

Coulomb Gap and Transport in Classical Electron Liquid

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The lattice model of a classical electron liquid with the Coulomb interaction and zero kinetic energy is considered. It is shown by both qualitative arguments and computer modeling that in this system the Coulomb gap exists near the chemical potential. Arguments are given that this is true for the nonideal quantum liquid as well. Nearest-neighbor hopping conductivity is studied at $d=2$. At low temperatures, the conductivity mechanism is shown to be a many-electron diffusion. At very small *external* disorder, the crossover from the diffusion to percolation has been found.

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In recent years many efforts have been made to study an interacting electron gas in attempts to obtain a phononless mechanism for superconductivity. The starting point in this field is usually the Hubbard model. I demonstrate here an important role of the long-range Coulomb interaction. Namely, I argue that in an electron liquid *without any external disorder* the same Coulomb gap exists as in a disordered system, and that the long-range interaction strongly affects the transport.

The Hamiltonian of the spinless fermions, which is the subject of the final discussion, is

$$H = \sum_{i,j} J_{ij} a_i^\dagger a_j + \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} (n_i - 1 + K)(n_j - 1 + K). \quad (1)$$

We are considering the very nonideal case, when the interaction is much larger than the overlap energy J_{ij} . Here $n_i=0,1$ are the occupation numbers. The average occupation number or the number of electrons per site is $1-K$, where $0 < K < 1$. The charge of the electrons is e . The system is neutral, because each site has a positive charge $(1-K)e$. Thus, the total charge of a site is $(1-K)e$ if $n_i=0$ and $-Ke$ if $n_i=1$. This is a lattice problem, but the lattice properties are minimized if $1-K \ll 1$.

At low enough temperatures and at small J_{ij} the system has an ordered distribution of the occupied sites. It is well known that the melting temperature is more than 100 times smaller than the characteristic energy of the electron-electron interaction for $d=2$ and $d=3$ [1,2]. Thus, the liquid remains strongly nonideal in a large range of temperatures.

The aim of this paper is to study the properties of the liquid well above the melting temperature but still in a very nonideal regime. We consider here the case when the temperature is much larger than the overlap energy, and give some arguments about the opposite case. If $T \gg J_{ij}$, the thermodynamic properties of the system can be studied, completely ignoring the overlap. Then, one obtains a still nontrivial Hamiltonian of the classical charged liquid:

$$H_{cl} = \frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}} (n_i - 1 + K)(n_j - 1 + K). \quad (2)$$

The Coulomb gap in disordered systems has been stud-

ied using a classical Hamiltonian [3]:

$$H = \sum_i \phi_i n_i + H_{cl}, \quad (3)$$

where the external disorder is introduced by the set of energies ϕ_i randomly distributed within the interval $(-A, A)$. It has been shown that the density of states (DS) $G(\epsilon)$ of the one-particle energies

$$\epsilon_i = \phi_i + \sum_{j \neq i} \frac{e^2}{r_{ij}} (n_j - 1 + K) \quad (4)$$

has a Coulomb gap near the chemical potential E_F with universal behavior around this point. In the two-dimensional case it has the form

$$G(\epsilon) = (2/\pi e^4) |\epsilon - E_F|. \quad (5)$$

I think the same gap exists in the system with an internal disorder only ($A=0$). If a temperature is, say, twice as large as the melting temperature, the correlation length of the electron liquid should be of the order of the average distance between electrons. In a liquid state a potential coming from distances which are larger than the correlation length can be considered as random. It is very weakly correlated with the occupation number of the site i . This random part of the potential in a liquid state can be considered as the random energies ϕ_i in Eq. (3). This is why I believe that the DS in such a liquid state has a Coulomb gap of the same nature as in an externally disordered system.

To support this point I have performed a computer modeling of the system with the Hamiltonian (2), using the Monte Carlo method. The program is basically the same as we have used [4] for the Hamiltonian (3). At first, electrons are randomly distributed on the lattice. Then different electron transitions are performed with the probability corresponding to the Gibbs ensemble at a given T until the system comes to equilibrium. The time average of the DS is calculated. Square and cubic arrays have been considered with periodic boundary conditions. A low-temperature run takes about an hour on a CRAY Y-MP8/864.

