

Statistics of the charging spectrum of a two-dimensional Coulomb-glass island

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The fluctuations of capacitance of a two-dimensional island are studied in the regime of low electron concentration and strong disorder, when electrons can be considered classical particles. The universal capacitance distribution is found, with the dispersion being of the order of the average. This distribution is shown to be closely related to the shape of the Coulomb gap in the one-electron density of states of the island. Behavior of the capacitance fluctuations near the metal-insulator transition is discussed. [S0163-1829(97)11416-3]

Capacitance C is conventionally understood as a well defined geometrical property of a metallic sample. For example, for a metallic sphere of radius R capacitance $C=R$, and when the sphere is large, in the first approximation capacitance does not depend on the distribution of impurities inside the sphere or on its charge. However, in very small metallic samples fluctuations of capacitance become observable. Recently, such fluctuations were measured in the semiconductor quantum dots as a function of the total charge of the dot using the Coulomb blockade phenomenon.^{1,2} In such an experiment a small quantum dot is weakly coupled to current leads while a gate is placed in the proximity of the dot and is used to vary its electrostatic potential. At low temperatures the charge of the dot is typically quantized and there is no significant current. However, the gate voltage can be tuned in such a way that the ground states with N and $N+1$ electrons are degenerate. At this gate voltage current can flow through the dot. The resulting conductance vs gate voltage comprises a series of sharp peaks (charging spectrum). The spacing between two peaks ΔV_g can be expressed in terms of the ground state energies E_N of the dot with N electrons:

$$e\alpha\Delta V_g = \Delta_N = E_{N+1} - 2E_N + E_{N-1} = e^2/C_N. \quad (1)$$

Here α is the geometrical coefficient and C_N is the capacitance of the dot with N electrons. This equation may be considered as a definition of the capacitance. For a macroscopic body with the positive background charge eN_0 , E_N has a simple form: $E_N = e^2(N - N_0)^2/2C$ and Eq. (1) gives $C_N = C = \text{const}$. For the quantum dot the charging energy Δ_N was found² to have surprisingly large relative fluctuations:

$$\delta \equiv \frac{(\langle \Delta_N^2 \rangle - \langle \Delta_N \rangle^2)^{1/2}}{\langle \Delta_N \rangle} \sim 0.15. \quad (2)$$

Here $\langle \rangle$ denotes the averaging over N . Much effort has been done to explain such large fluctuations. First, the experimental data were compared with the so-called constant interaction model in which $\Delta_N = e^2/C + \eta_N - \eta_{N-1}$, where η_N is the N th single-electron energy.² The fluctuations of the spacing between the nearest-neighbor levels are of the order of the average spacing E_F/N , where E_F is the Fermi energy. Hence, for a dot of radius R

$$\delta \sim \frac{E_F/N}{e^2/R} \sim \frac{r_s}{R}, \quad (3)$$

where $r_s = a_B$ is the screening radius of the two-dimensional electron gas, a_B is a semiconductor Bohr radius, which is close to 10 nm in GaAs. For this value of a_B and for $R \sim 200$ nm (see Ref. 2) Eq. (3) gives fluctuations that are substantially smaller than observed in the experiment. This discrepancy initiated the computer modeling and the analytical calculations of δ (see Refs. 2 and 3). When discussing theoretical results one should keep in mind that in all the theoretical works δ was obtained by averaging over the different realizations of disorder, instead of number of electrons N . Below we will also assume that in strongly disordered systems there is no difference between these two definitions of fluctuations.

Analytical diagrammatic calculations based on RPA confirm Eq. (3).³ On the other hand, the results of computer modeling^{2,3} agree with Eq. (3) for weak interactions (large r_s and a_B) and lead to larger and interaction independent δ for strong interactions, corresponding to low density electron gas. This fact was identified as a failure of RPA in the low density electron gas.³ It can be interpreted easily in terms of revision of equation $r_s = a_B$ at low densities $n \ll a_B^{-2}$. Indeed r_s cannot be smaller than the average distance between electrons $n^{-1/2}$ and at the small densities one should substitute $r_s = n^{-1/2}$ into Eq. (3). It is not clear yet whether such a simple modification of Eq. (3) can quantitatively explain numerical and experimental data,² which seem to indicate that δ is almost R independent. Hence it is challenging to understand what happens with $\delta(R)$ in the limit of a very low electron density.

