The quantum Coulomb glass within the Hartree-Fock approximation

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We study the influence of electron-electron interactions on the electronic properties of disordered materials. In particular, we consider the insulating side of a metal-insulator transition where screening breaks down and the electron-electron interaction remains long-ranged. The investigations are based on the quantum Coulomb glass, a generalization of the classical Coulomb glass model of disordered insulators. The quantum Coulomb glass is studied by decoupling the Coulomb interaction by means of a Hartree-Fock approximation and exactly diagonalizing the remaining localization problem. We investigate the behavior of the Coulomb gap in the density of states when approaching the metal-insulator transition and study the influence of the interaction on the localization of the electrons. We find that the interaction leads to an enhancement of localization at the Fermi level.

I. INTRODUCTION

The influence of electron-electron interactions on the electronic properties of disordered systems has attracted a lot of attention recently. Already disorder alone can lead to a metal-insulator transition (MIT) by means of spatial localization of the electronic states at the Fermi energy. This MIT, called the Anderson transition, has been investigated extensively within the last two decades. While the qualitative features of the Anderson transition are well understood by now, the description remains inconsistent at a quantitative level. In particular, the critical behavior is not completely understood and the results of several methods do not agree.

Moreover, today it is generally assumed that the MIT in most experimental systems cannot be described by a model of non-interacting electrons since the Coulomb interaction between the electrons plays a crucial role. The metallic regime of the disordered interacting electron system is comparatively well understood, at least qualitatively. Altshuler and Aronov showed that the single-particle density of states (DOS) displays a non-analyticity at the Fermi energy which was called the Coulomb anomaly. Later the perturbative treatment was extended into the whole metallic phase by means of a field-theoretic renormalization group method which permits a qualitative discussion of the MIT including the identification of the different universality classes. However, quantitative results are very difficult to obtain from these methods. This is in particular so since the e-expansion which has to be used to extrapolate to the physical dimension $d = 3$ is highly singular.

Whereas investigations in the metallic phase can be carried out by means of established diagrammatic methods analogous studies of the insulating phase are not possible. That is because the natural reference system for a perturbation theory, viz. a system having disorder and interactions but no overlap between the states at different sites, is an interacting system and diagrammatic methods cannot be applied since Wick’s theorem does not hold. Instead, the insulating limit itself represents a challenging many-body problem. Almost three decades ago Pollak predicted an interaction-induced reduction of the single-particle DOS at the Fermi energy in disordered insulators. Later Efros and Shklovskii defined the prototype model of disordered electronic systems in the insulating limit, the classical Coulomb glass model. They showed that the zero-temperature single-particle DOS has power-law gap at the Fermi energy which is called the Coulomb gap. This suggests the question whether Coulomb anomaly and Coulomb gap are manifestations of the same physical phenomenon on the metallic and insulating sides of the MIT, respectively. We will come back to this question in Sec. III. The physics of the classical Coulomb glass model has been investigated in much detail by several analytical and numerical methods and its static properties are comparatively well understood by now. In contrast, the nature of the transport mechanism is still controversially discussed.

Since experiments deep in the insulating regime are difficult to carry out most results on disordered insulators have been obtained from samples not too far away from the MIT. Here the (single-particle) localization length is still much larger than the typical distance between two sites and the description of the electrons in terms of classical point charges becomes questionable. Attempts to include the overlap between different states into the Coulomb glass model have been made earlier by mapping the problem onto a non-interacting model and applying the coherent potential approximation. However, in this method neither disorder nor interactions are treated completely and different results obtained this way contradict each other. Recently, localization in an interacting disordered system was investigated by the numerical analysis of the many-body spectrum of small clusters from which the authors inferred a delocalizing influence of the interactions.

We note, that in addition to these works which deal with the ground state properties of many-body systems possessing a finite particle density there has been a very active line of research concerning the behavior of just two interacting particles in a random environment. This
type of work concentrates on special highly excited states of the two-electron system which will, in general, behave differently from the ground state at finite particle density.

In this paper we investigate the physics of the disordered interacting electron problem (having finite particle density) on the insulating side of the MIT. In order to account for a finite overlap between the states we generalize the classical Coulomb glass model to a quantum model by including transfer matrix elements between different sites. We then study two main questions: (i) How does the single-particle DOS and, in particular, the Coulomb gap depend on the transfer between the sites? (ii) How does the Coulomb interaction influence the localization of the electrons?

