

Critical Behavior of Density of States in Disordered System with Localized Electrons

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The Coulomb gap in the density of states (DOS) of localized electrons is studied at different magnitudes of an external disorder A . Computer modeling has been done to find the DOS at the chemical potential G_F as a function of temperature and A . At a given filling factor all curves $G_F(T)$ obtained at different values of A and even from different distribution functions of the external disorder cross each other at one temperature T_c . We show that G_F obeys an equation with a fixed point. At this point the subsystem of electrons with energies close to the chemical potential becomes incompressible. A weak singularity of thermodynamic functions at $T = T_c$ is predicted and found by modeling.

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The interest in the Coulomb gap in the single-particle density of states (DOS) of two-dimensional localized electrons has been recently stimulated by observations of a tunneling gap in heterostructures [1] and quantum wells [2]. The problem of the Coulomb gap was originally associated with strongly disordered systems [3–7]. The following classical Hamiltonian has been studied traditionally [8]:

$$H = \sum_i \phi_i n_i + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} (n_i - \nu)(n_j - \nu). \quad (1)$$

The problem is formulated on a lattice, $n_i = 0, 1$ are occupation numbers of lattice sites, and ν is the average occupation number, i.e., the filling factor of the lattice. To make the system neutral, each site has a positive background charge νe . The external disorder is introduced by the set of random energies ϕ_i distributed uniformly within the interval $(-A, A)$.

Efros and Shklovskii [4] have proposed that the density of states $G(\epsilon)$ of the single-particle energies ϵ_i ,

$$\epsilon_i = \phi_i + \sum_{j \neq i} \frac{e^2}{r_{ij}} (n_j - \nu), \quad (2)$$

has a Coulomb gap near the chemical potential E_F . The low-temperature behavior of the DOS around E_F is *universal*: It depends neither on A nor on ν . In this Letter we discuss only two-dimensional systems. In this case, it has been predicted that, at $T = 0$,

$$G(\epsilon) = \frac{2}{\pi e^4} (\epsilon - E_F). \quad (3)$$

Computer simulations [5–8] mostly confirm this result; however, some deviations from the universal behavior have been reported [6,7].

At finite temperatures, the DOS at the chemical potential $G_F \equiv G(E_F)$ becomes nonzero, and it is of the order of T/e^4 . The universality of $G_F(T)$ follows from the universality of $G(\epsilon)$. At $A = 1$ the linear temperature behavior has been checked by a computer modeling in Ref. [9]. The result is that $G_F \approx 1.3T/e^4$. By doing computer modeling in a wide range of A at lower temperatures and at larger arrays than in Ref. [9], we show in this

Letter that G_F does depend on A . Only in the limit $A \rightarrow \infty$ the DOS G_F tends to a universal function $G_\infty(T)$, which is linear in temperature and is independent of A and ν . We have found a critical behavior at some temperature T_c . At this temperature G_F becomes independent of A and coincides with $G_\infty(T_c)$. We argue that there is also a singularity of a chemical potential at this point.

A computer modeling for the 2D case is done using the conventional Monte Carlo method with the Hamiltonian equation (1) on a square lattice with quasiperiodic boundary conditions (for details see Ref. [9]). Only the results for the DOS at the chemical potential $G_F \equiv G(E_F)$ are discussed here.

It has been shown [10] that the Coulomb gap exists also without any external disorder. In this case the system is ordered at $T = 0$. However, this ordered phase melts at a very low temperature, and an internal disorder provides a soft gap near E_F . We have proposed [11] the gap at $A = 0$ as an explanation of the gap in the tunneling density of states observed by Eisenstein, Pfeiffer, and West [2]. However, the DOS at the chemical potential G_F as a function of temperature has never been studied before in detail.

Our calculations show (see Fig. 1) that in a wide temperature range and at three different filling factors the DOS at the chemical potential G_F at $A = 0$ obeys the equation

$$G_0 \equiv G_F(A = 0) = 0.85 \exp \left\{ -0.3 \frac{e^2 [\nu(1 - \nu)]^{1/2}}{T} \right\}, \quad (4)$$

where lattice constant is of unit length. The physical reason for this law is as follows. Every electron pushes out other electrons creating a polarization around itself. Thus, all occupied sites are shifted down in the energy with respect to vacant sites. This is a kind of a polaron shift due to the other electrons. That is why the DOS consists of two peaks with the chemical potential between them. The states near the chemical potential appear as a result of thermal fluctuations destroying the polaron clouds around some sites. The probability of such fluctuation is propor-