In this paper we theoretically study the fluctuations of capacitance of the island in the extreme classical limit when the quantum kinetic energy of electrons is much smaller than both the disorder strength and Coulomb interactions. We consider the case of a large disorder when the ground state of the island is a Coulomb glass.⁴ Below we show that for a piece of Coulomb glass or, in other words, a Coulomb-glass island, the fluctuations are large, δ is of the order of unity, does not depend on R , i.e., is universal for a given shape of the island. For the square sample we find $\delta = 0.32$. (Previously a similar statement about giant, of the order of unity, relative fluctuations of the polarizability of the Coulomb-glass island was made in Ref. 5.)

We study probability density of Δ_N and show that it is a universal function of the ratio $x = \Delta_N / \langle \Delta_N \rangle$. We also discuss how the transition from the Coulomb glass to metal is reflected in the capacitance fluctuations.

When an electron is added to a large metallic sample its charge is distributed in the unique way according to the electrostatic theory. For this reason with addition of every electron the electric potential grows by the same amount e^2/C , or in other words $C = \text{const}$. In the Coulomb glass the electronic states are localized, so that every new electron is put into some localized site. Then electrons rearrange themselves in the vicinity of this site. However, it was shown in Ref. 5 that such rearrangement happens only with probability close to 1/2 on every scale. As a result the added charge in the majority of cases is localized in the region smaller than the size of the island. When next electron enters the island its charge is centered near another site in the island. The distance between this site and the position of the previous electron fluctuates between 0 and $2R$. As a result the difference between energies required to bring two sequential electrons, Δ_N and capacitance C_N experience roughly speaking hundred percent fluctuations.

To verify this reasoning we study the capacitance fluctuations numerically. We use the lattice model of the Coulomb glass suggested by Efros⁶ and widely used to study the Coulomb gap in the density of states (DOS). The Coulomb glass island is modeled by the square $M \times M$ lattice, with every site being either empty (occupation number $n_i = 0$) or occupied by one electron ($n_i = 1$). Electrons interact with each other by Coulomb interaction. The interaction energy between the nearest lattice sites is chosen to be the unit of energy and the lattice constant is the unit of length. Disorder is introduced by the random site energies ϕ_i which are distributed uniformly between -1 and 1 . The corresponding Hamiltonian has the form

$$H_{\text{class}} = \sum_i (\phi_i + u_i) n_i + \frac{1}{2} \sum_{i,j} n_i n_j / r_{ij}. \quad (4)$$

Here u_i is the potential due to the uniform background charge making the system electrically neutral for N electrons. We find the ground-state energies of $N-1$, N , $N+1$ electrons where N is the integer part of $M^2/2$ and then calculate Δ_N using Eq. (1). To find the ground state we use two different methods: the exhaustive enumeration and the simulated annealing. The first one is used for relatively small samples with $M \leq 5$. We enumerate *all* the possible states of N electrons on $M \times M$ lattice sites and find one with the lowest energy. In the second method we employ the simulated annealing technique, running the finite-temperature classical Monte Carlo for some time and taking the lowest-energy state. The convergence of the solution to the ground state has been checked by doubling the time of the simulation and making sure that the solution is not affected. The reliable results have been obtained by this method for $M \leq 8$. Δ_N has been calculated typically for 1000–2000 different realizations of disorder. We have obtained $\delta = 0.32$. Normalized distributions $F(x)$ of the ratio $x = \Delta_N / \langle \Delta_N \rangle$ for $M = 4, 5, 7, 8$ are shown in Fig. 1. We have found $\langle \Delta_N \rangle = 2.3/M$, in a good agreement with the inverse capacitance of metallic square of the same size. Remarkably,

