-transfer effects, i.e., the tunneling resistance is taken to be very large compared to the quantum resistance and (ii) use of the equilibrium approximation (4.11). It follows that the existing PCT theory is justified only in the low impedence regime, where the leads are the dominating environmental effects. On the other hand, our self-consistent theory in the form of Eqs. (4.8) and (4.9) supplemented by Eqs. (3.4), (3.5), (3.7), and (3.8) provides a generalized PCT theory.

B. Short-time approximation: quantum Langevin theory

Equation (4.3) indicates that the short-time behavior of the fluctuation function makes the dominating contribution. This motivates us to study the problem by means of the short-time approximation. In fact, in this case, there are two things which become apparent. First, it is straightforward, by using Eqs. (3.11) and (4.3), to obtain

$$b=\frac{e^2}{2C^2\hbar^2}\langle q^2\rangle, \tag{4.14}$$

where $\langle q^2\rangle$ is given by Eq. (3.11). Second, the probability density (4.9) can be derived explicitly as

$$P(E)=\frac{1}{2\hbar\sqrt{\pi b}}\exp\left\{-\frac{(E_c-E)^2}{4\hbar^2 b}\right\}$$
$$=\frac{C}{e\sqrt{2\pi\langle q^2\rangle}}\exp\left\{-\frac{C^2(E_c-E)^2}{2e^2\langle q^2\rangle}\right\}, \qquad (4.15)$$

where in the last step we have used Eq. (4.14). Next, we make a variable change $E\to qe/C$, and rewrite Eq. (4.15) as the charge probability density

$$\frac{e}{C}P(E+E_c)\to P(q)=\frac{1}{\sqrt{2\pi\langle q^2\rangle}}\exp\left\{-\frac{q^2}{2\langle q^2\rangle}\right\}. \qquad (4.16)$$

Substituting Eq. (4.16) into Eq. (4.8), we obtain

$$1=\frac{V}{Z(0)}+\frac{1}{eR_T}\int_{-\infty}^{\infty}dE\; P(E+E_c)$$
$$\times\left\{\frac{eV+E+E_c}{1-e^{\beta(eV+E+E_c)}}+\frac{eV-E-E_c}{1-e^{-\beta(eV-E-E_c)}}\right\}$$
$$=\frac{V}{Z(0)}+e\int_{-\infty}^{\infty}dq\; P(q)\{\Gamma^+(CV+q)-\Gamma^-(CV-q)\}, \qquad (4.17)$$

where

$$\Gamma^{\pm}(x)=\frac{(e/2)\pm x}{eCR_T}\,\frac{1}{1-e^{\beta(e/C)[(e/2)\pm x]}}. \qquad (4.18)$$

It is interesting to note that Eqs. (4.16)–(4.18) are the same as that of the quantum Langevin model,[6,7] if one uses the equilibrium approximation (4.11) to evaluate the $\langle q^2\rangle$ of Eq. (3.11). Thus, we have derived the quantum Langevin theory from the present self-consistent formulation.

In conclusion, we have presented a nonperturbative microscopically formulated treatment for the environmental effects on the Coulomb blockade of single-electron tunneling. Using the nonequilibrium Green's-function technique and the path-integral method, we have obtained self-consistent equations (3.4)–(3.8) for the Coulomb blockade in a single small tunnel junction. It is demonstrated that the PCT theory (4.8)–(4.13) and the QLE formalism (4.16)–(4.18) are just two special cases obtained from the present self-consistent theory under certain particular approximations.

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