Coulomb blockade at almost perfect transmission

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We study the equilibrium properties of a quantum dot connected to a bulk lead by a single-mode quantum point contact. The ground-state energy and other thermodynamic characteristics of the grain show periodic dependence on the gate voltage (Coulomb blockade). We consider the case of almost perfect transmission, and show that the oscillations exist as long as the transmission coefficient of the contact is less than unity. Near the points where the dot charge is half-integer, the thermodynamic characteristics show a nonanalytic behavior identical to that of the two-channel spin-$\frac{1}{2}$ Kondo model. In particular, at any transmission coefficient the capacitance measured between the gate and the lead shows periodic logarithmic singularities as a function of the gate voltage.

I. INTRODUCTION

The phenomenon of Coulomb blockade of tunneling has recently attracted a lot of interest, both theoretical and experimental.[1] It can be observed, e.g., by measuring conductance of a system of two macroscopic leads connected to a small metallic grain by tunnel junctions. At low temperature, tunneling of an electron into the grain leads to an increase of the electrostatic energy of the system by finite amount $E_C = e^2/2C_0$, where C_0 is the grain capacitance. Thus, the tunneling conductance becomes exponentially small, with the activation energy E_C. One can then add a gate electrode in order to control the electrostatic energy,

$$E_Q = \frac{(Q - eN)^2}{2C_0}. \tag{1}$$

Here, Q is the grain charge; parameter N is proportional to the gate voltage V_g. The activation energy is now a function of V_g. At the values of the gate voltage corresponding to $N = n + \frac{1}{2}$ the energies of states with charges en and $e(n+1)$ are equal, and the activation energy vanishes. Therefore, one observes periodic peaks of conductance as a function of the gate voltage.

Recently, the Coulomb blockade was observed in semiconductor heterostructures.[2] Unlike metallic systems, in a semiconductor device it is often possible to control the barrier height by adjusting the voltage on additional gate electrodes. In such experiments one can study the evolution of the Coulomb blockade as the transmission coefficient $\mathcal{T}$ of the tunnel barrier changes from 0 to 1. The experiments[3,4] indicate that the increase of the transmission coefficient leads to the suppression of Coulomb blockade. At $\mathcal{T} \sim 1$ instead of well-separated peaks, weak periodic oscillations of conductance $G(V_g)$ are observed. Experiment[3] indicates that the Coulomb blockade disappears at $\mathcal{T} = 1$. On the other hand, in the experiment[4] the Coulomb blockade oscillations were observed even when the conductance of the junction exceeded $e^2/\pi\hbar$. To resolve this contradiction, one needs a theory of the Coulomb blockade in the regime of strong tunneling, $\mathcal{T} \to 1$.

In this paper, we study the Coulomb blockade in a quantum dot connected by a controllable tunnel junction to a *single* electrode, Fig. 1(a). Conductance measurements in such a system are not possible. However, the Coulomb blockade shows up in the oscillations of the equilibrium characteristics of the system, e.g., its ground-state energy E, or the average charge $\langle Q \rangle$ of the dot. Experimentally the capacitance $C = \partial^2 E/\partial V_g^2$ between the gate and the lead can be measured.[5]

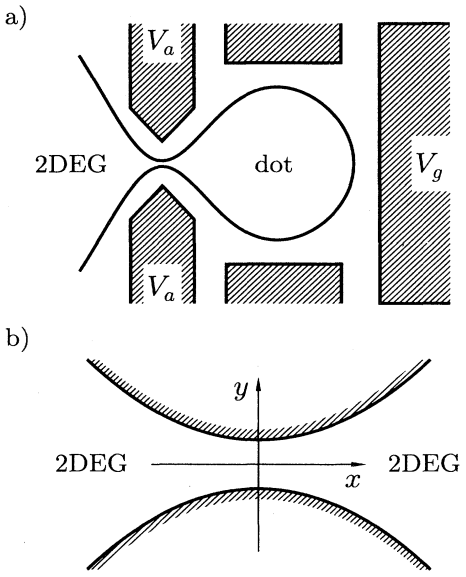

FIG. 1. (a) Schematic view of a quantum dot connected to a bulk 2D electrode. The dot is formed by applying negative voltage to the gates (shaded). Solid line shows the boundary of the 2D electron gas (2DEG). Electrostatic conditions in the dot are controlled by the gate voltage V_g. Voltage V_a applied to the auxiliary gates controls the transmission coefficient $\mathcal{T}$ through the constriction. (b) Constriction between two 2D regions. Inside the constriction the wave functions have 1D form (2).

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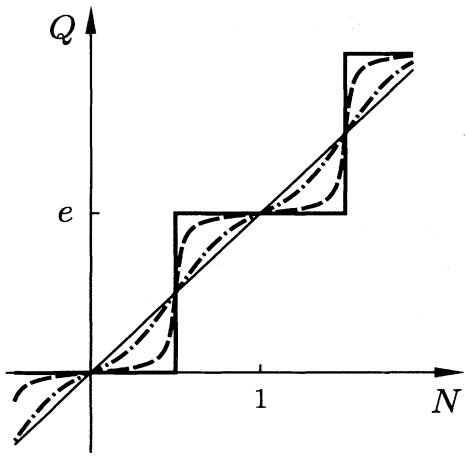

FIG. 2. The average charge Q of the dot as a function of dimensionless gate voltage N at different values of transmission coefficient: $\mathcal{T} = 0$ (solid line), $\mathcal{T} \ll 1$ (dashed line), $1-\mathcal{T} \ll 1$ (dash-dotted line), and $\mathcal{T} = 1$ (thin line).