The paper is organized as follows: In Sec. II we define the quantum Coulomb glass model and explain our calculational method. In Sec. III we present the results for the single-particle DOS and discuss the behavior of the Coulomb gap. The localization properties and the resulting phase diagram of the MIT are considered in Sec. IV and Sec. V is devoted to some conclusions and discussions.

II. THE QUANTUM COULOMB GLASS MODEL

In the insulating limit the overlap between the electronic states at different sites can be neglected and the electrons behave like classical point charges. The generic model for this regime is the classical Coulomb glass model, which consists of classical point charges in a random potential which interact via Coulomb interactions. The model is defined on a regular hypercubic lattice with $N = L^d$ ($d$ is the spatial dimensionality) sites occupied by $KN$ (spinless) electrons ($0 < K < 1$). To ensure charge neutrality each lattice site carries a compensating positive charge of $Ke$. The Hamiltonian of the classical Coulomb glass reads

$$H_{cl} = \sum_i (\varphi_i - \mu) n_i + \frac{1}{2} \sum_{i \neq j} (n_i - K)(n_j - K)U_{ij}.$$  (1)

Here $n_i$ is the occupation number of site $i$ and $\mu$ is the chemical potential. The Coulomb interaction $U_{ij} = e^2/r_{ij}$ remains long-ranged since screening breaks down in the insulating phase. We set the interaction strength of nearest neighbor sites to 1 which fixes the energy scale. The random potential values $\varphi_i$ are chosen independently from a box distribution of width $2W_0$ and zero mean.

Our goal is to describe the regime where the overlap between the states at different sites cannot be neglected but the system is still insulating. Therefore, we generalize the Coulomb glass model model to a quantum Coulomb glass model by adding hopping matrix elements between nearest neighbors. The Hamiltonian of the quantum Coulomb glass is given by

$$H = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + H_{cl},$$  (2)

where $c_i^\dagger$ and $c_i$ are the electron creation and annihilation operators at site $i$, respectively, and the sum runs over all pairs of nearest neighbor sites. In the limit $t \to 0$ the model reduces to the classical Coulomb glass, for vanishing Coulomb interaction but finite overlap it reduces to the usual Anderson model of localization.

In order to calculate the electronic properties we decouple the Coulomb interaction by means of a Hartree-Fock approximation giving

$$H_{HF} = -t \sum_{\langle ij \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) + \sum_i (\varphi_i - \mu)n_i + \sum_{i \neq j} n_i U_{ij} (n_j - K) - \sum_{i,j} c_i^\dagger c_j U_{ij} c_j^\dagger c_i,$$  (3)

where the first two terms contain the single-particle part of the Hamiltonian, the third is the Hartree energy and the fourth term contains the exchange interaction. (Note that in (3) several constant terms have been dropped.) $\langle \ldots \rangle$ represents the expectation value with respect to the Hartree-Fock ground state which has to be determined self-consistently. In this way the quantum Coulomb glass is reduced to a self-consistent disordered single-particle problem which we solve by means of numerically exact diagonalization giving the single-particle energies $\varepsilon_\nu$ and states $|\psi_\nu\rangle$. We note that the Hartree-Fock approximation is exact for both of the limiting cases mentioned above, viz. the classical Coulomb glass and the Anderson model of localization.

In this study we investigate three-dimensional quantum Coulomb glass systems with up to $N = 10^4$ sites and band fillings $K$ between 1/2 and 15/16. Due to the particle-hole symmetry of the Hamiltonian (2) this also covers the band fillings between 1/16 and 1/2. The disorder strength is fixed at $W_0 = 1$, and the overlap parameter $t$ varies from zero (classical limit) up to $t = 0.5$ which is above the MIT. In order to reduce the statistical error we average the results over 100 different configurations of the random potential $\varphi$.

