# Charge fluctuations in a Coulomb gap

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(Submitted 5 December 1991)
Zh. Eksp. Teor. Fiz. **102**, 194–200 (July 1992)

Charge fluctuations and the large-scale potential in the ground state of a disordered Coulomb system are studied. A universal law for the growth of charge fluctuations with the dimension is found for $2D$ systems: $q_R \sim R^{1/2}$. The relationship between the charge fluctuations, on the one hand, and the behavior of the density of states in the Coulomb gap and the screening depth for the weak field, on the other, is discussed.

## 1. INTRODUCTION

Much is unclear about the properties of the ground state of a disordered system of localized electrons. Wigner crystallization is disrupted if there is a large spread in the values of the random potential energy, but a correlation remains in the arrangement of the charges. The correlation is a consequence of the long-range nature of the interaction. One familiar manifestation of this correlation is the Coulomb gap in the electron energy distribution.[1] In this paper we examine the effect of an interaction on the bulk charge fluctuations and thus[3] on the large-scale fluctuations of the potential energy. These fluctuations play a fundamental role in problems involving the screening of a weak field, the carrier mobility,[6] a nonohmic conductivity, etc.

We restrict the discussion to $2D$ systems in the simple model proposed in Refs. 2 and 4. We study charge fluctuations as a function of size $R$ by numerical simulation. We find the result

$$q_R \sim R^{0,5}, \tag{1}$$

which is of universal applicability for various spreads in the values of the random potential. We discuss the effect of fluctuations on the screening of a weak external field, and we examine the behavior of the density of states of low-energy excitations.

## 2. NUMERICAL SIMULATION

We consider a simple square lattice with a lattice constant $a$. The occupation numbers $n_i$ take on the values 0 and 1. We say that there is an electron with a charge of $+1/2$ at a site if $n_i = 1$, while there is a hole with a charge of $-1/2$ there if $n_i = 0$. The values of the random potential $\Phi_i$, which creates the disorder in the system, are uncorrelated at the various sites. They are distributed uniformly between $-B/2$ and $+B/2$. The chemical potential is set equal to zero; this choice corresponds to a half filling in the macroscopic limit. The Hamiltonian of the system is

$$H = \sum_i \Phi_i n_i + {}^1/_2 \sum_{i \neq k} (n_i - {}^1/_2)(n_k - {}^1/_2) f_{ik}. \tag{2}$$

The summation is over all lattice sites; $f_{ik}$ is the energy of the Coulomb interaction between sites $i$ and $k$. To avoid effects due to a lowering of the dimensionality at the boundaries of the system, we require that the lattice sites at these boundaries be equivalent to those at the center of the sample. We impose this equivalence by means of periodic boundary conditions.[4] The energy of the Coulomb interaction is then given by $f_{ik} = 1/r_{ik}$, where

$$r_{ik}^2 = \sum_{\beta=1}^{d} (\min\{|x_{\beta i} - x_{\beta k}|, L - |x_{\beta i} - x_{\beta k}|\})^2. \tag{3}$$

The energy of an individual site is given by

$$\varepsilon_i = \Phi_i + \sum_{j \neq i} (n_j - {}^1/_2) f_{ij}. \tag{4}$$

We study the charge fluctuations in two steps. First we use a standard algorithm (discussed below) to determine the ground state of the system. We then make a direct study of the charge fluctuations for a given realization of the random potential. The final result is found by taking an average over a large number of realizations. For $2D$ systems of size $L \times L$ ($L = 20, 30, 40$) described by Hamiltonian (2), we use the procedure proposed in Ref. 5 to seek the ground state. This procedure can be outlined as follows. A random-number generator (with a return period of $1.6 \cdot 10^7$) is used to determine the random field $\Phi_i$. The initial distribution of electrons (or holes) is specified to be either a checkerboard pattern or the pattern

$$n_i^{(0)} = {}^1/_2(1 - \operatorname{sign} \Phi_i). \tag{5}$$

We then descend to the ground state at a fixed chemical potential, taking all the single and double interchanges into account.[5] In certain cases we also consider the interchange of three and four sites in the most compact arrangement (neighboring sites). In this manner we construct a ground state which is stable under the following interchanges:

I. the single interchanges (exchange with the reservoir)

$n_i = 1$, $\Delta H = \mu - \varepsilon_i > 0$,

$n_i = 0$, $\Delta H = \varepsilon_i - \mu > 0$.