Figure 1 shows the DS at $K=0.8$ for different temperatures. The array size L is in units of the lattice constant l ; energy and temperature are in units of e^2/l . The

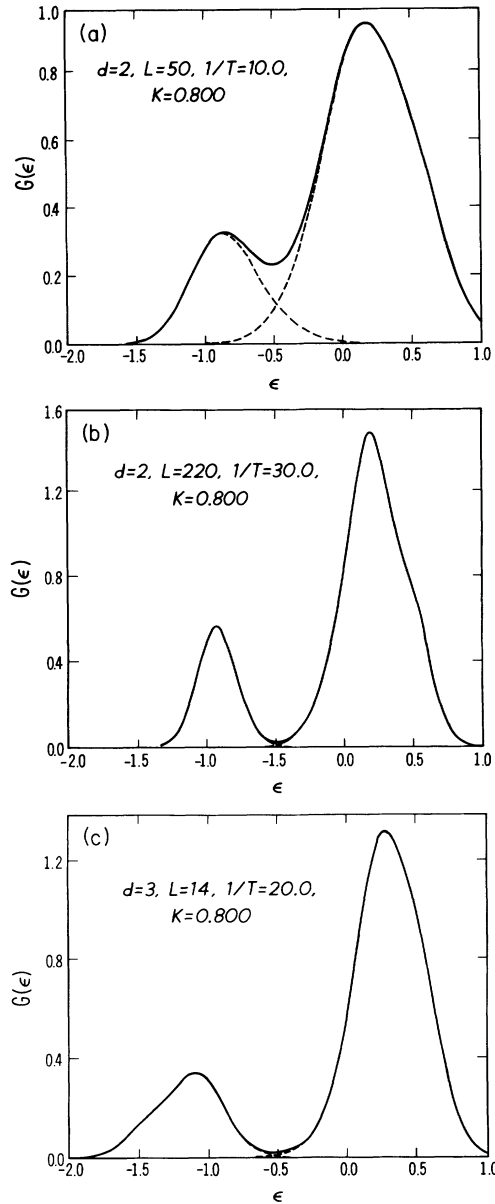


FIG. 1. DS of (a),(b) 2D and (c) 3D arrays as a function of energy as obtained by computer modeling at different temperatures at $K=0.8$. L is a linear size of a square array in units of a lattice constant l . Energy and temperature are in units of e^2/l . Dashed lines show separately the DS of occupied and vacant sites.

dashed lines show the DS of occupied and vacant sites separately so that their sum is equal to the total DS. The low-energy peak corresponds to the occupied sites. The chemical potential E_F is located at the intersection of the dashed lines.

A strong size effect has been found at low temperatures near E_F . In the 2D case the dimensionless ratio $g = \pi G(E_F)/2T$, taken at $T=0.05$, is about 1 at $L=10$, about 2 at $L=20$, and it tends to 2.5 at large L . The values of L for the 2D data in Fig. 1 are chosen to be

large enough for a given temperature, so that the data are almost size independent. Note that the same size effect is typical for the Coulomb gap with an external disorder. In that case the low-temperature limit of g at large L has been found to be about 2 (see Ref. [4]).

The following features confirm that the observed gap near the chemical potential is of the same nature as the Coulomb gap in the disordered system studied before: (i) pronounced minimum of the DS at the chemical potential E_F ; (ii) sharp temperature dependence of the DS in the vicinity of E_F at very low temperatures, while the peak positions are temperature independent; (iii) strong size effect in the same energy range, which is the result of the long-range interaction and of the failure of the screening.

An important aspect of the system without external disorder is that we are restricted to the temperatures well above the melting temperature. But we are also restricted by the smearing of the Coulomb gap around E_F due to the temperature. This double restriction makes it difficult to find a universal law similar to (5).

