01 Nov 1998

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Recommended Citation

T. Vojta et al., "Do Interactions Increase or Reduce the Conductance of Disordered Electrons? It Depends!," *Physical Review Letters*, vol. 81, no. 19, pp. 4212-4215, American Physical Society (APS), Nov 1998.
The definitive version is available at https://doi.org/10.1103/PhysRevLett.81.4212

Do Interactions Increase or Reduce the Conductance of Disordered Electrons? It Depends!

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(Received 16 June 1998)

We investigate the influence of electron-electron interactions on the conductance of two-dimensional disordered spinless electrons. We present an efficient numerical method based on diagonalization in a truncated basis of Hartree-Fock states to determine with high accuracy the low-energy properties in the entire parameter space. We find that weak interactions *increase* the dc conductance in the strongly localized regime while they *decrease* the dc conductance for weak disorder. Strong interactions always decrease the conductance. We also study the localization of single-particle excitations at the Fermi energy which turns out to be only weakly influenced by the interactions. [S0031-9007(98)07553-X]

PACS numbers: 72.15.Rn, 71.30.+h, 71.55.Jv

The influence of electron-electron interactions on the transport in disordered electronic systems has been investigated intensively within the past two decades [1,2]. Recently, the problem has reattracted a lot of attention after experimental [3] and theoretical [4] results challenged established opinions.

It is well accepted [5] that noninteracting electrons in three dimensions (3D) undergo a localization-delocalization transition at finite disorder. In contrast, all states are localized in 2D and 1D even for infinitesimal weak disorder [6]. However, today it is believed that the metal-insulator transition (MIT) in most experimental systems cannot be explained based on noninteracting electrons. The metallic phase of disordered interacting electrons has been studied intensively within the perturbative renormalization group (RG) [2], leading to a qualitative analysis of the MIT and the identification of different universality classes. One of the results is that the lower critical dimension of the MIT is $d_c^- = 2$ as it is for noninteracting electrons. Therefore it came as a surprise when experiments [3] on Si-MOSFETs revealed indications of a MIT in 2D. Since these experiments are performed at low electron density where the Coulomb interaction is particularly strong compared to the Fermi energy, interaction effects are a likely reason for this MIT. A complete understanding has, however, not yet been obtained. Explanations were suggested based on the perturbative RG [7], nonperturbative effects [8], or the transition being a superconductor-insulator transition rather than a MIT [9].

Theoretically, surprising results have been obtained for just two interacting particles in the *insulating* regime [4]. It was found that two particles can form a pair whose localization length is much larger than that of a single particle. Later an even larger delocalization was suggested for clusters of three or more particles [10]. In the case of a repulsive electron-electron, these delocalized states have rather high energy; thus their relevance for the low-energy properties of a degenerate system is not clear. It has been argued that the many-particle problem can be reduced to a few interacting quasiparticles above the Fermi surface [11]. This is, however, only possible if the interactions do not change the nature of the ground state. All in all, not even the qualitative influence of interactions is understood in the insulating regime.

We have numerically studied disordered 2D spinless electrons. Our calculations are summarized in Fig. 1 which is the main result of this Letter. It shows that the influence of repulsive electron-electron interactions on the dc conductance is opposite for high and low kinetic energies (i.e., weak vs strong disorder). The conductance of strongly localized samples ($t = 0.01$ to 0.03) is considerably enhanced by a weak interaction. With increasing kinetic energy the relative enhancement decreases as does the interaction range where the enhancement occurs. The conductance of samples with the highest kinetic energies ($t = 0.3$ and 0.5) is reduced even by weak interactions. In contrast, sufficiently strong interactions always reduce the conductance. This is not surprising since, for large enough interaction strength, the system will form a Wigner glass.

These findings shed some light on seemingly contradicting numerical results on the transport of disordered spinless electrons in the literature. Studies [12] of a 2D

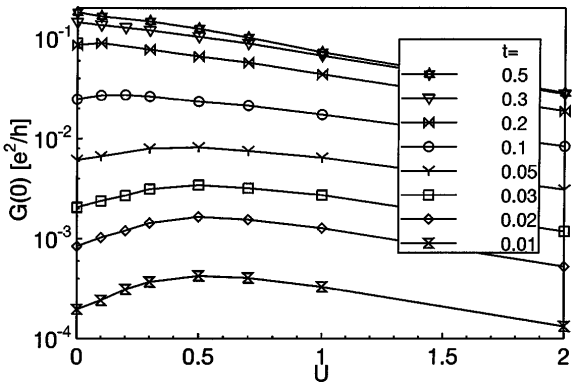

FIG. 1. dc conductance $G(0)$ for a system of 5^2 sites as a function of interaction strength U for different kinetic energies t. The disorder is fixed at $W = 1$. The statistical accuracy is better than the symbol size.