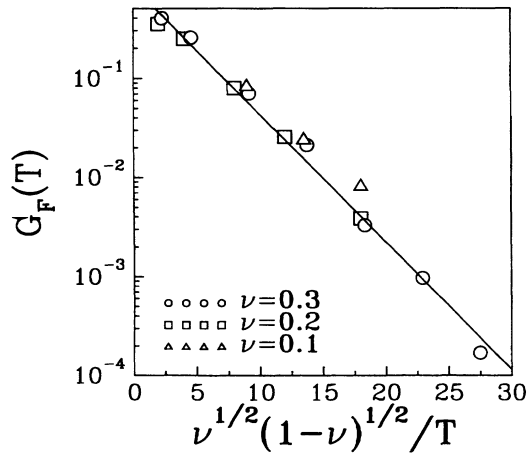


FIG. 1. DOS at the chemical potential vs temperature for $A = 0$ and different filling factors as obtained by computer modeling with $s = \infty$ and at system size 300×300 . The solid line shows the fit, given by Eq. (4).

tional to $\exp(-R_{\min}/T)$, where R_{\min} is a minimum work to create such fluctuation. Because of electron-hole symmetry of the Hamiltonian this work is of the order of $[\nu(1-\nu)]^{1/2}$ in the units of interaction between the nearest neighbors. This is an interpretation of Eq. (4). It differs essentially from the explanation of the Coulomb gap at large disorder. In the latter case the interaction between low energy excitations provides the upper boundary for the DOS. It follows from this Letter that at $A = 0$ the interaction between polarons also becomes important when the average distance between them is of the order of e^2/T .

One can see that there is a dramatic difference in low-temperature behavior of the DOS at the chemical potential with and without the external disorder. The exponential dependence of the DOS at $A = 0$ transforms with increasing A into a linear one. In order to study a crossover between these two regimes one must compute G_F down to very low temperatures. However, such calculations are hampered by a strong size effect. To reduce it we screen the long-range part of the Coulomb interaction by introducing a second metallic plane, parallel to the layer with electrons, at a distance s from it. Then the interaction potential between two electrons has the form

$$V(r) = e^2 \left[\frac{1}{r} - \frac{1}{\sqrt{r^2 + 4s^2}} \right]. \quad (5)$$

At large distances $V(r)$ looks like a dipole potential, and G_F now tends to some finite value as T goes to zero. The DOS for such interaction was calculated by Mogilyanskii and Raikh [12] using a generalized self-consistent equation. Their result for the DOS at the chemical potential reads

$$G_{\infty}(T, s) = \frac{0.085}{e^2 s} + \frac{0.86T}{e^4}. \quad (6)$$

We show here that this expression is a good approximation for the limit of G_F at $A \rightarrow \infty$.

For computer modeling we used $s = 3$ and $s = 5$ in units of the lattice constant. These large values do not change DOS substantially anywhere except the close vicinity of E_F , but eliminate the size effect. The simulation shows that the behavior of G_F at zero disorder is not changed qualitatively by the screening, only the numerical coefficients in Eq. (4) slightly depend on s . Therefore, at finite s , the transition from zero to large disorder manifests itself as a transition from zero to finite G_F at $T = 0$.

The results of the computer simulation for the DOS at the chemical potential G_F as a function of T are shown in Figs. 2(a)–2(d) at different values of A , s , and ν . The DOS G_F changes with A within the interval limited by the function G_0 at small A and by the function G_{∞} at large A . One can see that universality of G_F with respect to A and ν appears only in the limit of large A , where G_F is close to Eq. (6). At finite A the DOS is not universal.

The most interesting feature of Fig. 2 is that all curves cross each other at the same temperature $T_c \approx 0.04$. Both T_c and $G_F(T_c)$ depend on s at large s very slightly, and, obviously, tend to some universal constants as $s \rightarrow \infty$. To make this picture even more general we change the rectangular distribution of random energies ϕ in the interval $(-A, A)$ to a Gaussian distribution with mean square fluctuation equal to A . One can see from Fig. 2(d) that this changes neither T_c nor DOS at $T = T_c$.

