Single-Electron Box and the Helicity Modulus of an Inverse Square *XY* Model

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We calculate the average number of electrons on a metallic single-electron box as a function of the gate voltage for arbitrary values of the tunneling conductance. In the vicinity of the plateaus the problem is equivalent to calculating the helicity modulus of a classical inverse square *XY* model in one dimension. By a combination of perturbation theory, a two-loop renormalization group calculation, and a Monte Carlo simulation in the intermediate regime we provide a complete description of the smearing of the Coulomb staircase at zero temperature with increasing conductance. [S0031-9007(97)03141-4]

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One of the most elementary devices which exhibits the effect of Coulomb blockade [1,2] is the so called single-electron box, first realized by Lafarge *et al.* [3]. It consists of a small metallic island which is connected to an outside lead by a tunnel junction and is coupled capacitively to a gate voltage V. By elementary electrostatics the classical Coulomb energy for a given integer number n of additional electrons on the box is [3]

$$E_n = \frac{U}{2}(n - n_x)^2 \tag{1}$$

up to an irrelevant constant. Here $U = \frac{e^2}{C+C_g}$ is an effective single electron charging energy and $n_x = C_g V/e$ the continuous polarization charge induced by the gate. Obviously, on varying n_x, the actual integer value of n is the one minimizing E_n. As a result, $n(n_x)$ is a staircase function with unit jumps at $n_x = \frac{1}{2}$ (mod 1). The basic requirements for such a device to work are twofold: First, it is obvious that the temperature T (we set $k_B = 1$) has to be much smaller than the relevant charging energy. This point is easily taken into account by considering a thermal distribution of the energies E_n [3]. The thermal average $\langle n\rangle(n_x)$ will then approach the simple straight line at $T \gg U$ (note that n is measured over a sufficiently long time interval, giving a continuous $\langle n\rangle$ even though the number of additional electrons in the box is an integer at any given instant of time). Second, however, there is an intrinsic broadening of the staircase even at $T = 0$ since the tunneling probability through the junction is necessarily finite. As a consequence, the number of electrons in the box is not strictly conserved and the variable n exhibits quantum fluctuations, which are neglected in a simple electrostatic description. A quantitative measure of these fluctuations is provided by the average tunneling probability at the Fermi energy ε_F which determines the dimensionless tunneling conductance [4]

$$g = \pi^2 |t|^2_{\varepsilon_F} \rho_{\text{box}} \rho_{\text{lead}} =: \frac{h}{4e^2 R_t}\,. \tag{2}$$

Here t is the transfer matrix element [see (3)] and ρ are the densities of states at ε_F. Obviously the perfect staircase at $T = 0$ is realized only in the limit $g \to 0$, while we expect that $\langle n\rangle(n_x) \to n_x$ even at zero temperature if $g \gg 1$. In the following we will give a quantitative description of the behavior of $\langle n\rangle(n_x)$ near the plateaus at $n_x = 0$ (mod 1) for arbitrary values of g.

We start from a tunneling Hamiltonian [4]

$$\hat{H} = \frac{U}{2}(\hat{n} - n_x)^2 + \sum_{ab} t_{ab} c_a^\dagger c_b + \text{H.c.} + \hat{H}_0 \tag{3}$$

describing the Coulomb energy of the box and the transfer of electrons between states b and a from the box (index b) to the lead (index a) and vice versa. The contribution $\hat{H}_0$ is the Hamiltonian of noninteracting Fermions on both sides of the junction which act as reservoirs. The Coulomb interaction is incorporated only by the classical capacitive energy, which is a good description for metallic systems [1,2]. In the following we shall employ an effective model for the thermodynamics of the box which is obtained by integrating out the Fermionic degrees of freedom. Using a second order cumulant expansion in the transfer term, which is exact in the experimentally relevant limit of a large number of conductance channels, the reduced partition function $Z = \text{Tr}\,\frac{\exp(-\beta\hat{H})}{Z_0}$ can be written as a path integral [4]