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model in the *diffusive* regime yielded that interactions decrease the conductance. The same conclusion was drawn from density-matrix RG studies [13] and exact diagonalizations [14] in 1D. In contrast, for 2D models in the *localized* regime [15,16], it was found that interactions lead to a delocalization. Up to now, it has been unclear whether these inconsistent results are due to being in different parameter regions (weak vs strong disorder), different quantities studied (conductance, many-particle level statistics, or charge stiffness), or long-range vs short-range interactions. The results of this Letter suggest that being in different parameter regions is the most likely reason for the differences between the results cited above. A result similar to ours was obtained recently [17] in a study of the ground state phase sensitivity in 1D. It was found that, for small disorder, repulsive (nearest-neighbor) interactions reduce the phase sensitivity while, for large disorder, the phase sensitivity shows pronounced peaks at certain values of the interaction.

In the remainder of the Letter we explain the model and the calculational method and further discuss the results. We consider a 2D quantum Coulomb glass model [15,16,18,19]. It is defined on a square lattice with $M = L^2$ sites occupied by $N = KM$ spinless electrons ($0 < K < 1$). To ensure charge neutrality each site carries a compensating charge of Ke. The Hamiltonian reads

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i \varphi_i n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K) U_{ij}, \qquad (1)$$

where $c_i^\dagger$ and c_i are the creation and annihilation operators at site i, $n_i = c_i^\dagger c_i$, and $\langle ij \rangle$ denotes all pairs of nearest neighbors. $U_{ij} = e^2/r_{ij}$ represents the Coulomb interaction which is parametrized by its nearest-neighbor value U and t is the kinetic energy. The random potential values φ_i are chosen from a box distribution of width $2W$ and zero mean. (We always set $W = 1$.) Two important limiting cases of the quantum Coulomb glass are the Anderson model of localization (for $U = 0$) and the classical Coulomb glass (for $t = 0$).

The numerical simulation of disordered many-particle systems is one of the most complicated problems in computational physics. First, the size of the Hilbert space grows exponentially with the system size, making exact diagonalizations of the Hamiltonian impossible already for very small systems. Second, the presence of disorder requires the simulation of many different samples to obtain averages or distributions of physical quantities. For disordered interacting electrons the problem is made worse by the long range of the Coulomb interaction which has to be retained for a correct description of the insulating phase where screening breaks down.

In this Letter we suggest an efficient numerical method to simulate disordered interacting electrons. It is based on the idea of configuration interaction [20] adapted to disordered lattice models. The method, which we call the Hartree-Fock-based diagonalization (HFD), consists of three steps: (i) Solve the Hartree-Fock (HF) approximation of the Hamiltonian as in Ref. [18], (ii) use a Monte Carlo algorithm to find the low-energy many-particle HF states (Slater determinants), and (iii) diagonalize the Hamiltonian in the basis formed by these states [21]. The HF basis states are comparatively close in character to the exact eigenstates in the entire parameter space. Thus it is sufficient to keep only a small fraction of the Hilbert space to obtain low-energy quantities with an accuracy comparable to that of exact diagonalization. The HFD method is very flexible, it works well in any spatial dimension, and is capable of handling long-range and short-range interactions. A detailed description will be given elsewhere. Most of our calculations have been performed for lattices with 5^2 sites and 12 electrons keeping 500 basis states. We used periodic boundary conditions and the minimum image convention. We also studied 4^2 and 6^2 systems with $K = 0.25$ and 0.5 keeping up to 2000 out of 9×10^9 basis states.

We now turn to the conductance which we compute from linear response theory. The real (dissipative) part of the conductance (in units of e^2/h) is given by the Kubo-Greenwood formula [22],

$$\mathrm{Re}G^{xx}(\omega) = \frac{2\pi^2}{\omega} \sum_\nu |\langle 0| j^x |\nu\rangle|^2 \delta(\omega + E_0 - E_\nu), \qquad (2)$$

where ω denotes the frequency. j^x is the x component of the current operator and ν denotes the eigenstates of the Hamiltonian. Equation (2) describes an isolated system while in a real dc transport experiment the sample is connected to contacts and leads. This results in a finite lifetime τ of the eigenstates leading to an inhomogeneous broadening $\gamma = \tau^{-1}$ of the δ functions in (2) [23]. To suppress the discreteness of the spectrum of a finite system, γ should be at least of the order of the single-particle level spacing. For our systems this requires a comparatively large $\gamma \geq 0.05$. We tested different γ and found that the conductance *values* depend on γ but the qualitative results do not [24].