We propose the following one-parametric scaling theory to explain this very nontrivial property. The main

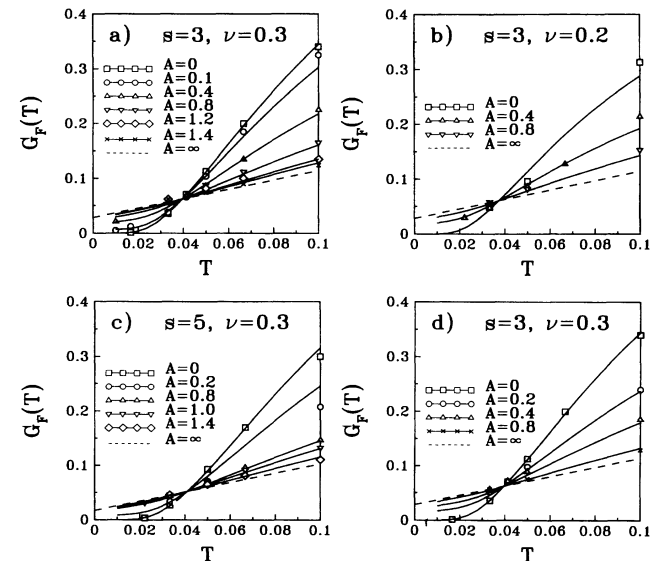


FIG. 2. DOS at the chemical potential G_F vs temperature for different A . The symbols show the results of computer modeling at system size 100×100 , the solid lines are plotted using Eq. (11), and the dashed lines show G_{∞} as obtained from Eq. (6). Plots (a)–(c) are for rectangular distribution ϕ_i , and plot (d) is for Gaussian distribution. Parameter A_0 in Eq. (11) is chosen to give the best fit. It is 0.5 for rectangular distribution and 0.32 for Gaussian.

concept in the theory of the Coulomb gap [4] is that the DOS in the energy interval of the order of T near the chemical potential E_F is determined by the interaction of electrons inside this interval only. Let us consider the electronic states within the energy interval of order T near E_F as a subsystem with a strong internal correlation and assume a weak correlation of these states with the other parts of the system. This subsystem is characterized by an electron density $n = G_F T$ and the temperature T . Now we assume an infinite s and the Coulomb interaction only. The only dimensionless parameter which determines the interaction inside the subsystem is the ratio of the interaction energy between electrons of the subsystem $e^2 n^{1/2}$ to the thermal energy T . This ratio is proportional to $\sqrt{G_F/G_\infty}$. The correlation energy of the subsystem depends on A through G_F only. To check directly this important assumption we have calculated the correlation function of occupied and empty sites within the energy interval of the order of T near E_F at $A = 0$ and $A = 1$, and we have shown that they perfectly scale into each other in units G_F [13].

The subsystem is in thermodynamic equilibrium with the rest of the system. Thus, the chemical potential μ of the subsystem is equal to E_F . However, μ can also be found through the total energy of the subsystem. Then, it will be a function of G_F , T , and the total electron density N . The dependence on N appears because in coordinate space the subsystem is dissolved in a total system. Then, μ contains the ratio of numbers of solute atoms and solvent atoms $G_F T/N$. However, μ depends on A through G_F only.

Differentiating the condition $E_F = \mu(G_F, T, N)$ with respect to A , one gets

$$\frac{\partial E_F}{\partial A} = \frac{\partial \mu}{\partial G_F} \frac{\partial G_F}{\partial A}, \quad (7)$$

where all derivatives are taken at constant T and N . From this equation we get

$$\frac{\partial G_F}{\partial A} = \left(\frac{\partial E_F}{\partial A} \right) f(G_F), \quad (8)$$

where

$$f(G_F) = \left(\frac{\partial \mu}{\partial G_F} \right)^{-1}. \quad (9)$$

The derivative $\partial E_F/\partial A$ is a smooth function of A which tends to a constant value as $A \rightarrow \infty$. Since $G_F \rightarrow G_\infty$ as $A \rightarrow \infty$, it follows from Eq. (8) that $f(G_\infty) = 0$. Thus, $G_F = G_\infty$ is a fixed point for Eq. (8). At all values of A the curves $G_F(T)$ cross the function $G_\infty(T)$ at the same temperature $T = T_c$ because, if $G_F = G_\infty$, the derivative $\partial G_F/\partial A = 0$. This explains the results shown in Fig. 2.

We assumed before that $s = \infty$ and the interaction is e^2/r . This is not an important limitation unless e^2/s is much less than the width of the Coulomb gap. Otherwise G_F depends on A even at large A [13] and, therefore, the fixed point disappears.

