Crossover from interaction induced localization to delocalization in disordered electron systems

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Abstract. We numerically investigate the transport properties of interacting spinless electrons in disordered systems. We use an efficient method which is based on the diagonalization of the Hamiltonian in the subspace of the many-particle Hilbert space which is spanned by the low-energy Slater states. Low-energy properties can be calculated with an accuracy comparable to that of exact diagonalization but for larger system sizes. The method works well in the entire parameter space, and it can handle long-range as well as short-range interactions. Using this method we calculate the combined effect of disorder and interactions on the Kubo-Greenwood conductance and on the sensitivity of the ground state energy to a twist in the boundary conditions. We find that the influence of the interactions on the transport properties is opposite for large and small disorder. In the strongly localized regime (small kinetic energy, large disorder) interactions increase the transport whereas for weak disorder (large kinetic energy) interactions decrease the transport.

Keywords: localization, interactions, quantum Coulomb glass

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1 Introduction

The influence of electron-electron interactions on Anderson localization has reattracted a lot of attention, in particular because recent experimental results show a metal-insulator transition (MIT) in the two-dimensional electron gas in Si-MOSFETs \cite{1}. This is in conflict with the theory of Anderson localization for non-interacting electrons. Since the electron density in the Si-MOSFETs is very low which makes the electron-electron interaction particularly important, it is generally assumed that some type of interaction effect is responsible for the MIT. A complete understanding has, however, not yet been obtained. There have been attempts to explain the experiments based on the perturbative renormalization group \cite{2}, non-perturbative effects \cite{3}, or the transition being a superconductor-insulator transition rather than a MIT \cite{4}.

We have investigated the influence of disorder and interactions on the transport of spinless electrons numerically. Within an effective single-particle theory at the Hartree-Fock level interactions always have a localizing effect \cite{4}. In order to go beyond the Hartree-Fock approximation we have developed \cite{6,7} an efficient method, the Hartree-Fock based diagonalization (HFD) which is related to the quantum-chemical configuration interaction approach. We have used this method to study the influence
of interactions on the conductance in one \([8]\), two \([6]\), and three \([9]\) dimensions. We found a delocalizing tendency of the interactions for strong disorder but a localizing one for weak disorder. Similar results have been obtained by means of the density-matrix renormalization group \([10]\) in one dimension and exact diagonalization in two dimensions \([11]\).

In this paper we compare the results for the Kubo-Greenwood conductance to those for the phase sensitivity, i.e., the reaction of the ground state energy to a twist in the boundary conditions. We only summarize the basic findings, the details will be published elsewhere.

2 Quantum Coulomb glass and Hartree-Fock based diagonalization

The generic model for spinless interacting disordered electrons is the quantum Coulomb glass \([5, 12]\). It is defined on a regular hypercubic lattice with \(g = L^d\) (\(d\) is the spatial dimensionality) sites occupied by \(N = Kg\) electrons \((0 < K < 1)\). To ensure charge neutrality each lattice site carries a compensating positive charge of \(Ke\). The Hamiltonian is given by

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

where \(c_i^\dagger\) and \(c_i\) are the electron creation and annihilation operators at site \(i\), respectively, and \(\langle ij \rangle\) denotes all pairs of nearest-neighbor sites. \(t\) is the strength of the hopping term, i.e., the kinetic energy, and \(n_i\) is the occupation number of site \(i\). We parametrize the Coulomb interaction \(U_{ij} = e^2/r_{ij}\) by its value \(U\) between nearest-neighbor sites. The random potential values \(\varphi_i\) are chosen independently from a box distribution of width \(2W_0\) and zero mean. The boundary conditions are periodic with an additional Bloch phase in one of the dimensions. The Coulomb interaction is treated in the minimum image convention.

A numerically exact solution of the quantum Coulomb glass requires the diagonalization of a matrix whose dimension increases exponentially with system size. This severely limits the possible sample sizes. In order to overcome this problem we have developed the HFD method. The basic idea is to work in a truncated Hilbert space consisting of the corresponding Hartree-Fock (Slater) ground state and the low-lying excited Slater states. For each disorder configuration three steps have to be performed: (i) find the Hartree-Fock solution of the problem, (ii) determine the \(B\) Slater states with the lowest energies, and (iii) calculate and diagonalize the Hamilton matrix in the subspace spanned by these states. The number \(B\) of new basis states determines the quality of the approximation, reasonable values have to be found empirically.

3 Kubo-Greenwood conductance and phase sensitivity

In order to characterize the transport behavior we have studied two quantities, the Kubo-Greenwood conductance and the phase sensitivity of the ground-state energy. The conductance \([3, 4]\) can be obtained from linear-response theory. It is essentially
Fig. 1 Logarithmically averaged (400 samples) d.c. conductance $G(0)$ for systems of $4 \times 4$ lattice sites and 8 electrons for different $U$ and $t$. The disorder strength is fixed to $W_0 = 1$, the broadening is $\gamma = 0.05$, and the HFD basis size is $B = 300$.

given by the current-current correlation function of the ground state. For an isolated finite system the conductance as a function of frequency consists of a finite number of $\delta$ peaks at the excitation energies of the system. In order to extrapolate to the d.c. conductance at zero frequency an inhomogeneous broadening $\gamma$ is assumed in our calculations which mimics the coupling to leads and contacts. This broadening introduces an additional empirical parameter. We have calculated the conductance for systems with up to 100 lattice sites. In Fig. 1 we show a typical result (for a comparatively small system which also allows the calculation of the phase sensitivity). For weak disorder (large kinetic energy $t$) the interactions always reduce the conductance while for strong disorder (small $t$) moderate interactions significantly increase the conductance. Sufficiently strong interactions always strongly suppress the conductance. This is the precursor of a Wigner crystal or Wigner glass. The behavior of the conductance can be attributed to the competition of two effects: First, the interactions destroy the phase of the electrons and thus the interference necessary for localization. This is particularly effective if the localization length is small to begin with. Second, the interactions introduce an additional source of randomness which tends to increase the localization.

It is well known [15] that in disordered systems there is a close relation between the charge stiffness (i.e., the 2nd derivative of the ground state energy with respect to a magnetic flux) and the conductance. A numerically simpler but related quantity is the phase sensitivity of the ground state. It is given by the difference between the ground-state energies for periodic and antiperiodic boundary conditions [16]. In Fig. 2 we show numerical results for the phase sensitivity of the same systems as considered in Fig. 1. For strong disorder (small $t$) the phase sensitivity shows the same qualitative behavior as the conductance. However, the interaction-induced enhancement of the phase sensitivity for moderate interactions is weaker than the enhancement of the conductance. For small disorder (large $t$) a crossover to a localizing effect of the
interactions starts, but to really reach the localizing regime seems to require still larger $t$. The differences between the results for the Kubo-Greenwood conductance and the phase sensitivity are not completely understood so far. However, a likely reason are the ambiguities in describing the contacts and in taking the zero-frequency limit.

In summary, we have studied the influence of electron-electron interactions on Anderson localization for spinless electrons in two dimensions. For strong disorder moderate interactions significantly enhance the transport.

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[16] Care has to be taken if (avoided) level crossings occur as a function of the boundary phase shift.