Most of the theoretical work on Coulomb blockade is devoted to the case of weak-tunneling, when the transmission coefficient of the tunnel barrier is small: $\mathcal{T} \ll 1$. At zero temperature, in the limit of very high barrier the charge of the dot $Q(N)$ is quantized in units of the elementary charge e, except for the degeneracy points $N = n+\frac{1}{2}$, where Q changes from ne to $(n+1)e$ (solid line in Fig. 2). However, if the small probability of tunneling through the barrier is taken into account, the charge of the dot is no longer a good quantum number. As a result the plateaus in $\langle Q(N)\rangle$ are not horizontal, with the slope proportional to $\mathcal{T}$, Ref. 6. This phenomenon is due to the quantum fluctuations of the dot charge caused by virtual processes of electron tunneling between the grain and the lead. Furthermore, the quantum fluctuations were shown[7] to smear the steps of the average grain charge Q at half-integer values of N, making $\langle Q(N)\rangle$ a continuous function (dashed line in Fig. 2).

In this paper, we present a theory of the Coulomb blockade near the strong-tunneling limit $\mathcal{T} = 1$. In Sec. II, we show that the Coulomb blockade in the system shown in Fig. 1(a) is described by a one-dimensional (1D) model. This allows us to use the bosonization approach, and treat the Coulomb interaction exactly. In agreement with experiment,[3] we find no contributions which are periodic in V_g in any measurable characteristic of the system at $\mathcal{T} = 1$. The backscattering on the barrier at $\mathcal{T} < 1$ can be treated in the bosonization approach as a small perturbation. In Sec. III, we calculate the first nonvanishing correction to the ground-state energy of the system $E(N)$, average grain charge $\langle Q(N)\rangle$, and capacitance $C(N)$. These corrections are periodic in N, with the period corresponding to the change of the grain charge by e. In the case of electrons with spin the corrections diverge logarithmically at low energies, indicating that the higher-order calculation is necessary. Such a calculation performed in Sec. IV removes the singularities at all values of N except half-integer ones. In Sec. V, we discuss the nonanalytic behavior of the thermodynamic characteristics of the system at $N = n + \frac{1}{2}$ using the analogy[7] between the Coulomb blockade problem and the two-channel Kondo model. We argue that the periodic logarithmic singularities in the capacitance measured between the gate and the lead should be observed at *any* value of the transmission coefficient $\mathcal{T} < 1$.

II. ONE-DIMENSIONAL MODEL

The system we study is shown in Fig. 1(a). The dot is connected to the lead by a narrow constriction formed by applying voltage V_a to the auxiliary gates. We assume that the width of the constricton in its center allows only a single transverse state below the Fermi level. In this sense the electron gas inside the constriction is one dimensional. As the electron moves away from the center of the constriction, the channel becomes wider, Fig. 1(b), and the number of transverse modes grows. Since the constriction is formed electrostatically, its boundaries are smooth and do not scatter the electrons.[8] Thus the constriction creates an ideal quantum point contact between two two-dimensional (2D) regions: the dot and the lead.

In the following, we will neglect the fact that the dot size is finite, i.e., the infinite system shown in Fig. 1(b) will be considered. The difference between the two systems is that an electron entering a finite dot will eventually return back to the lead through the constriction. The time τ between these two events is determined by the inverse width of the discrete energy levels in the grain. In the case of an ideal single-mode junction, the width is equal to the level spacing ε in the dot, and $\tau \sim \hbar/\varepsilon$. An important difference between noninteracting and interacting systems is that the latter has another energy scale, E_C. In particular, the typical frequency of charge fluctuations is $E_C/\hbar$ (see, e.g., Sec. III). Since in a 2D dot $E_C \gg \varepsilon$, the characteristic time $\hbar/E_C$ at which the Coulomb blockade develops is much shorter than τ. In the following, we will consider the limit $\tau \to \infty$ corresponding to the infinite system.

An important property of the infinite system shown in Fig. 1(b) is that it is essentially one dimensional. To see that, let us consider wave function $\Psi(x,y)$ of an arbitrary state penetrating the constriction. Near the center of the constriction the wave function is one dimensional:

$$\Psi_k(x,y) = \phi_0(y)e^{ikx}, \tag{2}$$

where $\phi_0(y)$ is the wave function of the ground state for the transverse motion, and wave vector k is determined by the energy corresponding to $\Psi(x,y)$. Since we consider an ideal contact characterized by the quantized value of conductance $G = e^2/\pi\hbar$, the wave function (2) does not have a scattered component $\phi_0(y)e^{-ikx}$. Outside the constriction the wave functions have a much more complicated form. In particular, they may be strongly affected by the disorder present in the 2D leads. Nevertheless, one can label any wave function by a single parameter k. Thus, the Hamiltonian of the system of electrons penetrating the constriction can be written as

$$H_0 = \int \left(E_0 + \frac{\hbar^2 k^2}{2m} \right) a_k^\dagger a_k dk, \tag{3}$$

where $a_k^\dagger$ is the creation operator for the electron in state $\Psi_k(x,y)$, and E_0 is the energy of the transverse motion corresponding to the wave function $\phi_0(y)$.

It is worth noting that Hamiltonian (3) does not describe the whole system of 2D electrons. For instance, the electrons with energies below E_0 do not penetrate the constriction and are not included in H_0. However, since we are interested in electron transport through the constriction, the existence of electron states confined in one of the electrodes, and therefore omitted in (3), does not affect our results.