II. the double interchanges (a hop within the system)

$$n_i = 1,\ n_j = 0,\ \Delta H = \varepsilon_j - \varepsilon_i - f_{ij} > 0.$$

III. the triple interchanges (a hop and exchange with the reservoir)

$$n_i = n_j = 1,\ n_k = 0\ (i \neq j),$$
$$\Delta H = \varepsilon_k - \varepsilon_i - \varepsilon_j + \mu + f_{ij} - f_{ik} - f_{jk} > 0,$$

$$n_i = 1,\ n_j = n_k = 0\ (j \neq k),$$
$$\Delta H = \varepsilon_j + \varepsilon_k - \varepsilon_i - \mu + f_{jk} - f_{ij} - f_{ik} > 0.$$

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TABLE I. Numerical-simulation data for systems with various values of $L$, $B$, and $K$.

| $B$ | $K$ | $L$ | $N_S$ | $\alpha$ | $C$ | Interchanges considered |
|---|---|---|---|---|---|---|
| 1,0 | 0,5 | 20 | 150 | 0,50±0,02 | 0,53±0,03 | I–IV |
| 1,0 | 0,5 | 30 | 150 | 0,50±0,01 | 0,54±0,03 | I–IV |
| 1,0 | 0,5 | 40 | 300 | 0,50±0,01 | 0,529±0,012 | I–II |
| 1,0 | 0,5 | 40 | 500 | 0,50±0,01 | 0,532±0,009 | I–IV |
| 2,0 | 0,5 | 40 | 150 | 0,50±0,01 | 0,88±0,06 | I–IV |
| 3,0 | 0,5 | 40 | 150 | 0,50±0,02 | 1,12±0,08 | I–IV |
| 4,0 | 0,5 | 40 | 150 | 0,50±0,01 | 1,30±0,16 | I–IV |
| 8,0 | 0,5 | 40 | 150 | 0,50±0,01 | 1,63±0,20 | I–IV |

*Note.* Interchanges I–IV, used in constructing the ground state, are described in Sec. 2 of this paper. The quantity $N_S$ is the number of systems over which the average was calculated.

IV. the quadruple interchanges (two hops)

$$n_i=n_j=1,\ n_k=n_l=0\ \ (i\neq j,\ k\neq l),$$
$$\Delta H=\varepsilon_k+\varepsilon_l-\varepsilon_i-\varepsilon_j+f_{ij}+f_{kl}-f_{ik}-f_{il}-f_{jk}-f_{jl}>0.$$

After the ground state has been constructed, the system is partitioned into nonintersecting squares of size $R\leqslant L$, and the mean square charge fluctuation $q_R{}^2$ is calculated for each square. This procedure was carried out for various values of $B$ and $L$ and for various initial charge distributions. As a result we found the following expression for the mean charge fluctuation as a function of the size of the square:

$$q_R{}^2=CR^{2\alpha}. \tag{6}$$

This expression is equivalent to a linear dependence of $\ln(q_R{}^2)$ on $\ln R$. Table I shows values of $C$ and $\alpha$ for various values of $B$, $K$, and $L$. We see from Fig. 1 that a linear law holds well in the interval $2\leqslant R\leqslant L/2$, while the periodic boundary conditions come into play at $R>L/2$. The value of the charge in the total volume, i.e., that for $R=L$, is close to zero in all cases, apparently because of the periodic boundary conditions. We should also point out that the first term of Hamiltonian (2) plays an important role when $B$ is large and the sizes $R$ are small. As was shown for the case $B=8.0$, the result is a deviation from the law $q_R\propto R^{0.5}$ at small values of $R$. The deviation is toward larger values of $\alpha$. For the case $B=0.5$ we studied the effect of the more complicated interchanges (of types III and IV) on the values of $C$ and $\alpha$. We see from Table I that the incorporation of these interchanges has no noticeable effect.