$$Z(n_x) = \int_{-\pi}^{\pi} d\theta \times \int_\theta^\theta \mathcal{D}\theta \exp\left\{-S[\theta] + i n_x \int_{-L/2}^{L/2} dx\, \frac{d\theta}{dx}\right\} \tag{4}$$

over a compact angular variable θ conjugate to the integer n. Here x is a dimensionless coordinate of a 1D system with length $L = \beta U$ where $L \to \infty$ as the physical temperature approaches zero. The action is given by $(-L/2 \le x \le L/2)$

$$S[\theta] = \frac{1}{2}\int dx \left(\frac{d\theta}{dx}\right)^2 + \frac{2g}{\pi^2}\int\int dx\, dx' \frac{\sin^2(\frac{\theta(x)-\theta(x')}{2})}{(x - x')^2}\,. \tag{5}$$

The long range part of the interaction has already been written in the form appropriate for $L \to \infty$. Introducing a two component unit spin $\mathbf{S}(x) = [\cos(\theta(x)), \sin(\theta(x))]$ at any point of the line, the action $S[\theta]$ is just the classical energy of an *XY* model with an inverse square interaction proportional to the conductance g. The first term, which arises from the classical charging energy $\frac{C}{2}V^2$, is then identical with the spin wave approximation to a short range interaction. Finally, the external charge n_x acts like a purely imaginary external torque on the *XY* model. Since $\int d\theta = 2\pi m$ determines an integer winding number $m \in Z$ which is a topological invariant for each configuration $\theta(x)$, the external charge appears as a pure boundary term. Defining the free energy per length by $f(n_x) = -\ln Z(n_x)/L$ the average number of electrons in the box can be expressed as

$$\langle \hat{n} \rangle = n_x - \frac{\partial f(n_x)}{\partial n_x}. \tag{6}$$

The fact that n_x arises only as a phase factor $e^{2\pi i m n_x}$ shows that $Z(n_x + 1) = Z(n_x)$ quite generally. Thus, all quantities are periodic in n_x with period 1 which allows one to restrict the discussion to the interval $-\frac{1}{2} < n_x \leq \frac{1}{2}$. In the following we confine ourselves to the zero temperature (i.e., thermodynamic) limit $L \to \infty$ and to the vicinity of $n_x = 0$. Taking $in_x = m_x$ to be a real torque for the moment, a finite value of m_x will induce a nonzero average gradient of the phase

$$\lim_{L\to\infty} \frac{1}{L} \left\langle \int dx \, \frac{d\theta}{dx} \right\rangle_{m_x} = \frac{m_x}{\gamma}, \tag{7}$$

which is linear in m_x in the limit $m_x \to 0$. The associated torsional rigidity γ is then precisely identical with the helicity modulus as defined by Fisher *et al.* [5]. It may be obtained from $f(n_x)$ via

$$\frac{1}{\gamma} = \frac{\partial^2 f(n_x)}{\partial n_x^2}\bigg|_{n_x=0}, \tag{8}$$

which is a measure for the sensitivity to a change in the boundary conditions. Using (6) the slope of the Coulomb staircase near $n_x = 0$ is related to the helicity modulus by

$$\chi = \frac{\partial \langle \hat{n} \rangle}{\partial n_x}\bigg|_{n_x=0} = 1 - \gamma^{-1}. \tag{9}$$

In the trivial limiting case $g = 0$ this describes the expected result $\chi^{(0)} = 0$, i.e., perfect plateaus. Indeed if $g = 0$, the helicity modulus is equal to one, being just the coefficient in front of the $\frac{1}{2}(\frac{d\theta}{dx})^2$ term [5]. In order to describe the behavior at finite g we apply three different methods.