The Hamiltonian (3) has a one-dimensional form. However, unlike in a usual 1D system, the density of states is determined by the 2D leads and is, therefore, energy independent. As a result the physical properties of the system at energy scales of order of Fermi energy E_F cannot be described by the 1D model. On the other hand, the low-energy properties of the system, such as conductance at low voltage and temperature $eV, T \ll E_F$, or Coulomb blockade that develops at energy scale $E_C \ll E_F$, can be described by the 1D model.

To consider the Coulomb blockade at $\mathcal{T} < 1$, we have to add scattering potential $V(x,y)$. We assume that this potential is localized inside the constriction, where one can use the simple 1D form (2) of the wave functions. Then the Hamiltonian describing such scattering also takes a 1D form

$$H' = \frac{1}{2\pi} \iint V(k-k') a_k^\dagger a_{k'} dk dk'. \tag{4}$$

Here, the 1D scattering matrix element $V(q)$ is determined as

$$V(q) = \iint V(x,y) |\phi_0(y)|^2 e^{-iqx} dx dy. \tag{5}$$

To complete our 1D formulation of the Coulomb blockade problem, we must show that the interaction Hamiltonian also has a 1D form. Assuming good screening within the 2D dot, we will describe the Coulomb interaction by the charging energy (1), with Q being the charge inside the dot. In the absence of a tunnel barrier the boundary of the dot is not well defined; we will assume it to be at the center of the constriction.[9] To find the explicit form of the charge operator, we note that there is an obvious relation between Q and the current operator:

$$\dot{Q} \equiv -\frac{i}{\hbar}[Q, H_0] = J(0), \tag{6}$$

where $J(0)$ is the operator of current at point $x = 0$. The current operator can be obtained by integrating the standard expression for the current density over the transverse coordinate y. The expression for the current density at $x = 0$ is local, and we can use the 1D form (2) of the wave functions inside the constriction. Then the current operator takes the form

$$J = \frac{e\hbar}{4\pi m} \iint (k + k') a_k^\dagger a_{k'} dk dk', \tag{7}$$

where m is the electron mass. Both H_0 and $J(0)$ have 1D forms in terms of operators a_k. Hence, the charge operator found from Eq. (6) is also essentially one dimensional:

$$Q = -i \frac{e}{2\pi} \iint \frac{a_k^\dagger a_{k'}}{k - k'} dk dk'. \tag{8}$$

Equations (3), (4), (1), and (8) present a complete 1D Hamiltonian of the system in k representation. It is more convenient to treat this Hamiltonian in coordinate representation, which can be obtained by making a Fourier transformation to the alternative 1D fermion operators:

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int a_k e^{ikx} dk. \tag{9}$$

Unlike the initial 2D wave functions $\Psi(x,y)$, these alternative operators are completely one dimensional.

As we already mentioned, we are interested in low-energy properties of the system. Thus, we can linearize the spectrum of electrons in Eq. (3) near the two Fermi points, and write the fermion creation operators in terms of left- and right-moving fermions: $\psi(x) = \psi_L(x) + \psi_R(x)$. The three parts of the Hamiltonian then transform to

$$H_0 = \hbar v_F \int \Big[\psi_L^\dagger(x)(i\nabla - k_F)\psi_L(x) - \psi_R^\dagger(x)(i\nabla + k_F)\psi_R(x) \Big] dx, \tag{10}$$

$$H' = \int V(x) \psi^\dagger(x) \psi(x) dx, \tag{11}$$

$$H_C = \frac{(Q - eN)^2}{2C_0}. \tag{12}$$

Here, v_F is the Fermi velocity; the 1D scattering potential $V(x)$ is obtained from the real 2D potential $V(x,y)$ by averaging over the electron density $|\phi_0(y)|^2$ in the transverse direction. The charge operator (8) takes the form

$$Q = \frac{e}{2} \int \Big[\psi_L^\dagger(x)\psi_L(x) + \psi_R^\dagger(x)\psi_R(x) \Big] \operatorname{sgn} x \, dx. \tag{13}$$

As expected, the operator (13) has the simple meaning of the charge transferred from the region $x < 0$ to the region $x > 0$.

To summarize, we established that the Coulomb blockade in a dot connected to a bulk electrode by means of a quantum point contact can be treated as a 1D problem.[10] This will greatly simplify the following discussion, since we can now bosonize the Hamiltonian (10)–(13) and treat the quartic in fermion operators interaction term (12) exactly.

III. PERTURBATION THEORY IN REFLECTION AMPLITUDE

A. Bosonized Hamiltonian

The bosonization technique[11] is applicable whenever the system behavior is determined by the low-energy

properties of the 1D electron system. As we already mentioned, the typical energy scale at which the Coulomb blockade becomes important is E_C. This energy is much lower than the Fermi energy, and the condition of applicability of the bosonization approach is satisfied. At low energies the electron system can be viewed as an elastic medium. Therefore the bosonized Hamiltonian can be written in terms of two variables: the displacement of the elastic medium $u(x)$ and its momentum density $p(x)$. The Hamiltonian (10) of noninteracting electrons takes the form:

$$H_0 = \int \left\{ \frac{p^2(x)}{2mn_0} + \frac{1}{2} mn_0 v_F^2 [\nabla u(x)]^2 \right\} dx. \quad (14)$$

Here, m is the electron mass, $n_0 = mv_F/\pi\hbar$ is the electron density. The two fields, displacement $u(x)$ and momentum density $p(x)$, satisfy the standard commutation relation,

$$[u(x), p(y)] = i\hbar\delta(x-y). \quad (15)$$

To bosonize the interaction Hamiltonian (12), we should find the expression for the charge transferred through the point $x = 0$. This can be done by substitution of the bosonized formula for the electron density $\psi_L^\dagger \psi_L + \psi_R^\dagger \psi_R \to -n_0 \nabla u$ into Eq. (13). Alternatively, one can just note the obvious relation $Q = en_0 u(0)$ between charge and displacement. In either case, we get

$$H_C = E_C [n_0 u(0) - N]^2. \quad (16)$$

It is important to emphasize that the interaction term (16) is quadratic in bosonic variables, and the Hamiltonian $H_0 + H_C$ of the system without scattering potential can be diagonalized exactly.

