Mesoscopic Charge Relaxation

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We consider charge relaxation in the mesoscopic equivalent of an *RC* circuit. For a single-channel, spin-polarized contact, self-consistent scattering theory predicts a universal charge relaxation resistance equal to half a resistance quantum independent of the transmission properties of the contact. This prediction is in good agreement with recent experimental results. We use a tunneling Hamiltonian formalism and show in Hartree-Fock approximation that at zero temperature the charge relaxation resistance is universal even in the presence of Coulomb blockade effects. We explore departures from universality as a function of temperature and magnetic field.

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There is increasing interest in the dynamics of mesoscopic structures motivated by the desire to manipulate and measure quantum phenomena as rapidly as possible. It is thus of great importance to characterize the time scales governing the electron dynamics in simple mesoscopic structures. An elementary but fundamental building block is the quantum coherent capacitor [1]. As in the classical case, the low frequency dynamics of a mesoscopic capacitor is determined by a charge relaxation time τ_{RC}. For a quantum coherent capacitor, the *RC* time can still be written as the product of a resistance and a capacitance, i.e., $\tau_{RC} = R_q C_\mu$. However, due to the coherent nature of electron transport through mesoscopic structures, both the electrochemical capacitance C_μ, which determines the charge on the capacitor, and the charge relaxation resistance R_q, which governs the charge fluctuations, now crucially depend on coherence properties of the system. The capacitance C_μ is related to the imaginary part of the ac conductance, but it can also be obtained by the differentiation of a thermodynamic (grand-canonical) potential [2–6]. The charge relaxation resistance R_q is related to the real part of the ac conductance and, therefore, requires a dynamic theory. In analogy to the classical *RC* circuit depicted in the upper left corner in Fig. 1, one has for the mesoscopic system

$$G(\omega) = -i\omega C_\mu + \omega^2 C_\mu^2 R_q + O(\omega^3). \qquad (1)$$

This equation will be taken as a definition of C_μ and R_q. If the cavity-reservoir connection permits the transmission of only a single spin-polarized channel, a self-consistent scattering matrix approach gives at zero temperature a resistance equal to half a resistance quantum [1]

$$R_q = \frac{h}{2e^2}. \qquad (2)$$

We emphasize that the factor of 2 is not connected to spin but is rather due to the fact that the cavity connects to only one electron reservoir. More astonishing, even counterintuitive, is the fact that Eq. (2) is independent of the transmission properties of the channel. For Eq. (2) to hold, it is essential that the entire reflection process at the cavity is quantum coherent. Indeed, treatments which take the metallic limit [2,3] (energy level spacing tends to zero) or treat transmission onto and off the cavity in the sequential approximation [7] do not lead to a universal R_q.

In a seminal experiment, Gabelli *et al.* [8] have recently measured both the in and out of phase parts of the ac conductance of a mesoscopic *RC* circuit. In their experiment, one "plate" of the capacitor consists of a submicrometer quantum dot (QD) and the other is formed by a macroscopic top gate. The role of the resistor is played by a tunable quantum point contact (QPC) connecting the QD to an electron reservoir. The results of this experiment are in good agreement with the theoretical predictions of Ref. [1]. In particular, in the presence of a strong magnetic field to spin polarize the electrons, they confirm the universality of the single-channel charge relaxation resistance. However, it is *a priori* unclear whether the results derived in Ref. [1] still hold in the presence of single charge effects [2–4], which must become important if the transmission through the QPC becomes small. Indeed, the experiment observes Coulomb blockade oscillations of the capacitance as a function of the gate voltage. It is the aim of the present work to present a theoretical description for the charge

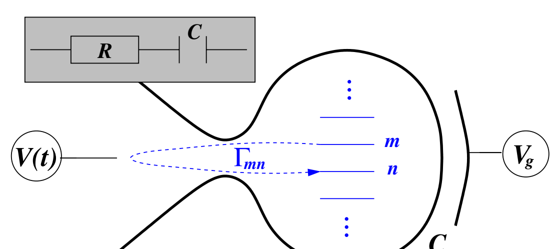

FIG. 1 (color online). Schematics of the mesoscopic capacitor. A cavity is connected via one lead to an electron reservoir at voltage $V(t)$ and capacitively coupled to a backgate with voltage V_g. The coupling matrix elements Γ_{mn} are defined in the text. The inset shows the corresponding classical *RC* circuit.

relaxation resistance in the presence of Coulomb blockade effects.