Perturbation theory.—While the nonlinearity of the $\sin^2$ in the action (5) makes an exact evaluation of the path integral impossible, we may expand the long range contribution down to second order in g. Evaluating the resulting averages $\langle \exp(\pm i\theta) \rangle$ with the remaining Gaussian action, the free energy can be calculated up to order g^2. After a straightforward but tedious calculation we obtain

$$\chi(g) = c_1 g + c_2 g^2 + \cdots \tag{10}$$

with $c_1 = \frac{4}{\pi^2}$ and $c_2 \approx -0.052$. For the coefficient c_2 we have evaluated a remaining definite integral numerically. The result (10) is identical with a previous calculation by Grabert [6], who has used direct perturbation theory to fourth order in t in the original Fermionic Hamiltonian (3). The agreement to order g^2 which we have verified to eight digits, confirms that the inverse square *XY* model employed here is a correct representation for the reduced thermodynamics of the original model.

Renormalization group (RNG).—To obtain the exact behavior of the helicity modulus at large values of g, we use the RNG. Indeed the limit $g \gg 1$ has previously been treated by approximate instanton calculations [7,8]. However, they give different results for the pre-exponential factor of the effective charging energy which is essentially the inverse of the helicity modulus. Here we will show that a definitive solution of this problem may be obtained by a two-loop RNG, which uniquely determines both the exponent and the g dependence of the prefactor of the correlation length ξ in the limit $g \gg 1$. Indeed the helicity modulus is directly proportional to the correlation length. To see this we define

$$\rho_m = 2\pi Z(n_x = 0)^{-1} \int_0^{2\pi m} \mathcal{D}\theta \exp\{-S[\theta]\} \tag{11}$$

as the probability for a given winding number m. It is then straightforward to show that the inverse helicity modulus

$$\gamma^{-1} = \lim_{L\to\infty} \frac{\langle (2\pi m)^2 \rangle}{L} \tag{12}$$

measures the normalized variance of the winding number with respect to the probability distribution (11). At $g \gg 1$ a given value of $\langle m^2 \rangle$ requires a system size which is larger by a factor of $\xi(g)$ than that at g of order 1 where $\xi(1) \sim O(1)$. Therefore, by applying (12) we have $\gamma(g) \sim \xi(g)$. In order to determine $\xi(g)$, we use the fact that $d = 1$ is the lower critical dimension of the inverse square *XY* model [9,10]. Since the kinetic energy term in (5) is irrelevant at $g \gg 1$ and $T_{\text{eff}} = \pi^2/g$ is the effective temperature of our classical *XY* model, we may perform a $d = 1 + \epsilon$ expansion around an ordered state at $\epsilon > 0$, which is effectively a low temperature expansion. It is convenient to generalize the *XY* spin $\mathbf{S}(x)$ to a $O(n)$ spin $\mathbf{S}$ parametrized by [11]

$$\mathbf{S}(x) = \left(\mathbf{\Pi}(x), \sqrt{1 - \mathbf{\Pi}^2(\mathbf{x})}\right). \tag{13}$$

Here the $\Pi_i(x), i = 1, \ldots, n-1$ are Goldstone modes whose expectation scales like $\langle \mathbf{\Pi}^2 \rangle \sim T_{\text{eff}}$. We thus expand the long range part of the action in powers of $\mathbf{\Pi}$. In Fourier space and with H as an external magnetic field which serves to regularize the infrared divergencies, the action takes the form ($d = 1$)

$$S = \int dq \frac{|q| + H}{2T_{\text{eff}}}\Big[\mathbf{\Pi}_q\mathbf{\Pi}_{-q} + \frac{1}{4}\mathbf{\Pi}_q^2\mathbf{\Pi}_{-q}^2 + \frac{1}{8}\mathbf{\Pi}_q^2(\mathbf{\Pi}^2)_{-q}^2\Big] \tag{14}$$

up to terms of order Π^8. Following the method of Amit [11] we calculate the β function by field theoretic renormalization using dimensional regularization. In one-loop order two diagrams contribute, only one of which diverges as $\epsilon \longrightarrow 0$. Because of cancellations, the fourteen two-loop diagrams reduce to three types of integrals yielding single and double poles in ϵ. The two-point function at zero external momentum is given by