We are primarily interested in the periodic dependence of the ground-state energy on the gate voltage, i.e., on N. One can easily see that after the transformation,

$$u(x) \to u(x) + N/n_0, \quad (17)$$

the Hamiltonian $H_0 + H_C$ does not depend on N. Hence we expect the Coulomb blockade to be completely suppressed by charge fluctuations in the absence of scattering potential, i.e., at $\mathcal{T} = 1$ (thin line in Fig. 2). To find the Coulomb blockade oscillations at $\mathcal{T} < 1$, one has to consider the effect of scattering on the potential of the barrier.[12]

In the bosonization approach, only the low-energy properties of the system are considered. The scattering on a localized potential is, therefore, characterized by two constants: the amplitudes of forward and backward scattering $V(0)$ and $V(2k_F)$ given by Eq. (5). In boson representation the scattering potential has the form:

$$H' = -V(0) n_0 \nabla u(0) - \frac{V(2k_F)}{\pi\hbar v_F} D \cos[2\pi n_0 u(0)], \quad (18)$$

where D is the high-energy cutoff (bandwidth). The first term in Eq. (18) does not change under the transformation (17) and does not lead to a dependence of the ground-state energy on N. On the contrary, the backscattering term becomes periodically dependent on N, and therefore leads to periodic dependence of all the thermodynamic properties on gate voltage. Below, we calculate the first nonvanishing periodic correction to the ground-state energy due to the backscattering.

B. Perturbation theory for spinless electrons

To find the first-order correction to the ground-state energy one has to calculate the average of the cosine term in Eq. (18) over the ground state of the quadratic Hamiltonian (14), (16). This can be performed along the same lines as in the Debye-Waller theory:

$$\delta E_1 = -\frac{1}{\pi} |r| D \cos[2\pi n_0 \langle u(0) \rangle] e^{-2\pi^2 n_0^2 \langle\langle u^2(0) \rangle\rangle}. \quad (19)$$

Here, we introduced the reflection amplitude r. [In the first order in backscattering potential, $r = V(2k_F)/i\hbar v_F$.] From Eq. (16), it is obvious that $\langle u(0) \rangle = N/n_0$. In a 1D elastic medium the average quantum fluctuation of the displacement $\langle\langle u^2 \rangle\rangle = \langle u^2 \rangle - \langle u \rangle^2$ diverges logarithmically due to the low-energy phonons. In our case, the phonons with energies below E_C are pinned down by the interaction term (16), see Ref. 13. Therefore the fluctuation of u is large, but finite. To find $\langle\langle u^2 \rangle\rangle$, we will explicitly diagonalize the Hamiltonian $H_0 + H_C$. This is achieved by the transformation

$$u(x) = \frac{N}{n_0} + \frac{1}{\sqrt{\pi}} \int_0^\infty u_k \cos(k|x| - \delta_k) dk, \quad (20)$$

$$p(x) = \frac{1}{\sqrt{\pi}} \int_0^\infty p_k \cos(k|x| - \delta_k) dk. \quad (21)$$

Here, the phase shift δ_k is defined as

$$\delta_k = \arctan\left(\frac{E_C}{\pi\hbar v_F k} \right). \quad (22)$$

In Eqs. (20) and (21), we neglected the odd modes proportional to $\sin kx$ because they do not contribute to $u(0)$ and, therefore, are decoupled from both interaction H_C and scattering H'. The fields u_k and p_k satisfy standard commutation relations $[u_k, p_{k'}] = i\hbar\delta(k - k')$. In terms of these fields the Hamiltonian $H_0 + H_C$ takes the form

$$H_0 + H_C = \int_0^\infty \left(\frac{p_k^2}{2mn_0} + \frac{1}{2} mn_0 (v_F k)^2 u_k^2 \right) dk. \quad (23)$$

It follows from Eq. (20) that the contribution of the low-frequency modes to the displacement $u(0)$ is suppressed by the factor $\cos\delta_k \sim \hbar v_F k / E_C$. This gives rise to the low-frequency cutoff in the logarithmic integral for $\langle\langle u^2(0) \rangle\rangle$. A simple calculation then gives

$$\langle\langle u^2(0) \rangle\rangle = \frac{1}{2\pi^2 n_0^2} \ln\left(\frac{\pi D}{\gamma E_C} \right). \quad (24)$$

Here $\gamma = e^{\mathbf{C}}$, with $\mathbf{C} \approx 0.5772$ being the Euler's constant. We can now find the periodic correction to the ground-state energy using Eq. (19),

$$\delta E_1 = -\frac{\gamma}{\pi^2}|r|E_C \cos 2\pi N. \quad (25)$$

As expected the amplitude of oscillations of the ground-state energy becomes of the order of E_C at $|r| \sim 1$.

The average charge $\langle Q \rangle$ in the dot can now be found using (12),

$$\langle Q \rangle = eN - \frac{e}{2E_C}\frac{\partial \delta E_1}{\partial N} = eN - \frac{\gamma}{\pi} e|r| \sin 2\pi N. \quad (26)$$

The period of oscillations corresponds to the change of the average number of particles in the dot by one. At weak reflection, $|r| \ll 1$, the amplitude of the oscillations of charge is small (dash-dotted line in Fig. 2).