III. SINGLE-PARTICLE DENSITY OF STATES

For several reasons, the single-particle DOS plays a special role in the investigation of the quantum Coulomb glass. First, it is the quantity investigated best for the classical Coulomb glass where it shows the well-known power-law Coulomb gap. One question we want to address in this section is whether the Coulomb gap remains intact in the presence of a small overlap. This question is of central importance for the justification of the classical model in experiments comparatively close to the MIT where the overlap between different impurity states cannot be neglected. Second, from field-theoretic studies on the metallic side of the MIT it was inferred that
the single-particle DOS at the Fermi energy is the order parameter of the disorder-driven MIT in interacting systems. Thus it should remain zero in the whole insulating phase and start to increase when crossing the MIT point. Third, in the metallic phase the DOS should display the aforementioned Coulomb anomaly, a square-root non-analyticity on top of a finite background.

In the context of the Hartree-Fock approximation the single-particle energies are simply given by the eigenvalues $\epsilon_\nu$ of the self-consistent Hartree-Fock Hamiltonian \((3)\). Thus, the single-particle DOS is defined by

$$ g(\epsilon) = \frac{1}{N} \sum_\nu \delta(\epsilon - \epsilon_\nu) . \quad (4) $$

Our numerical results for the single-particle DOS of the quantum Coulomb glass are comprised in Figs. 1 and 2. Note that the Hamiltonian is particle-hole symmetric for $K = 0.5$ (Fig. 1). Thus the Fermi energy does not depend on $t$. For $K = 0.75$, in contrast, the Fermi energy increases with $t$, and the shift of the gap position in Fig. 2 exactly matches the shift of the Fermi energy.

In order to address the questions raised at the beginning of this section we study the behavior of the DOS close to the Fermi energy. Let us first discuss our expectations: In the insulating phase the electrons are localized and cannot screen the Coulomb interaction. Consequently, the Hartree part of the interaction remains long-ranged while the exchange part which is proportional to the overlap of different states is small and short-ranged. In the insulating phase we can therefore apply a generalization of the Efros-Shklovskii argument to discuss the behavior of the leading terms of the DOS: The original argument shows that an empty state $j$ and an occupied state $i$ with an energetic distance smaller than $\delta$ must have a spatial distance larger than $e^2/\delta$ since the change $\Delta = \epsilon_j - \epsilon_i - e^2/r_{ij}$ of the system energy when moving the electron from $i$ to $j$ must be positive in the many-body ground state. If finite overlaps between different sites are included the electrons become somewhat delocalized and therefore the interaction is screened on short length scales of the order of the localization length. In contrast, the long-range part of the interaction remains unchanged. Since the DOS close to the Fermi energy is determined by the long-range tail of the interaction we expect it to remain unchanged as long as the electrons are localized. However, the region of validity of the classical result shrinks to zero with increasing delocalization and vanishes when the electronic states become extended. Thus the Coulomb gap should become narrower with increasing $t$ and vanish at the MIT.

On the other hand, with increasing delocalization of the electrons the exchange interaction becomes larger and longer-ranged. Since the exchange interaction is responsible for the Coulomb anomaly $^{16}$ we expect the DOS to show a crossover from the Coulomb gap behavior to a Coulomb anomaly behavior. To be precise, if the system is close to the MIT but still insulating the DOS should show Coulomb-gap-like behavior in a narrow interval around the Fermi energy and Coulomb-anomaly-like behavior for energies a bit away from the Fermi level.

In Fig. 3 we present a log–log plot of the single-particle DOS in the Coulomb gap region for the system with band filling $K = 0.5$. The data presented are compatible with the above expectations. For small $t$ we find a power-law behavior with an exponent close to 2 as expected for the Coulomb gap in 3D. With increasing $t$ the exponent becomes smaller and approaches 0.5 as expected for the Coulomb anomaly (if the constant background is small).

We are, however, not able to explicitly demonstrate the crossover from the Coulomb gap to the Coulomb anomaly at fixed $t$ as a function of energy . The main reason is that the investigation of the DOS very close to the Fermi energy is hampered by strong finite size effects. The usual problem, viz. that a finite system always possesses a discrete spectrum, is made worse by the long-range character of the interaction. Since the maximum system size
FIG. 3. Log–log plot of the density of states of the quantum Coulomb glass for $W_0 = 1$, $K = 0.5$. The lower dashed line represents the analytical result for the DOS in the classical model ($t = 0$), the upper dashed line corresponds to a square-root behavior with arbitrary prefactor and the dotted line is the reliability limit due to the cut-off of the Coulomb interaction, see text.