$$\Gamma^{(2)}(0,H) = \frac{H}{T} - \frac{n-1}{2\epsilon}H^{1+\epsilon} + TH^{1+2\epsilon}\Big[\frac{(n-1)(n-2)}{4\epsilon} + \frac{3(n-1)^2}{8\epsilon^2}\Big] \tag{15}$$

in two-loop order, where $T = T_{\text{eff}}/2\pi^2$ is a rescaled effective temperature. $\Gamma^{(2)}$ can be made finite by introducing renormalized parameters [10]

$$t = \kappa^{\epsilon}Z^{-1}T, \qquad h = Z^{-\frac{1}{2}}H \tag{16}$$

and fields

$$\mathbf{\Pi}_R = Z^{-1/2}\mathbf{\Pi}, \qquad \Gamma_R^{(2)} = Z\Gamma^{(2)}. \tag{17}$$

The renormalization constant Z turns out to be

$$Z = 1 + \frac{n-1}{\epsilon}t + \Big[\frac{(n-1)^2}{\epsilon^2} + \frac{n-1}{2\epsilon}\Big]t^2 + O(t^3). \tag{18}$$

This implies that under a reduction $\Lambda \longrightarrow \Lambda\exp(-l)$ of the cutoff the parameter $g^{-1} = 2T$ at $\epsilon = 0$ scales like

$$\frac{dg^{-1}}{dl} = \frac{1}{2g^2} + \frac{1}{4g^3} + O(g^{-4}). \tag{19}$$

By integrating this differential equation, we find that the associated correlation length diverges like

$$\xi(g \gg 1) = c(g)g^{-1}\exp(2g) \tag{20}$$

with a function $c(g)$ which is finite as $g \longrightarrow \infty$. The exponential behavior is typical for a system at its lower critical dimensionality, and is also obtained in an instanton approach [4,9]. However, the prefactor proportional to g^{-1} which is fixed by the coefficient of the two-loop contribution in (19) and which implies that

$$\chi(g \gg 1) = 1 - \bar{c}g\exp(-2g) \tag{21}$$

is quite different from the g^2 [7] or g^3 [8] prediction of the instanton calculation. In fact, a very similar situation arises in the closely related $O(n)$ nonlinear σ model in two dimensions. Because of the scale invariance of the action there are instantons of arbitrary size and the calculation cannot be controlled in the thermodynamic limit. It is only the two-loop RNG which allows one to determine the correct prefactor of ξ [12], although—in contrast to the instanton results—it does not fix the numerical constant $\bar{c}$. It should also be pointed out that the finite correlation length (20) does not imply an exponential decay of $\langle\mathbf{S}(x)\mathbf{S}(0)\rangle$. Indeed it can be shown [13] that this correlation function asymptotically decays like $1/x^2$ for all $0 < g < \pi^2/2$ and—possibly—even more slowly for larger values of g. For our discussion of the helicity modulus, however, the detailed behavior of $\langle\mathbf{S}(x)\mathbf{S}(0)\rangle$ is irrelevant.

Monte Carlo simulation.—In order to bridge the gap between the perturbative result (10) valid for small g and the asymptotic behavior (21) we have performed a Monte Carlo simulation of the inverse square *XY* model (5) including the short range interaction term for values of g between 0.1 and 5. Following previous work [14,15] we have sampled the winding number probabilities ρ_m defined in (11) using the standard Metropolis algorithm with periodic boundary conditions on a discrete chain with up to 2000 spins. We have checked carefully that further increase in the system length does not change our results for the helicity modulus. To estimate the statistical error we have performed about 40 runs for each choice of the parameters g and L. The calculations were done with HP 700 workstations and a CRAY T90 and took about one hour of CPU time per run. The numerical data are shown in Fig. 1. Evidently the slope of $\langle\hat{n}\rangle$ versus n_x follows the perturbative result (10) closely up to values around $g \approx 1$ and finally approaches $\chi = 1$