A modeling of the phonon-assisted hopping conduction in this system has also been performed. It has been assumed that the probability of an electron transition from an occupied site i to an empty site j has the form

$$\gamma_{ij} = \gamma_0 \exp(-\Delta_{ij}/T), \quad (6)$$

where Δ_{ij} is the work to transfer an electron from i to j if this work is positive, and zero otherwise. The tunneling probability γ_0 comes from the overlap and it is supposed to be nonzero for nearest neighbors only. A homogeneous electric field E has been applied in the x direction, so that Δ_{ij} has an extra term eEx_{ij} . Periodic boundary conditions have been used so that an electron leaves the sample, say, through the left boundary and appears simultaneously at the right boundary. The conductivity has been calculated as an electric current in the x direction divided by E . It is found to be approximately Ohmic at $E \leq 0.3T/el$. Only the two-dimensional case is discussed below.

The program of modeling was the same as in Ref. [4] where the Hamiltonian (3) has been considered. However, the results are drastically different.

In the case of external disorder the hopping conductivity is a percolation process. For the nearest-neighbor hops it has an activation energy of the order of half the separation between peaks of the DS. Without external disorder the 2D conductivity has been found to *increase* with decreasing temperature and *it becomes temperature independent* in a wide temperature interval (Figs. 2 and 3). At $K=0.8, 0.82$ there is also a small drop at very low temperatures. I argue below that this is a result of a proximity to the ordering. Besides, it is shown here that a random walk approximation (RWA) describes conductivity very well in all temperature ranges (excluding the low-temperature drop). Thus, it is a diffusion rather than a percolation process.

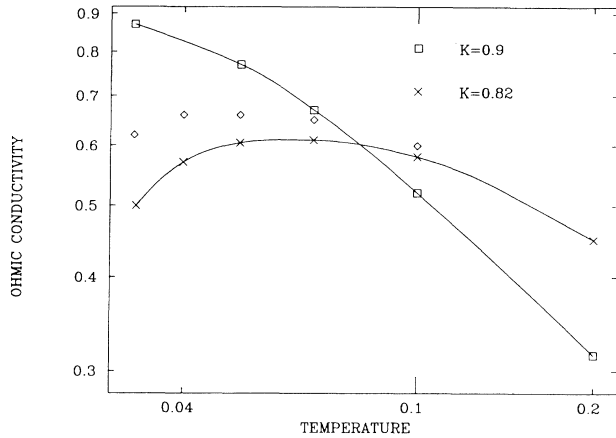


FIG. 2. Ohmic conductivity (in units $\gamma_0 l$) as obtained by computer modeling as a function of temperature at $K=0.9$ (squares) and $K=0.82$ (crosses). The diamonds show the conductivity at $K=0.82$ as calculated from the RWA [Eq. (7)] with function $F(r_{ij})$ obtained by computer modeling at $E=0$. The diamonds are only in those points where an essential difference between two approaches has been found. At $K=0.9$ it has not been found.

In the 2D case the conductivity in the RWA has the form [4]

$$\sigma = \frac{\gamma_0 e^2}{8 T l^2} \sum_j F(r_{ij}) r_{ij}^2, \quad (7)$$

where $F(r_{ij})$ is the probability of the transition $i \leftrightarrow j$ at zero electric field, and the sum includes only the four nearest neighbors on a square lattice. The conductivity has been calculated independently from Eq. (7) using $F(r_{ij})$ as obtained from computer modeling at zero electric field. The results are shown in Figs. 2 and 3. At $K=0.9$ no reliable difference has been found in the conductivity as obtained by the current calculation and by the RWA. At $K=0.8, 0.82$ one can see the difference at low temperatures, but it is not very large.

It is obvious that the RWA must work if the temperature is much larger than the energy distance between the peaks of the DS. Then $F = 2K(1-K)$ and

$$\sigma = \gamma_0 e^2 K(1-K)/T. \quad (8)$$

This explains the high-temperature behavior. Equation (8) was used to test the program.