Finally, the periodic correction to the capacitance measured between the gate and the lead can be found as $\delta C_1 = \partial^2 \delta E_1 / \partial V_g^2$. It also exhibits periodic oscillations as a function of the gate voltage.

In the above discussion, we completely ignored the spins of electrons. The spinless case can probably be realized in an experiment in a high magnetic field. However, in the absence of magnetic field one should take the spins into account. We will now demonstrate that the spin degree of freedom affects the above results dramatically.

C. Perturbation theory for electrons with spin

To take into account electron spins, we consider a model with two channels corresponding to two spin directions:

$$H_0 = \int \left\{ \frac{p_1^2 + p_2^2}{2mn_0} + \frac{mn_0 v_F^2}{2}\left[(\nabla u_1)^2 + (\nabla u_2)^2\right] \right\} dx, \quad (27)$$

$$H_C = E_C \{ n_0 [u_1(0) + u_2(0)] - N \}^2, \quad (28)$$

$$H' = -\frac{1}{\pi}|r| D \{ \cos[2\pi n_0 u_1(0)] + \cos[2\pi n_0 u_2(0)] \}. \quad (29)$$

The expressions for H_0 and H' are obtained by a straightforward generalization of Eqs. (14) and (18) to the two-channel case. [In Eq. (29), we neglected the forward scattering terms.] The two channels are coupled through the interaction term (28) which depends only on the sum $u_1(0) + u_2(0)$ representing the total charge brought into the dot. Thus, it is natural to transform the Hamiltonian to charge and spin modes $u_{c,s} = (u_1 \pm u_2)/\sqrt{2}$ (and similarly for momentum densities $p_{c,s}$). In the new variables the Hamiltonian (27)–(29) takes the form:

$$H_0 = \int \left\{ \frac{p_c^2 + p_s^2}{2mn_0} + \frac{mn_0 v_F^2}{2}\left[(\nabla u_c)^2 + (\nabla u_s)^2\right] \right\} dx, \quad (30)$$

$$H_C = E_C \left[\sqrt{2}\, n_0 u_c(0) - N \right]^2, \quad (31)$$

$$H' = -\frac{2}{\pi}|r| D \cos\left[\sqrt{2}\,\pi n_0 u_c(0)\right] \cos\left[\sqrt{2}\,\pi n_0 u_s(0)\right]. \quad (32)$$

One can easily calculate the first-order correction to the ground-state energy following the discussion of the spinless case. An important difference between these two cases is that now we have two modes, and only one of them is pinned down by Coulomb interaction (31). Therefore, the quantum fluctuation $\langle\langle u_s^2 \rangle\rangle$ of the displacement in the spin channel diverges logarithmically. This leads to a strong suppression of the oscillations of the ground-state energy. The amplitude of these oscillations is $|r|\sqrt{E_C \varepsilon}$, where ε is the low energy cutoff of the order of the level spacing in the dot. In the limit of large dot ($\varepsilon \to 0$) the first-order correction to the ground-state energy vanishes. Thus, in order to obtain the Coulomb blockade oscillations one has to perform the calculation up to the second order in barrier potential.

The second-order correction to the ground-state energy can be presented in the form

$$\delta E_2 = \frac{1}{\hbar}\mathrm{Im} \int_0^\infty \langle H'(t) H'(0) \rangle \, dt. \quad (33)$$

From the explicit form (32) of the perturbation H' it follows that the correlator $\langle H'(t) H'(0) \rangle$ factorizes into charge and spin parts. The spin part is easily calculated:

$$\langle \cos[\sqrt{2}\,\pi n_0 u_s(0,t)] \cos[\sqrt{2}\,\pi n_0 u_s(0,0)] \rangle = \frac{1}{2iDt}. \quad (34)$$

The slow decay of the correlator at large t is due to the low-frequency modes. In the charge channel the low-frequency components of $u(0)$ are suppressed. As a result at $t \gg \hbar/E_C$, the charge part of the correlator $\langle H'(t) H'(0) \rangle$ saturates

$$\langle \cos[\sqrt{2}\pi n_0 u_c(0,t)] \cos[\sqrt{2}\pi n_0 u_c(0,0)] \rangle = \frac{2\gamma E_C}{\pi D}\left(\cos^2 \pi N - \frac{\pi^2 \hbar^2}{4E_C^2 t^2} \sin^2 \pi N \right). \quad (35)$$

The substitution of Eqs. (34) and (35) into the expression for the second-order correction (33) gives the integral which diverges logarithmically at large t. The divergence can be cut off at $t \sim \hbar/\varepsilon$ (or at $t \sim \hbar/k_B T$ if the correction to the free energy at a finite temperature is being calculated). The result has the form

$$\delta E_2 = -\frac{4\gamma}{\pi^3}|r|^2 E_C \ln\left(\frac{E_C}{\varepsilon}\right) \cos^2 \pi N. \quad (36)$$

In the limit of large dot $E_C/\varepsilon \to \infty$, and the second-order result diverges. This indicates that the terms of higher orders in $|r|$ should be taken into account.

IV. HIGHER-ORDER CALCULATION OF THE GROUND-STATE ENERGY

To proceed with the higher-order calculation, we will first simplify our Hamiltonian (30)–(32). Since the logarithmic divergence arises at small energy scales $E \ll E_C$, we do not have to treat the charge fluctuations exactly. At such low energies the charge fluctuations are suppressed by the interaction term, and one can replace $\cos[\sqrt{2}\,\pi n_0 u_c(0)]$ in Eq. (32) by its value averaged over the unperturbed ground-state. After this simplification the charge-related part of the Hamiltonian completely decouples and can be excluded.