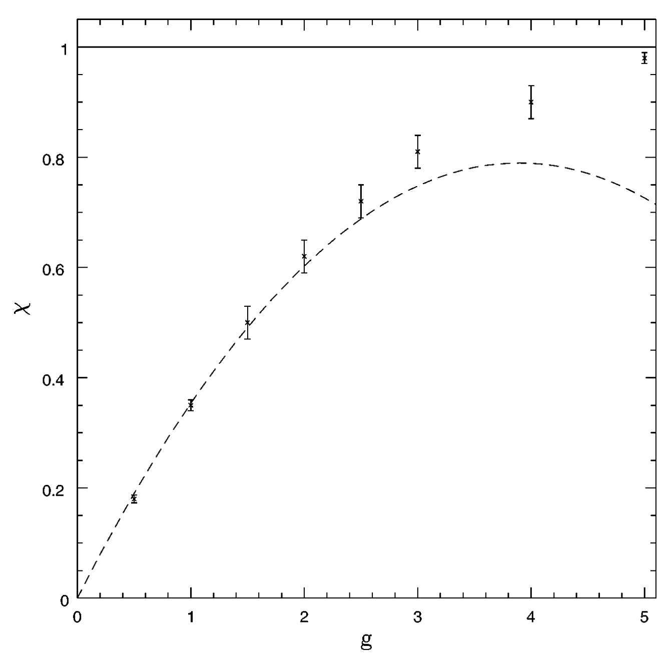

FIG. 1. MC results for the zero temperature slope χ of the Coulomb staircase at $n_x = 0$ as a function of the dimensionless conductance g. The dashed line is the perturbative result (10).

exponentially fast as predicted by (21). Assuming that the asymptotic behavior (21) is already valid for $g > 3$, the MC results allow one to determine the constant in (21), giving $\overline{c} = 80$ from a two-point fit. One should note that a prefactor of this magnitude has also been obtained for the low-temperature behavior of the correlation length of the nonlinear σ-model [16]. It is difficult to estimate, however, whether the asymptotic behavior has already been reached at these values of g. Unfortunately, the exponential increase of the correlation length does not allow us at present to verify numerically our analytical result (21) for the g dependence of the prefactor [17]. Indeed the situation is again analogous to the much studied $O(n)$ nonlinear σ-model in $d = 2$. While the purely numerical constant equivalent to $c(\infty)$ in (20) was determined approximately by Shenker and Tobochnik [16] via a Monte Carlo RG method, the exact coupling constant dependence of the prefactor which follows from the two-loop RNG [18] has only been verified in recent years by extremely extensive numerical computations [19]. Since the range of physical interest in the single electron box problem is restricted to g values smaller than about five (i.e., $R_t \geq 1.3\ \mathrm{k}\Omega$, see Fig. 1) it is evident that our present numerical results fully cover the experimentally accessible regime.

In conclusion, we have calculated the zero temperature smearing of the Coulomb staircase in the single electron box for arbitrary values of the tunnel conductance g. In contrast to previous work on this problem, which has concentrated on the behavior near $n_x = \frac{1}{2}$ and $g \ll 1$ [20], we have discussed the slope at the center of the plateaus. It has been shown that this is determined by the helicity modulus of an inverse square *XY* model. Quantitative MC simulations in the physically relevant regime $g = 0.1$–5 yield the expected crossover between perturbation theory and the asymptotic behavior. Moreover, the two-loop RNG calculation uniquely determines the analytical behavior at large conductance and shows that previous instanton calculations are problematic. Further support for our result is given by the case of the $O(n)$ nonlinear σ-model in two dimensions, where the RNG result for the behavior of the correlation length has been verified by the exact solution [21].

Regarding the experimental situation, the conductance in the existing measurements [3] had a fixed value of order $g_{\mathrm{exp}} \approx 0.02$, i.e., well in the perturbative regime. In fact the first order correction in (10) was used to calibrate the slope at $n_x = 0$ to zero. To verify our results one therefore needs measurements with different and considerably larger values of g at temperatures where the thermal broadening is negligible.

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