Using the data in Table I, we plotted $\ln C$ versus $\ln B$. As Fig. 2 shows, this plot is linear and can be described by $C\propto B^{\beta}$, where $\beta\approx 0.63$.

We studied the behavior of the density of states in the case $B=0.5$, $L=40$. We found $g(\varepsilon)\propto\varepsilon^{1.2}$ in the energy interval $0.025<\varepsilon<0.16$, and $g(\varepsilon)\propto\varepsilon^{1.5}$ in the interval $0.16<\varepsilon<0.6$ (Fig. 3). This result supports the data found in Ref. 7. The typical value of the energy at which the behavior of the density of states, $g(\varepsilon)$, changes is

$$\varepsilon_c=0,16\pm 0,02. \tag{7}$$

## 3. EFFECT OF CHARGE FLUCTUATIONS ON THE PROPERTIES OF THE SYSTEM

*A. Density of States.* A numerical analysis of the behavior of the density of states in a Coulomb gap, which we carried out for systems of dimensionality $d=2$, reveals substantial deviations from the Shklovskiĭ–Éfros law $g(\varepsilon)\propto|\varepsilon|$ as $\varepsilon\to 0$. Corresponding deviations were observed in Refs. 4 and 5. Summarizing the results of a recent study[7] of $2D$ systems with a size of $200\times 200$ and our own results for systems with a size of $40\times 40$, we conclude that the density of states behaves in the following way. At $|\varepsilon|>\varepsilon_c$ we have

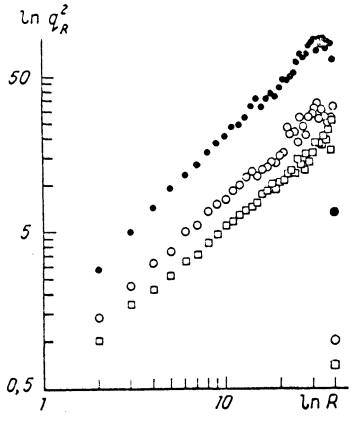


FIG. 1. Charge fluctuations versus the size $R$ in $2D$ systems with $L=40$ and $K=0.5$, for various maximum values of the random potential, $B$. □—$B=1.0$; ○—4.0; ●—8.0

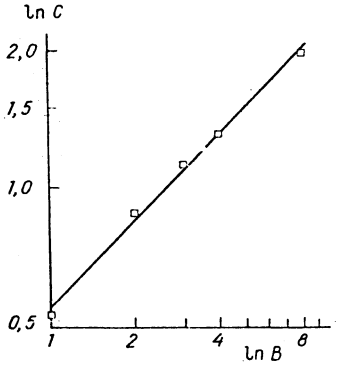


FIG. 2. Relationship between the coefficient $C$ [see (6)] and the maximum value of the random potential, $B$, for systems with $L=40$, with a ground state constructed through the use of interchanges of types I–IV.