In a random system, different samples will have different conductance values. Figure 2 shows the probability distribution $P\{\log[G(0)]\}$ for systems in the localized regime with and without interactions. Both distributions show the same qualitative behavior; they are close to normal distributions corresponding to very broad distributions of the conductances themselves. The arithmetic average of the conductance is therefore not a good measure of the typical behavior. We use instead the logarithmic (i.e., geometrical) average $G_{\mathrm{typ}} = \exp\langle \log(G) \rangle$ [25], usually over 400 disorder configurations.

In Figs. 3 and 4 we present results on the dependence of the conductance on the interaction for two sets of

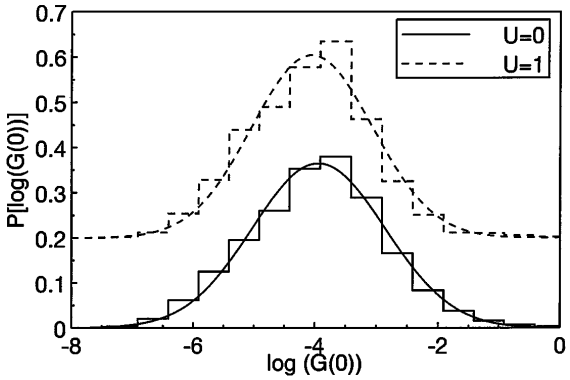

FIG. 2. $P\{\log[G(0)]\}$ for $W = 1$, $t = 0.1$, and $\gamma = 0.05$. The histograms represent 2000 samples. The smooth lines are fits to Gaussians. The data for $U = 1$ have been shifted by 0.2.

parameters. In Fig. 3 the kinetic energy is very small ($t = 0.03$). Thus the system is in the strongly localized regime, as we also estimated from the single-particle participation number $P_{\mathrm{sp}} \approx 2$. Here a weak Coulomb interaction ($U = 0.5$) leads to an *increase* of the conductance at low frequencies. If the interaction becomes stronger the conductance decreases and finally ($U = 2$) falls below the value of noninteracting electrons. We emphasize that the increase of the conductance for weak interactions is a true correlation effect: Within the HF approximation [18], interactions always lead to a decrease of the conductance. The behavior is qualitatively different at higher kinetic energy ($t = 0.3$) as shown in Fig. 4. Here the system is approaching the diffusive regime ($P_{\mathrm{sp}} > 10$). Already, a weak interaction ($U = 0.5$) leads to a reduction of the low-frequency conductance compared to noninteracting electrons. If the interaction becomes stronger the conductance is decreased further. We have performed analogous calculations for kinetic energies $t = 0.01$–0.5 and interaction strengths $U = 0$–2. The resulting dc conductances are those presented in Fig. 1.

We also checked for system size and filling factor dependences by simulating systems with 4^2 and 6^2 sites, and filling factor $K = 0.25$ in addition to 0.5. We found

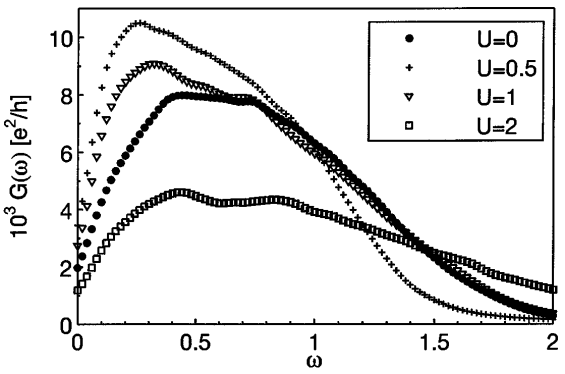

FIG. 3. $G(\omega)$ for $W = 1$, $t = 0.03$, $\gamma = 0.05$.