Near the fixed point Eq. (8) can be written in the form

$$\frac{\partial G_F}{\partial A} = -\frac{G_F - G_\infty}{A_0}. \quad (10)$$

Assuming that this expansion works in a wide range of A and T with a constant value of A_0 , we get

$$G_F(T) = G_\infty(T) \left[1 - \exp\left(-\frac{A}{A_0}\right) \right] + G_0(T) \exp\left(-\frac{A}{A_0}\right). \quad (11)$$

Here G_0 and G_∞ are given by Eqs. (4) and (6). Equation (11) should be considered as an extrapolation, but it fits well the results of computer simulation shown in Fig. 2. The value of A_0 is approximately 0.5 for a rectangular distribution of random energies ϕ_i and $A_0 \approx 0.32$ for a Gaussian distribution. The unit of A_0 is the interaction energy between nearest neighbors.

Since $G_F T$ is the electron density of the subsystem, we obtain from Eq. (9) that the compressibility of the subsystem $(\partial \mu/\partial n)^{-1} = T(\partial \mu/\partial G_F)^{-1}$ becomes zero at $G_F = G_\infty$. The reason is that at $T = T_c$ the state of the subsystem at any A is the same as at $A = \infty$. In this state the DOS G_F is described by Eq. (6), it is universal, and it cannot be changed by any change of A or ν . One can show that at $\nu < 0.5$ the derivative $\partial E_F/\partial A < 0$. Then it follows from Eqs. (7)–(10) that the compressibility of the subsystem is positive at $T > T_c$, when $G_F > G_\infty$ and negative otherwise. Zero compressibility means that the chemical potential μ has a singularity at $G_F = G_\infty$. Thus, on a diagram $G_F(T, A)$ the plane $G_F = G_\infty(T)$ separates the states with positive and negative compressibility of the subsystem. Figure 2 shows that one cannot cross this plane by changing A . However, at any value of A one can cross it by changing T over the point $T = T_c$. The incompressible state must provide the singularity of thermodynamic functions of the subsystem in this point. The contribution of this singularity to the thermodynamics of the total system should be small as the ratio of the electron density in the subsystem to the total density at $T = T_c$. The subsystem density is $G_F(T_c)T_c$. At $\nu = 0.3$ and $s = 3$ this product is about 2.8×10^{-3} per lattice site. Thus, in our case this is at least 100 times smaller than the total density ν .

To check this conclusion we have performed a calculation of the chemical potential of the system $E_F(T)$ near T_c . One can show that the occupation of a site with energy ϵ is described by the Fermi function [11]. Thus, E_F has been found as an energy where the DOS of occupied and empty states are equal to each other. Our results at $A = 0.4$ are shown in Fig. 3. We have averaged E_F through six different sets of ϕ with array size 100×100 . Without a singularity one should expect $E_F(T) = E_F(0) \{1 + \text{const} \times [T/E_F(0)]^2\}$ dependence at $T \ll E_F(0)$. We see instead a maximum at $T = T_c$ in the scale corresponding to the above estimate.

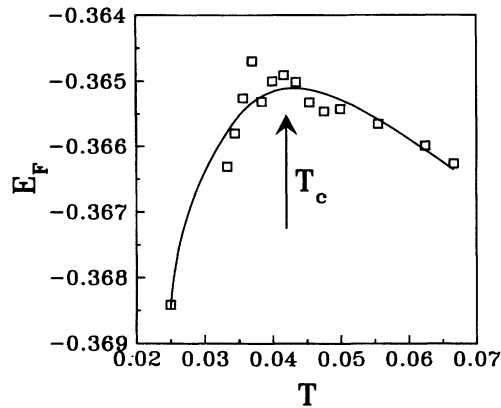


FIG. 3. Chemical potential E_F vs temperature as obtained by computer modeling at $A = 0.4$, $s = 3$, and $\nu = 0.3$. The results are averaged over six sets of ϕ with array size 100×100 . Solid line is a guide for the eye.

Finally, we have found that the universal linear temperature dependence of G_F is valid only in the limit of large A , where it fits the solution of the self-consistent equation. The new equation for G_F has been proposed which has a fixed point at $T = T_c$. This equation explains the unusual behavior of $G_F(T, A)$ and a singularity of E_F at $T = T_c$.

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