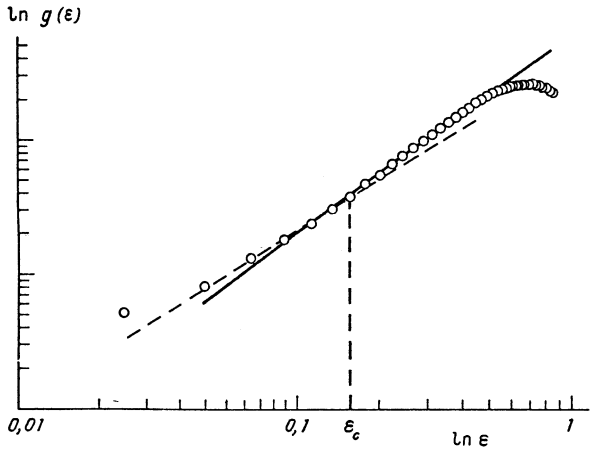


FIG. 3. Density of states versus the energy for system with $L = 40$, $B = 1.0$, and $K = 0.5$, with a ground state constructed through the use of interchanges of types I–IV. The dashed and solid lines are least-squares fits of the points in the energy intervals $0.05 < \varepsilon < 0.16$ and $0.16 < \varepsilon < 0.6$, respectively.

$g(\varepsilon) \propto |\varepsilon|^{1.5}$, while at $|\varepsilon| < \varepsilon_c$ we have $g(\varepsilon) \propto |\varepsilon|^{1.2}$.

A point of fundamental importance is that the values found for $\varepsilon_c$ in Ref. 7 ($\varepsilon_c = 0.08$) and in the present study ($\varepsilon_c = 0.16$) are quite different. We think that the difference stems from a dependence of $\varepsilon_c$ on the dimensions of the system. The existence of a typical value of the charge fluctuation, $q_R$, mandates a new energy scale, $\Delta\varepsilon \sim q_R/R$. A trivial estimate shows that the energies $\varepsilon_c$ for systems with $L = 200$ and with $L = 40$ are the same as the typical minimum energy of large-scale fluctuations, $\Delta\varepsilon_L \sim q_L/L \sim L^{-1/2}$. We would thus expect a relationship between the charge fluctuations and the behavior of the density of states at low energies. We can present some rather crude arguments which reveal the nature of this relationship.

We assume that the density of states has a power-law behavior near the Coulomb gap:

$$g(\varepsilon) \propto |\varepsilon|^{\nu_d} \quad \text{as} \quad |\varepsilon| \to 0. \tag{8}$$

From our standpoint (see also Ref. 3), this behavior stems from large-scale fluctuations of the charge density, whose structure is in turn determined by $g(\varepsilon)$. What is the nature of this interrelationship? We assume that a charge fluctuation $q > 0$ is created in a $d$-dimensional sphere of radius $R$. This fluctuation creates a field $q/r$ outside the sphere. If the energy of a site is in the interval $(-q/r, 0)$, then the energy becomes positive as a result, and the electron leaves this site and goes off to infinity. The probability for such an event is

$$W(r) = \int_{-q/r}^{0} d\varepsilon g(\varepsilon) \sim g(q/r)\, q/r \sim \frac{q^{\nu+1}}{r^{\nu+1}}. \tag{9}$$

Summing this quantity over all sites outside the sphere, we find the total screening charge:

$$q_1 = -\int_{R}^{\infty} dV\, W(r). \tag{10}$$

We assume

$$d - 1 < \nu, \tag{11}$$

An integration in (10) then yields

$$q_1 \sim -q^{\nu+1} R^{d-\nu-1}. \tag{12}$$

We see that a small charge is screened almost not at all, while a very large charge, on the contrary, induces an even larger charge. It is thus clear that for a given radius there exists a characteristic charge

$$q_R \propto R^{\alpha}, \tag{13}$$

which screens itself completely. From (12) we then find

$$\nu = (d-1)/(1-\alpha). \tag{14}$$

This derivation is obviously valid only if the sphere is small in comparison with the dimensions of the system, $L$. The behavior of the density of states should thus change when we pass through the energy $q_L/L$, and this is what is seen in the numerical simulation.