The mesoscopic RC circuit along with the principal model parameters is shown in Fig. 1. $V(t) = V_{\rm ac}\cos(\omega t)$ is the time-dependent voltage applied to the electron reservoir, while V_g is the voltage applied to the gate and C is the geometrical capacitance between the QD and the gate. The matrix elements Γ_{mn}, to be defined below, describe the indirect coupling between the dot states m and n via the reservoir.

Our first goal is to show that in the single-channel case R_q is universal also in the Coulomb blockade regime. For that purpose, we treat the cavity at the Hartree-Fock (HF) level [9,10]. The starting point of our calculation is the relation

$$I(t) = -e\frac{\partial}{\partial t}\Im\{\mathrm{Tr}[G^<(t,t)]\}, \quad (3)$$

which expresses the tunneling current through the QPC as a function of the lesser (matrix) Green function (GF) $G^<(t,t')$ of the dot. We are primarily interested in the regime where the modulation and thermal energies are small compared to the level spacing in the dot. Treating the dot as zero-dimensional, the Hamiltonian of this system is [11]

$$H = H_L + H_D + \sum_{k\sigma,n}(t^\sigma_{k,n}c^\dagger_{k\sigma}d_{n\sigma} + \mathrm{H.c.}), \quad (4)$$

where $H_L = \sum_{k\sigma}E_{k\sigma}(t)c^\dagger_{k\sigma}c_{k\sigma}$, with $E_{k\sigma}(t) = E^0_{k\sigma} + eV(t)$, describes the (noninteracting) electrons in the isolated lead and $t^\sigma_{k,n}$ is the tunneling matrix element between a reservoir momentum state k and the nth single particle dot state, both with spin σ. A change in the gate voltage is modeled as a shift of the Fermi energy E_F in the reservoir, and we set $V_g = 0$. The Hamiltonian of the dot reads $H_D = \sum_{n\sigma}\epsilon_{n\sigma}d^\dagger_{n\sigma}d_{n\sigma} + E_c(\hat{N}_{\rm dot} + \mathcal{N}(t))^2$. Here $E_c = e^2/2C$ is the electrostatic charging energy, $\hat{N}_{\rm dot} = \sum_{m\sigma}d^\dagger_{m\sigma}d_{m\sigma}$ is the particle number in the dot, and $e\mathcal{N}(t) = CU(t)$ gives the polarization charges between the dot and gate produced by the time-dependent voltage at the reservoir [12]. This polarization charge, in turn, leads to a time-dependent (Hartree) potential $U(t)$ inside the dot, and we may write $H_D = \sum_{n\sigma}\tilde{\epsilon}_{n\sigma}(t)d^\dagger_{n\sigma}d_{n\sigma} + E_c\hat{N}^2_{\rm dot}$, with $\tilde{\epsilon}_{m\sigma}(t) = \epsilon_{m\sigma} + eU(t)$. In HF approximation, the retarded (advanced) GF of the dot takes the form [13,14]

$$G^{R(A)}(t,t') = e^{i\phi_U(t,t')}G^{R(A)}_{\rm eq}(t-t'), \quad (5)$$

where $G^{R(A)}_{\rm eq}(t-t') = G^{R(A)}(t,t')_{V_{\rm ac}=0}$ is the equilibrium retarded (advanced) HF Green function and $\phi_U(t,t') = \int_t^{t'} d\tau U(\tau)$. The equal time lesser GF is obtained via the Keldysh equation [13,15]

$$G^<(t,t) = \int dt_1 \int dt_2 G^R(t,t_1)\Gamma^<(t_1,t_2)G^A(t_2,t). \quad (6)$$