To explain the low-temperature results the following mechanism is proposed. At $1-K \ll 1$ the energy difference between neighboring sites is typically of the order of $W = (e^2/l)(1-K)^{3/2}$, because electrons are located close to the minimum of the potential energy. Because of the Coulomb field of other moving electrons this difference fluctuates and sometimes it is very small. Electrons hop in the moments of "fair weather," when the difference is not larger than a few T . These occur with a probability of the order of T/W . Substituting $F \approx T/W$

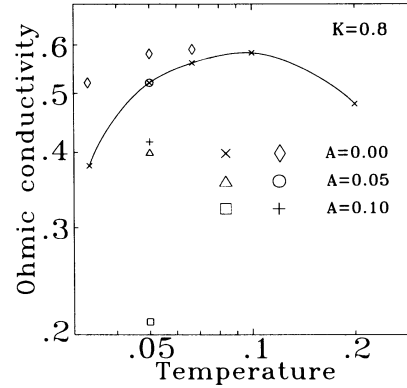


FIG. 3. The same as in Fig. 2 at $K=0.8$. At $T=0.05$ the conductivity with an external disorder ($A > 0$) has been calculated. The signs \diamond , \circ , and $+$ stand for the RWA.

into Eq. (7), one gets that conductivity is independent of T . This mechanism is a many-electron diffusion.

The low-temperature value of the conductivity at $K=0.9$ is larger than at $K=0.82$ (see Fig. 2). This is not trivial because the carrier concentration at $K=0.82$ is nearly twice as large. But it can be understood in terms of the above mechanism. A simple scaling law gives the low-temperature concentration dependence. The conductivity depends on the temperature through a factor T/W only. Then it can be written as a product of two unknown functions:

$$\sigma = q(1-K)f(T/W), \quad (9)$$

where $q(1-K)$ is independent of T , and f depends on $1-K$ only through W . It follows from Eq. (8) that $f(x) \sim 1/x$ at $x \gg 1$ and that $q \sim 1/\sqrt{1-K}$. To provide the low-temperature saturation of the conductivity, $f(x)$ should be constant at small x . Thus, we get that the low-temperature conductivity is proportional to $1/\sqrt{1-K}$, in good agreement with the computer results.

Equation (7) is valid if each hop is independent of the previous one. A simple estimate shows that the fair weather deteriorates with high probability before the electron can hop back. This is because the electron "pulses" its neighbors, and their potentials change "the weather." However, this is not enough to provide the diffusion in the ordered phase or in an externally disordered system, where electrons "walk" around the equilibrium positions only.

I suggest that the low-temperature drop of the conductivity and deviation from the RWA at $K=0.8, 0.82$ (see Figs. 2 and 3) is a result of proximity to the ordering. The deviation is larger at $K=0.8$ because at this density the ordered phase is a square lattice, and the melting temperature should be larger than at $K=0.82$. At $K=0.9$ this temperature is $\approx \sqrt{2}$ times smaller than at $K=0.8$ due to lower density.

The crossover from a diffusion to a percolation process

with an increase of an external disorder is also studied here. Pollak and Ortuno (see review [5]) have argued that the electron-electron interaction prevents using the percolation approach in the theory of hopping conduction in disordered systems. It is shown here that this is the case for internal disorder only. In fact, the novel diffusion conductivity is pinned by a very small external disorder. The same computation has been performed using Hamiltonian (3) with very small A . The results are shown in Fig. 3. At $T=0.05$ a dramatic decrease of the conductivity with increasing A has been observed at $A=0.05, 0.1$. The RWA yields results very far above the data obtained by current calculations. The temperature dependence has not been studied yet, but the data suggest that an activation energy appears proportional to A . At such a small A one cannot see any changes in the DS. Thus, the random potential essentially does not change its magnitude. The data show that pinning of soft modes with energy of the order T appears when $A \approx T$. This means that in the presence of an external disorder the fair weather is permanent in some parts of the lattice and it never occurs in the others. Thus, an external disorder prevents soft modes from participating in the dc conductivity, and the dc transport mechanism becomes a percolation process.

To summarize, the following results have been obtained.

The Coulomb gap is shown to exist in a classical liquid above the melting temperature. At $|\epsilon - E_F| \gg T$ the DS is independent of T and is characteristic of the ground state of the system. Coming back to Hamiltonian (1), one can predict that the same gap exists in a liquid state at $T=0$ if an overlap is the cause of a melting, provided

it is still much smaller than the interaction. The overlap determines the DS near E_F in this case, but far from this point the DS can be obtained from the same classical Hamiltonian (2). An important manifestation of the Coulomb gap is the drop of the tunneling current at zero bias.

The effect of many-electron diffusion has been found, and the crossover from diffusion to percolation has been studied. This may also be important for the diffusion of interacting impurities on the lattice [6].

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