IV. LOCALIZATION PROPERTIES

The usual criteria for localization are defined for non-interacting electrons only, and their generalization to many-body systems is not straightforward. Within the Hartree-Fock approximation, however, we do obtain effective single-particle states and energies so that the usual localization criteria can be applied.

A. Participation number

One of the simplest measures to study the localization properties is the participation number $P$ which describes how many sites are effectively occupied by a single-particle state $|\psi_\nu\rangle$. Thus the inverse participation number measures the degree of localization. It is defined as the second moment of the spatial probability distribution of the state

$$P^{-1}_\nu = \frac{1}{N} \sum_i |\langle \psi_\nu |i \rangle|^4$$

(5)

where the sum runs over all sites $i$. In practice it is often averaged over all states with a certain energy $\varepsilon$

$$P^{-1}(\varepsilon) = \frac{1}{g(\varepsilon)} \frac{1}{N} \sum_\nu P^{-1}_\nu \delta(\varepsilon - \varepsilon_\nu) .$$

(6)

In Figs. 4 and 5 we show the results for the inverse participation numbers of systems with $N = 10^3$ sites and band filling factors of $K = 0.5$ and 0.75, respectively.

The most remarkable feature of these results is the strong enhancement of $P^{-1}$ close to the Fermi energy which can be as large as one order of magnitude (note the logarithmic scale in the figures). This enhancement of $P^{-1}$ corresponds to a much stronger localization at the Fermi level compared to the rest of the band. It is a direct consequence of the Coulomb gap in the DOS which means a reduction of the number of states that can be hybridized by a certain overlap $t$. Based on this argument it is also easy to understand how the enhancement depends on the overlap $t$: For very small $t$ all states remain strongly localized so that there is no room for a large enhancement. The largest enhancement is obtained for moderate values of $t$ which are still smaller than the width of the Coulomb gap. In this case the states away
from the Fermi level are considerably delocalized while the hybridization at the Fermi energy is still hampered. For overlaps $t$ larger than the width of the Coulomb gap hybridization becomes easier also at the Fermi level and thus the enhancement of $P^{-1}$ is diminished. Note that in contrast to non-interacting electrons the participation numbers depend on the band filling since the electronic states are influenced by the interaction with the other electrons.

A comparison (see Fig. 6) of the inverse participation numbers of the quantum Coulomb glass and of non-interacting electrons shows that in the interacting system the electrons are more strongly localized all over the band but the enhancement is strongest close to the Fermi energy.

Although the inverse participation number is a useful quantity to study qualitative features of localization it is not well suited to quantitatively determine the MIT and its properties. The reason is that determining the MIT from the participation numbers amounts to detecting changes in the size dependence of $P^{-1}$ which is much harder than detecting changes of $P^{-1}$ itself. ($P$ should remain finite for $N \to \infty$ for localized states but scale with $N$ for extended states.) We therefore use a different method based on the properties of the eigenvalue spectrum of the Hamiltonian which is explained in the following subsection.

### B. Level statistics

The mobility edge, i.e. the energy that separates extended from localized states, can be found by using the statistical properties of the energy levels as was done for the Anderson model of localization. In this method the distribution $P$ of nearest-neighbor level spacings $s$ of the (unfolded) spectrum of eigenvalues $\varepsilon_n$ is considered. In accordance with the literature we use the notation $P(s)$ for this distribution, it should not be confused with the participation number $P$ discussed in Sec. IV.A. At the MIT the level spacing distribution function displays a sharp transition from the Poisson ensemble (PE, for the insulating phase) via the critical ensemble (at the transition point) to the Gaussian orthogonal ensemble (GOE, in the metallic phase). For finite system sizes a smooth crossover between the three ensembles is observed instead of the sharp transition for the infinite system.

Within the Hartree-Fock approximation the quantum Coulomb glass is equivalent to an Anderson model of localization having an unusual disorder distribution and additional disordered transfer elements. As in the Anderson model, the MIT can therefore be determined by the crossover of the level spacing distribution $P(s)$.