Here $\Gamma^<(t,t') = i\Gamma e^{i\phi_V(t,t')}\hat{f}(t-t')$, with $\phi_V(t,t') = \int_t^{t'} d\tau V(\tau)$ is the lesser coupling self-energy and $\hat{f}(t-t') = (1/2\pi)\int dE e^{-iE(t-t')}f(E)$ is the Fourier transform of the Fermi function. $\Gamma^\sigma_{mn} = 2\pi\rho_L t^{\sigma*}_m t^\sigma_n$ are the coupling matrix elements in the wide band limit [13]. Here and in the following, we use the matrix notation $A_{m\sigma,n\sigma'} \equiv A^\sigma_{mn}\delta_{\sigma\sigma'}$, which takes advantage of the fact that spin is conserved in Eq. (4). An important property of the coupling matrix elements is that $\Gamma^\sigma_{mn}\Gamma^\sigma_{kl} = \Gamma^\sigma_{ml}\Gamma^\sigma_{kn}$, from which it immediately follows that for arbitrary matrices A and B

$$\mathrm{Tr}[\Gamma^\sigma A\Gamma^\sigma B] = \mathrm{Tr}[\Gamma^\sigma A]\mathrm{Tr}[\Gamma^\sigma B], \quad (7)$$

where the trace is over a basis of dot states with spin σ. Since we are interested in the linear conductance, we expand (6) to linear order in V and U and find after double Fourier transformation

$$G^<(E,E') = G^R_{\rm eq}(E)\Gamma^<_1(E,E')G^A_{\rm eq}(E') + O(U^2,V^2), \quad (8)$$

where $\Gamma^<_1(E,E')$ is the double Fourier transform of $\Gamma^<_1(t,t') = i\Gamma(1 + i\phi(t,t'))\hat{f}(t-t')$, with $\phi(t,t') \equiv \phi_V(t,t') - \phi_U(t,t')$. With (3) and (8), the linear response tunneling current at frequency ω becomes $I(\omega) = g(\omega)\times[V(\omega) - U(\omega)]$, with

$$g(\omega) = -i\frac{e\omega}{2\pi}\int dEF(E,\omega)\mathrm{Tr}[G^R_{\rm eq}(E)\Gamma G^A_{\rm eq}(E-\omega)], \quad (9)$$

where $F(E,\omega) = [f(E+\omega) - f(E)]/\omega$ and we have set $\hbar = 1$. To obtain the ac conductance $G(\omega) = I(\omega)/V(\omega)$, we need the internal potential $U(\omega)$. For this, we note that, in the present single lead system, the displacement current $-i\omega e\mathcal{N}(\omega)$ is equal to the tunneling current so that $g(\omega)[V(\omega) - U(\omega)] = -i\omega CU(\omega)$ and, consequently [16], $U(\omega) = g(\omega)V(\omega)/[-i\omega C + g(\omega)]$. Expanding the conductance to second order in frequency, we then obtain after restoring the units

$$R_q = -\frac{h}{2e^2}\frac{\int dEf'(E)\mathrm{Tr}[D(E)^2]}{(\int dEf'(E)\mathrm{Tr}[D(E)])^2}, \quad (10)$$

where $f' = df/dE$ and $D(E) \equiv G^R_{\rm eq}(E)\Gamma G^A_{\rm eq}(E)$. Using (7), we have $\mathrm{Tr}[D^\sigma(E)^2] = \mathrm{Tr}[D^\sigma(E)]^2$ and, hence, at zero temperature

$$R_q = \frac{h}{2e^2}\frac{\sum_\sigma \nu_\sigma(E_F)^2}{(\sum_\sigma \nu_\sigma(E_F))^2}, \quad (11)$$

where $\nu_\sigma(E) \equiv \mathrm{Tr}[D^\sigma(E)]/2\pi$ is the density of spin σ states in the dot. Equations (9) and (11) are the central results of this work. In particular, Eq. (11) demonstrates that for a single (spin-polarized) channel R_q is still given by Eq. (2).