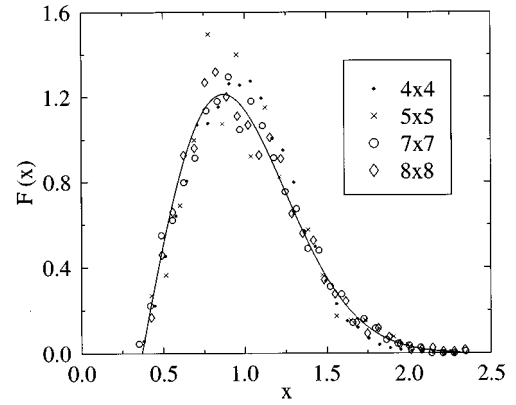


FIG. 1. The inverse capacitance distribution is presented for different sample sizes. The line is the fit by Eq. (5).

$F(x)$ does not depend on M . We emphasize also that contrary to the predictions of the constant interaction model the inverse capacitance of the Coulomb glass island can be both larger and *smaller* than that of the metallic island of the same shape. The fit in Fig. 1 is given by

$$F(x) = \begin{cases} 0, & x < x_0 \\ 4(x-x_0)\exp[-2(x-x_0)^2], & x \geq x_0, \end{cases} \quad (5)$$

where $x_0 = 0.37$. Two interesting features of $F(x)$ are clearly seen. First, this function has a termination point at $x = x_0$. One can easily check that Δ_N corresponding to this point is equal to the smallest possible Coulomb interaction: $1/r_{\text{max}}$, where $r_{\text{max}} = (M-1)\sqrt{2}$ is the maximum distance between sites in the square $M \times M$. Second, $F(x+x_0)$ is identical to the Wigner surmise for the nearest-neighbor distance distribution of the levels of a random matrix. We shall show below that this is only an interesting coincidence.

Now we would like to interpret both features establishing the relation between $F(x)$ and the one-electron DOS $g(\epsilon)$ of the Coulomb-glass island. The energy of the one-electron excitation localized at i th site can be written as

$$\epsilon_i = \phi_i + u_i + \sum_j \frac{n_j}{r_{ij}}. \quad (6)$$

For an empty site, for example, it is the energy required to bring an electron from infinity to this site. When averaging this DOS over different realizations of the disorder potential or, in other words, over different samples, we match the chemical potential in them (μ averaging).⁴ The chemical potential of the island is situated halfway between the largest energy of the occupied states and the lowest energy of the empty ones. The corresponding DOS is shown in Fig. 2. The important feature of this DOS is a linear Coulomb gap, which at the small energies crosses over to the hard gap related to the finite size effects.⁴ Linear dependence of the DOS for $|\epsilon| > 0.2$ agrees with the analytical expression for an infinitely large sample

$$g(\epsilon) = \frac{2}{\pi} |\epsilon| \quad (7)$$

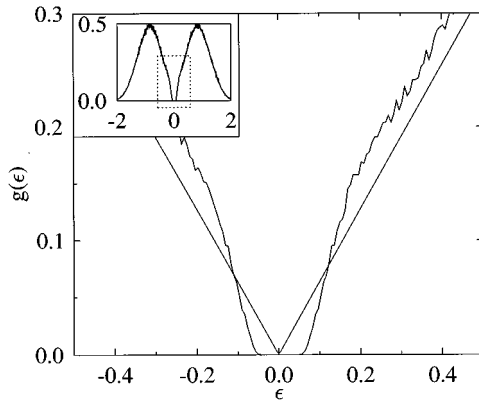


FIG. 2. DOS for the 8×8 sample averaged over disorder. The main picture shows the region near the Fermi level. The Coulomb gap in the density of states for an infinitely large sample [Eq. (7)] is presented by the straight lines. The inset shows the general view of the DOS.

derived in Refs. 6 and 7. The total width of the hard gap is equal to $1/r_{\max}$, where r_{\max} is the maximum distance between two points in the island. Indeed, the energy that is required to transfer an electron from site i to an empty site j is equal to

$$\Delta_{i \rightarrow j} = \epsilon_j - \epsilon_i - \frac{1}{|r_i - r_j|} \geq 0. \quad (8)$$

The minimum difference between the energies of empty and occupied states cannot exceed the minimum interaction energy within the island and hence is greater than or equal to $1/r_{\max}$.