Another simplification is made possible by the fact that the barrier potential depends only on the spin mode displacement at $x = 0$. Therefore, the odd elastic modes

proportional to $\sin kx$ are not coupled with H' and can be excluded. To this end, we will change the variables: $u_{e,o}(x) = [u_s(x) \pm u_s(-x)]/\sqrt{2}$, and similarly for the momentum densities $p_{e,o}(x)$. Thus, we arrive at a Hamiltonian

$$H_0 = \int_0^\infty \left\{ \frac{p_e^2}{2mn_0} + \frac{mn_0 v_F^2}{2} (\nabla u_e)^2 \right\} dx, \tag{37}$$

$$H' = -\left(\frac{8\gamma E_C D}{\pi^3} \right)^{1/2} |r| \cos \pi N \cos[\pi n_0 u_e(0)]. \tag{38}$$

The bandwidth D, here, should be taken of the order of the charging energy E_C, because only at such small energies the charge fluctuations can be neglected.

The Hamiltonian (37), (38) is very similar to the Hamiltonian (14), (18) of noninteracting electrons in the presence of scattering potential. The important difference is that the cosine in Eq. (38) has an argument that is twice smaller than the one in Eq. (18). The latter represents a product of two fermion operators $\psi^\dagger(0)\psi(0)$. Similarly, Eq. (38) can be interpreted as a sum of two fermion operators: $\psi^\dagger(0) + \psi(0)$. To support this observation, we will rewrite the Hamiltonian in terms of an alternative bosonic field,

$$\Phi(x) = -\pi n_0 u_e(|x|) + \frac{\operatorname{sgn} x}{\hbar n_0} \int_0^{|x|} p_e(x')dx'. \tag{39}$$

Unlike the old variables $u_e(x)$ and $p_e(x)$ defined at $x > 0$, the field $\Phi(x)$ is defined on the whole x axis and has the same number of degrees of freedom. The commutation relations for the new variables have the form: $[\Phi(x), \Phi(y)] = i\pi \operatorname{sgn}(x - y)$.

In terms of the field Φ, the Hamiltonian (37), (38) takes the form

$$H_0 = \frac{\hbar v_F}{4\pi} \int_{-\infty}^\infty [\nabla \Phi(x)]^2 dx, \tag{40}$$

$$H' = -\left(\frac{8\gamma E_C D}{\pi^3} \right)^{1/2} |r| \cos \pi N \cos \Phi(0). \tag{41}$$

Expression (40) obviously coincides with the well-known form of the bosonized Hamiltonian of a 1D gas of noninteracting right-moving electrons (see, e.g., Ref. 11). In this case, the operator $\sqrt{D/2\pi\hbar v_F}\, e^{i\Phi(x)}$ is identified as the electron annihilation operator $\psi(x)$. Consequently, the Hamiltonian (40), (41) can be debosonized to the following form:

$$H_f = \int_{-\infty}^\infty \left[\xi_k b_k^\dagger b_k - \lambda(b_k^\dagger + b_k) \right] dk, \tag{42}$$

where b_k and $b_k^\dagger$ are the new fermion operators in k representation, electron energy $\xi_k = \hbar v_F k$ is measured from the Fermi level, and $\lambda = \sqrt{2\gamma \hbar v_F E_C/\pi^3}\, |r| \cos \pi N$.

The Hamiltonian (42) contains a term linear in fermion operators b_k and $b_k^\dagger$. If it is treated perturbatively, one obtains the result (36). However, it is possible to take into account all the higher terms of the perturbation theory. This can be done by transforming the Hamiltonian (42) to a quadratic form. One such transformation based on the Jordan-Wigner transformation to a spin chain was suggested by Guinea.[14] We will use a simpler transformation:

$$b_k = (c + c^\dagger)\, c_k. \tag{43}$$

One can easily check that if c and c_k are fermion operators, the operators b_k have correct anticommutation relations. After this transformation, we get a Hamiltonian quadratic in fermion operators,

$$H_q = \int_{-\infty}^\infty \left\{ \xi_k c_k^\dagger c_k - \lambda \left[c_k^\dagger (c + c^\dagger) + (c + c^\dagger) c_k \right] \right\} dk. \tag{44}$$

The Hamiltonian H_q is very similar to the Hamiltonian of a resonant impurity at the Fermi level. Unlike the latter, H_q does not conserve the number of particles and should be diagonalized by a Bogoliubov transformation. As a result, we get the diagonal form

$$H_q = E + \int_0^\infty \xi_k \left(C_k^\dagger C_k + \tilde{C}_k^\dagger \tilde{C}_k \right) dk, \tag{45}$$

where E is the ground-state energy of our Hamiltonian. The two branches of the excitation spectrum correspond to some linear combinations of particle and hole states. One of the branches is not affected by coupling to the impurity level: $\tilde{C}_k = (c_k + c_{-k}^\dagger)/\sqrt{2}$. The other branch has some admixture of operators $c^\dagger$ and c,

$$C_k = \frac{\xi_k}{\sqrt{\xi_k^2 + \Gamma^2}} \frac{c_k - c_{-k}^\dagger}{\sqrt{2}} - \sqrt{\frac{\hbar v_F \Gamma}{2\pi(\xi_k^2 + \Gamma^2)}} (c + c^\dagger) + \frac{\Gamma}{\pi \sqrt{\xi_k^2 + \Gamma^2}} \int_{-\infty}^\infty \frac{d\xi_{k'}}{\xi_k - \xi_{k'}} \frac{c_{k'} - c_{-k'}^\dagger}{\sqrt{2}}, \tag{46}$$

where the principal value of the integral is assumed. The parameter $\Gamma = 4\pi\lambda^2/\hbar v_F$ has the meaning of the width of the resonant level.