In the following, we use Eq. (11) to investigate the magnetic field dependence of R_q. We consider here a dot with two spin degenerate levels with bare energies $\epsilon_{1\sigma}$ and $\epsilon_{2\sigma} = \epsilon_{1\sigma} + \Delta$, respectively. In the numerical calculations, we set $\Delta = 1$ and $2E_c = 2.5$. We are interested in the regime of low magnetic field, where the Zeeman splitting $\Delta_B = \mu_B gB \le \Delta$. For simplicity, we further assume that $\Gamma^\uparrow_{mn} = \Gamma^\downarrow_{mn} \equiv \gamma$, for $m,n \in \{1,2\}$. The equilibrium

HF retarded GF of the dot may be written as $G^R_{\rm eq}(E) = [G^R_0(E)^{-1} - \Sigma^R_{\rm HF} + i\Gamma/2]^{-1}$, with the noninteracting equilibrium GF of the isolated dot $(G^R_0(E))_{mn} = \delta_{mn}(E - \epsilon_m + i0^+)^{-1}$ and the HF self-energy

$$(\Sigma^R_{\rm HF})^\sigma_{mn} = 2E_c\Big[\delta_{mn}\sum_{l\sigma'}\langle n_{l\sigma'}\rangle - \langle d^\dagger_{m\sigma}d_{n\sigma}\rangle\Big]. \qquad (12)$$

The most important feature of this self-energy is that it correctly excludes the unphysical self-interaction terms ($m = n = l$ and $\sigma = \sigma'$) of the Hartree approximation and, consequently, leads to the appearance of the Coulomb gap across E_F, which is the essential spectral signature of the Coulomb blockade effect. The "mean fields" $\langle d^\dagger_{m\sigma}d_{n\sigma}\rangle$ are determined self-consistently [17] by solving the set of equations

$$\langle d^\dagger_{m\sigma}d_{n\sigma}\rangle = \frac{1}{2\pi}\int_{-\infty}^{\infty} dEf(E)[G^R_{\rm eq}(E)\Gamma G^A_{\rm eq}(E)]^\sigma_{mn}. \qquad (13)$$

Because of the interaction, $\nu_\sigma(E)$ depends on the level occupancies, and we must distinguish two cases. Solving Eq. (13) numerically in the strongly blockaded regime $\pi\gamma \ll \Delta + 2E_c$, we find that R_q is nonuniversal even as $B \to 0$ (upper left panel in Fig. 2). This is due to the fact that the dot charge is strongly quantized in this regime, as shown in the lower left panel in Fig. 2, which leads to a gap of order $2E_c + \Delta\delta_{\sigma\sigma'} + (1 - \delta_{\sigma\sigma'})\Delta_B$ between the highest occupied state with spin σ and the lowest unoccupied state with spin σ'. There are thus four well separated (separation $\sim e^2/C$), narrow (width $\sim\gamma$) resonances in the total density of states $\sum_\sigma \nu_\sigma$ as a function of E_F. We can understand the particular behavior of R_q shown in the upper left panel in Fig. 2 at specific values of the Fermi energy. If E_F is on a resonance with spin σ, then $\nu_{\sigma'}(E_F) \cong \nu_\sigma(E_F)\delta_{\sigma\sigma'}$. Therefore, on resonance, i.e., for $E_F \in \{\epsilon_{1\sigma}, \epsilon_{2\sigma}, \epsilon_{1\bar\sigma} + 2E_c + \Delta_B, \epsilon_{2\bar\sigma} + 2E_c + \Delta_B\}$, we expect to have $R_q \cong h/2e^2$ according to (11). Furthermore, in the middle between two consecutive resonances $\nu_\sigma(E_F) = \nu_{\bar\sigma}(E_F)$, and so R_q takes on its minimal two-channel value $h/4e^2$. In the opposite limit of strong coupling $1 \lesssim \pi\gamma/2E_c$, the Coulomb blockade is smeared out, and the charge on the dot is not strongly quantized anymore (see lower right panel in Fig. 2). Thus, at very low magnetic fields, the two spin states are nearly simultaneously charged and the degeneracy is not appreciably lifted. Therefore, $R_q \cong h/4e^2$ at low magnetic fields as shown in the upper right panel in Fig. 2. As Δ_B increases, the broad resonances in the density of states corresponding to the two spin degenerate levels split into consecutively overlapping resonances, and R_q starts to increases except in the middle between two neighboring resonances. Finally, a crossing of the two innermost resonances is observed for $\Delta_B \cong 0.75$. Such a crossing occurs when the Zeeman splitting approaches the effective level spacing $\Delta + 2E_c(\langle n_{1\sigma}\rangle - \langle n_{2\bar\sigma}\rangle)$, which interestingly is seen to be smaller than the bare level spacing here. This effect is