Let us now explain how the one-electron DOS can be used to find $F(x)$. Strictly speaking the one-electron energies are not directly related to the ground-state energies and capacitance. The excitations relevant to capacitance are electronic polarons introduced by Efros.⁶ Their energies $\tilde{\epsilon}_i$ can be used to calculate Δ_N . Indeed, $\tilde{\epsilon}_i$ is defined as the energy required to bring an electron to the site i and rearrange the other electrons in order to reach minimum of the total energy. From this definition it is obvious that the minimum polaron energy of the empty states is $E_{N+1} - E_N$, and the maximum polaron energy of the occupied states is $E_N - E_{N-1}$. It is clear that Δ_N is just the energy gap between these two polaron states. It is known, however, that in two dimensions the polaron energies are very close to the one-electron ones.⁴ This means that Δ_N can be well approximated by the energy difference between the lowest empty and the highest occupied *one-electron* states. This immediately explains the existence of the termination point of $F(x)$: Δ_N cannot be smaller than the smallest interaction between two electrons within the island. Moreover the function $F(x)$ can be related to the one-electron DOS $g(\epsilon)$ in the following way.

As the inverse capacitance of an island is equal to the difference between the lowest empty and the highest occupied states' energies, our problem is to find the distribution function of this difference. The probability $P(\Delta \geq \epsilon)$ to have it bigger or equal than certain value ϵ is equal to the prob-

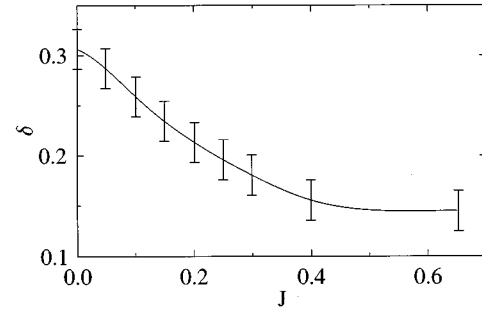


FIG. 3. Relative inverse capacitance fluctuations of 4×4 island as a function of the hopping matrix element J .

ability not to find energy levels in the region $-(\epsilon/2) < \epsilon' < \epsilon/2$. Assuming the Poissonian statistics of the level distribution we arrive at

$$P(\Delta \geq \epsilon) = \exp\left(-M^2 \int_{-(\epsilon/2)}^{\epsilon/2} g(\epsilon') d\epsilon'\right). \quad (9)$$

Here $g(\epsilon)$ is assumed to be normalized to unity: $\int_{-\infty}^{\infty} g(\epsilon') d\epsilon' = 1$. The expression in the exponential is the average number of electrons in the band of energies $[-(\epsilon/2), \epsilon/2]$. The probability density of Δ is, hence, equal to

$$\begin{aligned} F(\epsilon) &= -\frac{dP(\Delta \geq \epsilon)}{d\epsilon} \\ &= 2Ng\left(\frac{\epsilon}{2}\right) \exp\left(-2M^2 \int_0^{\epsilon/2} g(\epsilon') d\epsilon'\right). \end{aligned} \quad (10)$$

This expression establishes the general relationship between the one-electron DOS and the inverse capacitance distribution function for the Coulomb glass island. Having been applied to the numerically obtained DOS it gives a very good agreement with the actual $F(\epsilon)$. Substituting Eq. (7) into Eq. (10) one arrives at the Gaussian asymptotic behavior of $F(x)$: $\ln F(x) \propto -x^2$, $1 \ll x \ll M$. This asymptotic, however, does not persist in three dimensions, where the DOS has a different form.