The correction δE to the ground-state energy of the Hamiltonian H_q can be found, e.g., by averaging Eq. (45) over the unperturbed ground state,

$$\delta E = -\int_0^\infty \xi_k \langle C_k^\dagger C_k \rangle_0 dk. \tag{47}$$

The resulting integral over k is logarithmically divergent at the upper limit due to the second term in the right-hand side of Eq. (46). However, as we already mentioned, the bandwidth in our Hamiltonian should be E_C. Unlike in the case of the perturbation theory, the logarithmic integral now has an intrinsic cutoff Γ at low energies. This low-energy cutoff is due to the higher-order terms in λ. As a result the correction to the ground-state energy is now finite, $\delta E = -(\Gamma/2\pi) \ln(E_C/\Gamma)$. In our original notations, this result has the form

$$\delta E = -\frac{4\gamma}{\pi^3} |r|^2 E_C \ln \left(\frac{1}{|r|^2 \cos^2 \pi N} \right) \cos^2 \pi N. \tag{48}$$

To summarize, the chain of transformations has lead

us from bosonized Hamiltonian (27)–(29) to simple form (44). The transformations are exact at low energies. They uncover the low-energy cutoff Γ for the logarithmic divergence of the second-order perturbation theory.

It is important to note that Γ vanishes at half-integer values of N. At these points the logarithm in Eq. (48) diverges. Due to the prefactor, correction δE is not divergent, but still has a nonanalytic behavior at $N = n + \frac{1}{2}$. The nonanalyticity shows up in the capacitance $C = \partial^2 E/\partial V_g^2$, measured between the gate and the lead:

$$\delta C(N) = \frac{8\gamma}{\pi}|r|^2\beta^2 E_C \ln\left(\frac{1}{|r|^2\cos^2\pi N}\right)\cos 2\pi N. \quad (49)$$

Here, β is the parameter controlling the relation between N and the gate voltage, $N = \beta V_g$; its value is determined by the system geometry. One can easily see that the capacitance is logarithmically divergent at half-integer N. The nature of these singularities is discussed in the next section.

V. ANALOGY TO THE TWO-CHANNEL KONDO MODEL

The logarithmic divergence of the capacitance (49) at half-integer N was found for the case of strong tunneling. It is instructive to compare it with the similar divergence in capacitance[7] in the weak-tunneling case:

$$\delta C(N) = -2\beta^2 E_C \frac{1}{|t|}\exp\left(\frac{\pi}{4|t|}\right)\ln\left(\frac{1}{|2N-1|}\right). \quad (50)$$

Here, t is the transmission amplitude; expression (50) is written for the vicinity of the point $N = \frac{1}{2}$. Both expressions (49) and (50) predict a logarithmic singularity at $N = \frac{1}{2}$, with the factors in front of the logarithm being of the same order at $|t| \sim |r| \sim 1$. It is, therefore, natural to conjecture that the logarithmic divergencies of capacitance exist not only in the limiting cases of weak and strong tunneling, but at any value of the transmission coefficient.

To support this idea, we shall first outline the arguments leading to the divergence (50) of capacitance in the weak-tunneling case. The solution[7] was based on the mapping of the Coulomb blockade problem onto an anisotropic multichannel Kondo model. At N close to $\frac{1}{2}$, one can consider the perturbation theory in tunneling amplitude and neglect all the terms involving virtual states with a charge different from 0 and 1. This restriction on the possible charge states is due to the large charging energy associated with all other states. Thus, all the relevant terms of the perturbation theory are constructed in such a way that first an electron tunnels through the barrier from left to right, changing the dot charge from 0 to 1, then another electron tunnels from right to left returning the dot to the state with $Q = 0$, then one more electron tunnels from left to right leading to $Q = 1$, and so on. One can note that the same structure of the perturbation theory takes place for the Kondo model with anisotropic coupling $J_\perp(\sigma^+S^- + \sigma^-S^+)$. Instead of the two types of electrons, left and right, we now have two other types, spin-up and spin-down. Furthermore, each electron scattering on the impurity flips its own spin, e.g., from up to down, and the spin of the impurity, down to up. This means that the next electron scattered on the impurity has to flip its spin from down to up, then from up to down, etc. This leads to the same structure of the perturbation theory as in the Coulomb blockade problem.

A small deviation of the system from the point $N = \frac{1}{2}$ gives rise to the energy difference between the states with $Q = 0$ and $Q = 1$. It is completely analogous to the effect of magnetic field h in the Kondo problem. Thus, the capacitance of the system $C \sim \partial^2 E/\partial N^2$ is analogous to the magnetic susceptibility of the Kondo impurity $\chi_i = \partial^2 E/\partial h^2$. The latter is inversely proportional to the Kondo temperature, which leads to the exponentially large factor in Eq. (50).

Finally, the presence of the real spin of electrons (conserved in the tunneling process) should be interpreted as a "color" for the electrons in the Kondo model. Thus, the spin-$\frac{1}{2}$ case maps onto the two-channel Kondo model. The latter is known[15–18] to exhibit some non-Fermi-liquid properties. These include the logarithmic divergence of the susceptibility at $h = 0$, resulting in the logarithmic singularity in Eq. (50).