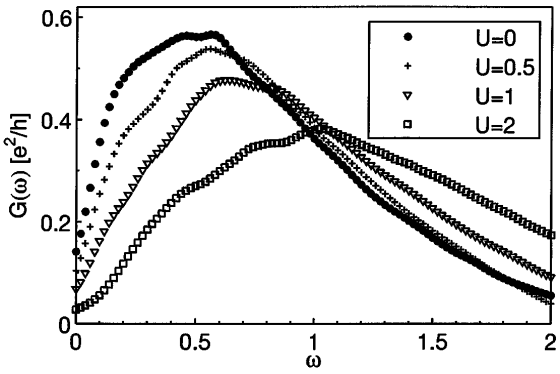

FIG. 4. Same as Fig. 3 but for $t = 0.3$.

the qualitative picture (as presented in Fig. 1) to be the same in all cases. As an example, Fig. 5 shows the interaction dependence of $G(0)$ for $t = 0.01$ for the different systems studied. Clearly, the interaction-induced enhancement of the conductance exists in all cases. Moreover, the relative enhancement seems to increase from the 4^2 system to the 6^2 system. (A comparison of even and odd linear system sizes is problematic since at half filling a regular array of charges is impossible for odd sizes. Moreover, any *quantitative* comparison of different sizes would require a more realistic description of the broadening.)

In order to find out to what extent the behavior of the conductance is reflected in single-particle localization properties, we also computed the single-particle return probability

$$R_p(\varepsilon) = \frac{1}{N} \sum_j \lim_{\delta \to 0} \frac{\delta}{\pi} G_{jj}(\varepsilon + i\delta) G_{jj}(\varepsilon - i\delta). \quad (3)$$

Here $G_{ij}(\varepsilon)$ is the single-particle Greens function. $R_p(\varepsilon)$ is the generalization of the inverse participation number $P_{\mathrm{sp}}^{-1}(\varepsilon)$ (of a single-electron state) to a many-particle system. Figure 6 shows a typical result for $R_p(\varepsilon)$. We performed analogous calculations for $t = 0.01$–0.5 and $U = 0$–2. For all cases, we obtain the same qualitative behavior: Close to the Fermi energy the return probability

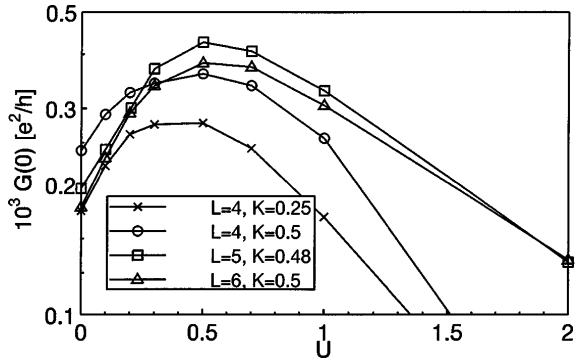

FIG. 5. Comparison of $G(0)$ for $W = 1$, $t = 0.01$, and different system sizes and filling factors.

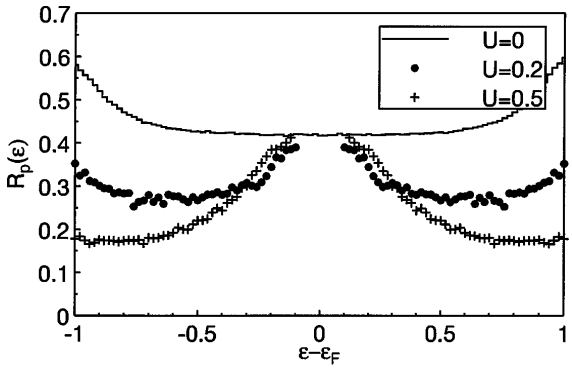

FIG. 6. $R_p(\varepsilon)$ for $W = 1$, $t = 0.1$. The data are averaged over 2000 disorder configurations (10 000 for noninteracting electrons).

is only weakly influenced by the interaction. Directly at the Fermi energy, which is not accessible in our simulations because of our still too small system sizes, there may develop a slight enhancement of the return probability as a result of the Coulomb gap in the single-particle density of states. Such an enhancement has already been observed within the HF approximation [18]. Within the results obtained in this Letter, the effect, if any, is weaker than within HF. For energies away from the Fermi energy the single-particle excitations in the interacting system become strongly *de*localized compared to the noninteracting case. The interaction dependence of the conductance discussed above is, however, not reflected in the single-particle return probability.

In summary, we have used the Hartree-Fock-based diagonalization method to investigate the transport properties of disordered interacting spinless electrons. We have found that a weak Coulomb interaction can enhance the conductivity of localized samples considerably while it reduces the conductance in the case of weaker disorder. If the interaction becomes stronger it eventually reduces the conductance also in the localized regime. Let us finally mention that, although we show that intereactions can enhance the conductivity in certain parameter regions, this does not directly provide an explanation for the MIT in 2D [3] since the importance of the spin degrees of freedom for this transition is established experimentally [26]. We emphasize, however, that our method is very easy to generalize to electrons with spin. Work in this direction is in progress.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft.

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