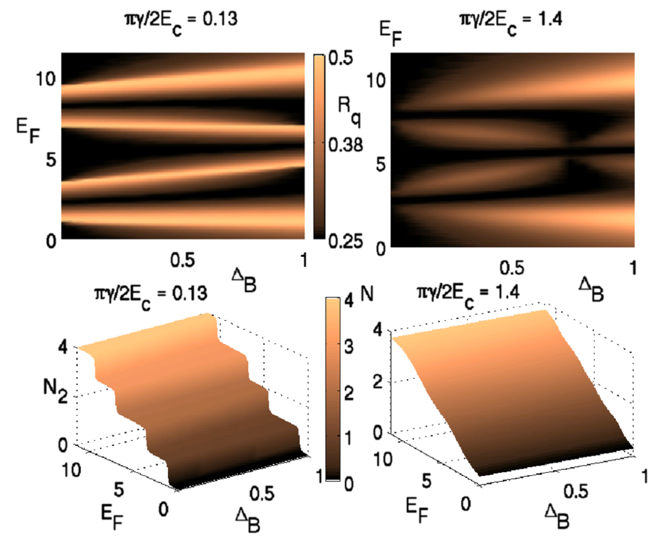

FIG. 2 (color online). Magnetic field dependence of the charge relaxation resistance R_q. The upper panels show R_q as a function of the Zeeman splitting Δ_B and the Fermi energy E_F for weak $\pi\gamma/2E_c = 0.13$ and strong $\pi\gamma/2E_c = 1.4$ coupling. All energies are given in units of the bare level spacing Δ. The lower panels show the corresponding total dot charge.

peculiar to the strongly coupled regime and is due to enhanced exchange interactions, which favor the consequent population of states with equal spins [18,19]. At the crossing point, the densities of both spin states are equal and R_q takes on its minimal value.

As a second application, we investigate the temperature dependence of R_q in the high magnetic field limit, where the incoming electrons are effectively spin-polarized and there is only a single transmitting channel through the QPC. We consider here a quantum dot with two (bare) levels ϵ_1 and $\epsilon_2 = \epsilon_1 + \Delta$ and suppress the now superfluous spin index. In the low temperature regime $k_BT \ll \gamma$, we may expand $\nu(E)$ and $\nu(E)^2$ around E_F, assuming that these functions vary slowly in the range $E_F \pm k_BT/2$. This yields to first nonvanishing order in $k_BT \equiv \beta^{-1}$

$$R_q \cong \frac{h}{2e^2}\bigg(1 + \frac{\pi^2}{3\beta^2}\bigg[\frac{\nu'(E_F)}{\nu(E_F)}\bigg]^2\bigg), \qquad (14)$$

where $\nu'(E) \equiv \frac{\partial\nu(E)}{\partial E}$. Thus, in HF approximation, the lowest order correction is proportional to the square of the energy derivative of the density of states at the Fermi energy. This explains the presence of the peaks seen in Fig. 3, to the left and right of the two resonances at $E_F = \epsilon_1 = 1$ and $E_F = \epsilon_2^* = \epsilon_1 + 2E_c + \Delta$, for the two lowest temperatures $\beta = 100$ and $\beta = 12.5$. The fact that, for $\beta = 12.5$, R_q does not identically vanish at resonance where $\nu'(E_F) = 0$ is due to higher order terms in the low temperature expansion, which involve nonvanishing higher order derivatives of ν. The dotted horizontal line at $R_q = h/2e^2$ marks the zero temperature result. In the opposite limit of very high temperature $k_BT \gg \Delta + 2E_c$, where