The result (50), for the capacitance in the weak-coupling regime, was obtained using the exact solution of the Kondo model.[15] Another approach based on the renormalization group treatment[19] allows one to find some low-energy properties of the system at any coupling strength. The main idea of this technique is that at low energies the effective coupling constant in the Kondo model grows, and the system approaches the strong-coupling fixed point. This fixed point is stable, and the low-energy properties of the system are determined by the leading irrelevant perturbation. Therefore the low-energy behavior is universal, i.e., independent of the initial conditions. The stable fixed point for the multichannel Kondo problem was studied in detail by conformal field theory methods.[16] In particular, the logarithmic behavior of the susceptibility in the two-channel Kondo model was rederived.

To apply this method to the Coulomb blockade problem one should first find the fixed points. There are two obvious fixed points: $\mathcal{T} = 0$ and 1. As we already discussed, the weak-tunneling fixed point $\mathcal{T} = 0$ corresponds to the weak-coupling fixed point in the Kondo model. This fixed point is, therefore, unstable. It is then natural to assume that the strong-tunneling fixed point $\mathcal{T} = 1$ maps to the strong-coupling fixed point of the Kondo model. To test this hypothesis one should first show that the $\mathcal{T} = 1$ fixed point is stable. This can be done by calculating the scaling dimension of the perturbation H' in the Hamiltonian (30)–(32). The correlator $\langle H'(t)H'(0)\rangle$ can be found from Eqs. (34) and (35). At half-integer values of N (corresponding to zero magnetic field in the Kondo model) it decays as $1/t^3$. Thus the scaling dimension of the perturbation H' is $\frac{3}{2}$, and the fixed point is stable.

The stability of the $\mathcal{T} = 1$ fixed point suggests that

at half-integer N the system with any value of transmission coefficient $\mathcal{T}$ approaches the strong-tunneling limit. We, therefore, can argue that periodic logarithmic divergences of the capacitance (49) and (50) are a general property of the system and should be observed at any value of the transmission coefficient. In particular, the divergence of capacitance at weak tunneling (50) can be interpreted as a consequence of the divergences (49) in the strong-tunneling limit.

The last statement can be tested by calculation of the so-called Wilson ratio in the strong-tunneling limit. Indeed, since the weak-tunneling properties of the Coulomb blockade problem were found by mapping to the Kondo model, one expects the correction to the heat capacity to have a nonanalytic temperature dependence $\delta c_i \sim k_B T \ln(E_C/k_B T)$, and its ratio to the correction to the susceptibility to be universal.[16,18] If the low-energy behavior of the weak-tunneling model is controlled by the strong-tunneling fixed point, the same must be valid for the model (30)–(32). A straightforward calculation of the correction to the heat capacity in the second order in H' gives

$$\delta c_i = \frac{\pi\gamma|r|^2}{E_C} k_B T \ln(E_C/k_B T). \tag{51}$$

Taking into account the relation $h = 2E_C(N - \frac{1}{2})$ between the effective magnetic field h in the Kondo model and the deviation of N from a half-integer value, we can find the susceptibility from Eq. (36) as $\delta\chi_i = (2E_C)^{-2}\partial^2\delta E_2/\partial N^2$. The result is

$$\delta\chi_i = \frac{2\gamma|r|^2}{\pi E_C} \ln(E_C/k_B T). \tag{52}$$

The ratio $k_B T\delta\chi_i/\delta c_i$ now takes the universal value $2/\pi^2$, in agreement with the theory of the two-channel Kondo model.[16,18]

Finally, it is instructive to discuss the relation between our quadratic Hamiltonian (44) describing the low-energy properties of the Coulomb blockade problem and the similar Hamiltonian for the Toulouse limit of the two-channel Kondo model. The latter was obtained by Emery and Kivelson[17] and has the following form:

$$H = iv_F \int_{-\infty}^{\infty} \psi^\dagger(x)\frac{\partial\psi(x)}{\partial x}dx + \frac{J_x}{\sqrt{2\pi a}}[\psi^\dagger(0) + \psi(0)][d^\dagger - d] + h(d^\dagger d - 1/2). \tag{53}$$

Unlike in the Hamiltonian (53), the second part of Eq. (44) is proportional to the weak magnetic field: $\lambda \propto h$. However, one can still bring the Hamiltonian (53) to the form identical to (44). A linear transformation of fermion operators analogous to (46) allows one to absorb the second term of Eq. (53) into the kinetic energy term. After such a transformation the third term of Eq. (53) takes the form, which is identical to the second term of Eq. (44) at low momenta. Therefore, at low energies the Hamiltonians (44) and (53) are equivalent. This proves our conjecture that the strong-tunneling fixed point is identical to the strong-coupling fixed point of the two-channel Kondo model.

VI. CONCLUSION

In this paper, we have studied the Coulomb blockade in the limit of the barrier transmission coefficient $\mathcal{T}$ close to unity. The Coulomb blockade oscillations of the dot charge and capacitance persist as long as $\mathcal{T} < 1$. As $\mathcal{T}$ approaches unity, the sharp peaks in the system capacitance transform into a weak oscillation with periodic logarithmic divergences at the points where the dot charge is half-integer.

The analogy between the Coulomb blockade and Kondo problem discussed in Sec. V allowed us to conclude that the logarithmic divergences in capacitance should be observed at any value of $\mathcal{T}$. Of course, the exact calculation of the capacitance in terms of the transmission and reflection amplitudes is possible only in the limits $\mathcal{T} \ll 1$ and $1 - \mathcal{T} \ll 1$.

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