The basic assumption used in deriving (13) is that the screening can be described satisfactorily by introducing induced charges in the one-particle approximation, (9). The effective of spatial correlations of the density of states is ignored in this approach. A spatial variation of the distribution of charges with energies close to zero was observed in Ref. 4. The corresponding variations found in our own calculations are shown in Fig. 4. These factors apparently explain why the estimate of the exponent $\nu = 2$ from (14) and from the value $\alpha = 0.5$ found above is high in comparison with the result of the numerical simulation, $\nu = 1.5$.

*B. Screening of a weak field.* We assume that the system is in an electric field such that the potential difference across the boundaries is small in comparison with the Coulomb gap. In this case the screening of the field $U$ should occur over that length scale $l$ over which the fluctuation in the potential energy, $q_R/R$, is comparable to the scale of the field $U$, i.e., over which the system begins to "feel" the field. We thus find an estimate of the penetration depth:

$$l \sim U^{-1/(1-\alpha)}. \tag{15}$$

We have been unable to test (15) numerically because

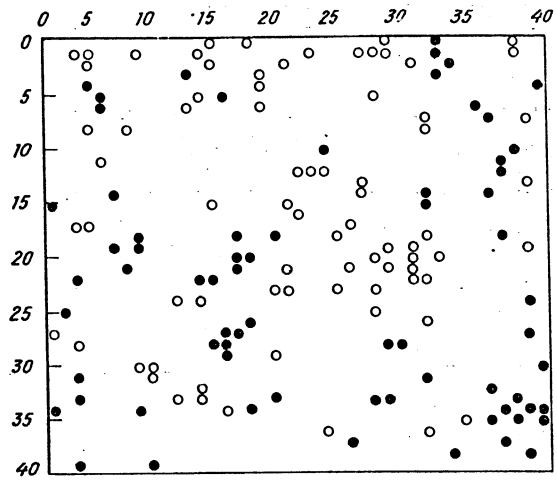


FIG. 4. Spatial distribution of states whose one-particle energies lie in the interval $-0.4 < \varepsilon < 0.4$ in the case of a $2D$ system with $L = 40$, $B = 1.0$, and $K = 0.5$. The ground state of the system was constructed through the use of interchanges I–IV. Filled symbols—cases in which there is an electron at the site; open symbols—cases in where there is a hole at the site.

of the very large dimensions which the system must have in the case of weak fields. Nevertheless, relation (15) can be tested experimentally. The capacitance of a capacitor filled with a highly disordered semiconductor is described by

$$C=\varepsilon S/l, \tag{16}$$

where $\varepsilon$ is the dielectric constant, $S$ is the area of the plates, and $l$ is the field penetration depth. If the potential difference between the plates is small in comparison with the Coulomb gap (which is usually on the order of $10^{-2}$ eV), while it is large in comparison with the temperature, then we would expect that the capacitance would have a field dependence $C \propto U^2$ for the value $\alpha = 0.5$.

## CONCLUSION

We have shown that bulk charge fluctuations can play an important role in a disordered Coulomb system. In $2D$ systems, such fluctuations grow with the dimension in accordance with the universal law $q_R \propto R^{\alpha}$, where $\alpha = 1/2$. The value of $\alpha$ does not change when more-complex excitations are taken into account; it is furthermore independent of the value of $B$. The charge fluctuations mandate a new energy scale $\varepsilon_c \sim L^{-1/2}$, which is manifested in the behavior of the density of states. At $\varepsilon < \varepsilon_c$ the density of states has a behavior $g(\varepsilon) \propto |\varepsilon|^{1.2}$, while at $\varepsilon > \varepsilon_c$ it has a behavior $g(\varepsilon) \propto |\varepsilon|^{1.5}$. Working from the behavior of the charge fluctuations, we have described the screening of a weak field, and we have estimated the screening depth.

We wish to thank A. G. Aronov and Yu. M. Kagan for their interest in this study and for useful discussions, A. Möbius for stimulating discussions, and E. I. Levin, F. G. Pikus, and N. V. Prokof'ev for critical comments.

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Translated by D. Parsons