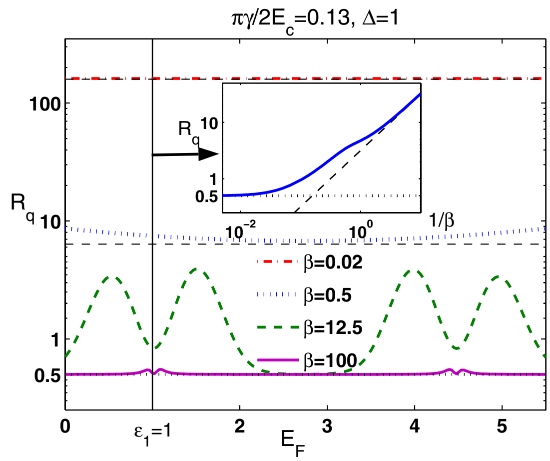

FIG. 3 (color online). Charge relaxation resistance R_q as a function of Fermi energy E_F for different temperatures. The lower three curves are for a two level dot. The uppermost curve is the high temperature asymptote. The inset shows R_q as a function of temperature for $E_F = \epsilon_1$.

$-f'(E) \cong \beta/4$ and in the weakly coupled regime $\gamma \ll \Delta$, where the density of states is well approximated by a sum of displaced Lorentzians of width γ, we can estimate the remaining integrals in the numerator and denominator of (10) as $-\int dEf'(E)\nu(E)^2 \cong \beta M/4\pi\gamma$ and $-\int dEf'(E)\nu(E) \cong \beta M/4$, respectively, where M is the number of density of states peaks under the broad curve $f'(E)$. Therefore, at very high temperature, we find

$$R_q \cong \frac{h}{e^2}\frac{2}{\pi\gamma M\beta}. \tag{15}$$

This high temperature limit is shown as a dashed horizontal black line in Fig. 3 for the two highest temperatures. In the present two level system, $M = 2$ and as expected the agreement with the numerical integration of (10) is good for the highest temperature $\beta^{-1} = 50 \gg \Delta + 2E_c = 3.5$. For the intermediate temperature $\Delta = 1 < \beta^{-1} = 2 < \Delta + 2E_c = 3.5$, there is already a significant deviation from the asymptotic result. In the inset in Fig. 3, we show R_q as a function of the temperature on the first resonance at $E_F = \epsilon_1$. The dashed line corresponds to the high temperature asymptote (15), and the dotted line is the low temperature limit (14).

In this work, we have analyzed the charge relaxation of a mesoscopic capacitor in the linear regime of coherent dynamical transport. We have shown that the single-channel zero temperature charge relaxation resistance R_q is universal even in the presence of single charge effects, described in the Hartree-Fock approximation. This shows, in particular, that charge relaxation of a quantum coherent capacitor is faster than one could naively expect based on classical arguments. We obtain the magnetic field dependence of R_q in the two-channel case (electrons with spin), where we identify two qualitatively different regimes of weak and strong coupling. In the former, the degeneracy of both spin states is lifted by the interaction at all field strengths and R_q is nonuniversal. In the latter regime, the degeneracy is lifted only at finite field, and at zero field R_q is universal and equal to its minimum two-channel value $h/4e^2$. The finite temperature behavior of R_q for a two level spin-polarized system is, to lowest order, determined by the logarithmic derivative of the density of states with respect to energy. In the multilevel case, the HF approximation gives a reasonable qualitative picture of the underlying physics. The important case of $B = 0$, for a single strongly coupled level in the dot, requires a treatment of Kondo physics and will be discussed elsewhere [20].

Our work demonstrates that mesoscopic charge relaxation is a physically very interesting process and provides a basis for the understanding of experimental data in the low and high magnetic field ranges.

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