Let us now examine what happens with δ when a hopping term is added to the classical Hamiltonian, given by Eq. (4):

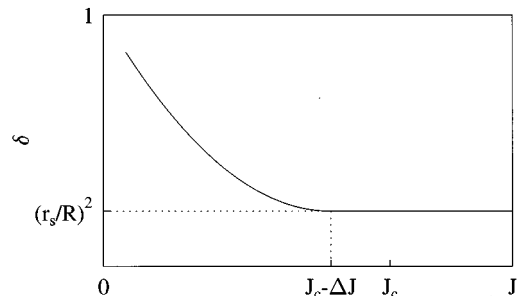


FIG. 4. The relative inverse capacitance fluctuations of the three-dimensional island as given by Eq. (12) for $J < J_c - \Delta J$ and by Eq. (13) for $J > J_c - \Delta J$.

$$H = H_{\text{class}} - J \sum_{\langle i,j \rangle} a_i^\dagger a_j. \quad (11)$$

Here J is the hopping matrix element and a_i^\dagger is the creation operator of the electron at site i . The summation is carried over the neighboring sites. The ground states of this Hamiltonian were found numerically using the Lanczos algorithm. The system considered was of size 4×4 lattice sites, with up to 7, 8, and 9 electrons. The results are depicted in Fig. 3. As it is seen that δ decreases by a factor of 2 from $J=0$ to $J=0.4$. Such a decay is consistent with the tendency of metallic samples to have smaller capacitance fluctuations. At the same time the shape of $F(x)$ becomes more symmetric in agreement with Refs. 2 and 3. Unfortunately we were not able to do such calculations for $M > 4$. Hence the existing numerical data leave open the challenging question of how the crossover happens between $\delta \sim 1$ in the classical case and Eq. (3) in the quantum one for large enough samples. Below we try to answer this question concentrating on the three-dimensional case where the insulator-metal transition happens at some critical value $J = J_c$. We assume that this transition is accompanied by the divergency of the wavefunction correlation length ξ and the dielectric constant κ : $\xi = |J_c - J|^{-\nu}$ and $\kappa = |J_c - J|^{-\zeta}$. It was argued that $\kappa \sim (\xi/r_s)^2$, where r_s is the screening radius of the three-dimensional degenerate Fermi gas, or $\zeta = 2\nu$ (see Ref. 8). When J approaches J_c from the insulator side the growth of κ plays a very important role in the distribution of charge of the added electron, even when ξ is still much smaller than a sample size R . It is well known that if a localized charge is put inside a dielectric sample with $\kappa \gg 1$ the sample becomes polarized in such a way that almost all of the added charge appears on its surface in the form of induced charge. Only a

small fraction of charge e/κ remains localized inside. If the second electron is added to the sample at the distance r from the first the interaction energy between these two consecutively added electrons fluctuates by $e^2/\kappa R \ll e^2/R$, provided that r fluctuates in the range $0 < r < 2R$ for a sphere of radius R . Therefore

$$\delta \sim 1/\kappa \sim (r_s/\xi)^2 \sim (J_c - J)^{2\nu}. \quad (12)$$

Equation (12) is valid only if $\xi \ll R$, or $J < J_c - \Delta J$, where $\Delta J = (r_s/R)^{1/\nu}$. At $\xi = R$ the relative capacitance fluctuations saturate at

$$\delta \sim (r_s/R)^2. \quad (13)$$

Equation (13) is the three-dimensional analog of Eq. (3). It can also be obtained from the assumption that fluctuations of Δ_N are equal to the fluctuations of the spacing between the one-electron quantum levels. Predicted behavior of function $\delta(J)$ is schematically depicted in Fig. 4. We conjecture that in the two-dimensional case, where as it is commonly believed ξ grows monotonically with J , the crossover from $\delta \sim 1$ to Eq. (3) happens in the similar way: $\delta \sim r_s/\xi$ at $r_s \ll \xi \ll R$ and $\delta \sim r_s/R$ at $\xi \gg R$. Schematically this behavior is similar to the one shown in Fig. 4. Our numerical results do not contradict this prediction.

In conclusion, we have found the large universal relative fluctuations of capacitance of the Coulomb-glass island and described a scenario of their decay when the system undergoes the insulator-metal transition.

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