In Fig. 7 we show examples for the distribution. For $t = 0.1$ the spectrum is close to PE (the states are localized as will be shown later) while for $t = 0.2$ the spectrum is close to GOE (the states are extended). In order to determine the location of the MIT in parameter space the crossover from PE to GOE has to be described quantitatively. Following Ref. 19 we fit the numerically obtained distributions $P(s)$ to the phenomenological formula:

$$P_{phe}(s) = A s^\beta (1 + C s^\beta)^{f(\beta)} \exp \left[ -\frac{\pi^2}{16} \beta s^2 - \frac{\pi}{4} (2 - \beta) s \right]$$

with $f(\beta) = 2^3 (1 - \beta/2)/\beta - 0.16874$. This formula interpolates smoothly between PE and GOE. It contains only a single free parameter since the first two moments of the level spacing distribution $P(s)$ are normalized:

$$\int ds \, P(s) = \int ds \, s \, P(s) = 1.$$
We then study the dependence of the fit parameters $A$, $C$ and $\beta$ on the single-particle energy $\varepsilon$ and overlap strength $t$. The parameter $\beta$ shows a particular strong dependence close to the mobility edge. From Ref. [18] it is known that the critical ensemble corresponds to $\beta \approx 0.875$ which we use as a criterion to determine the transition point. The resulting dependence of the mobility edge on energy and overlap is presented in Figs. 8 and 9. Close to the Fermi energy the mobility edge is shifted to larger overlaps (or, equivalently, smaller disorder), so the location of the mobility edge also reflects the enhancement of localization at the Fermi energy.

C. Metal–insulator transition

In a system of non-interacting electrons the states and energy levels do not depend on the filling of the band. Changing the filling factor simply leads to a shift of the Fermi energy within the otherwise unchanged band. When the Fermi energy crosses the (fixed) mobility edge the system undergoes a MIT. In a system of interacting electrons, however, the mobility edge changes with filling factor $K$. Therefore, separate calculations have to be done for different filling factors to determine the phase diagram. The MIT occurs when the states at the Fermi energy delocalize (or localize). This means that Figs. 8 and 9 yield only one data point each for the phase boundary. We have carried out the corresponding calculations for filling factors $K = 7/8$ and $15/16$, too. The resulting phase diagram of the MIT is displayed in Fig. 10 and compared to the analogous phase diagram for the Anderson model of localization. We find that the phase boundary of the quantum Coulomb glass is shifted to significantly larger values of the overlap $t$ compared to non-interacting electrons if the Fermi energy is well within the band. As discussed above this is a direct consequence of the Coulomb gap in the single-particle DOS. For band fillings close to $K = 1$ the critical $t$ of the quantum Coulomb glass remains almost unchanged since the form of the Coulomb gap does not depend on its position in the band whereas the critical $t$ of the Anderson model is reduced because the DOS of the Anderson model decreases near the band edges.

V. CONCLUSIONS

To summarize, we have investigated the combined influence of disorder and interactions on the properties of electronic systems on the insulating side of the MIT. Our work is based on the quantum Coulomb glass model. We have decoupled the interaction by means of the Hartree-Fock approximation and numerically diagonalized the remaining disordered single-particle problem. The resulting single-particle DOS shows a Coulomb gap in the
whole insulating phase which becomes narrower when approaching the MIT. The reduced DOS at the Fermi energy leads to an enhancement of localization compared to the rest of the band and also compared to non-interacting electrons. In this concluding section we will discuss some aspects of the results that have not yet been covered. First, we want to discuss the justification of the Hartree-Fock approximation. On a qualitative level, there are several possible influences of the Coulomb interaction on Anderson localization with competing effects. On the one hand, the Coulomb interaction leads to a reduction of the density of states at the Fermi energy which enhances localization. This process is contained in the Hartree-Fock approximation as discussed in Sec. 11 and as we have demonstrated in this paper. On the other hand one may argue that any interaction leads to transitions between the states of the non-interacting system thus giving the electrons additional hopping possibilities and reducing localization. This second point is not well described within the Hartree-Fock approximation. We have therefore started to compare the results of this paper to that of exact diagonalizations of small lattices. Preliminary results show that the large enhancement of localization at the Fermi level is also found by the exact diagonalizations while the average degree of localization in the band is overestimated by the Hartree-Fock approximation in some parameter regions. Further studies along these lines are in progress. We also note that, as is well known, the Hartree-Fock approximation of the 3D homogeneous interacting electron system produces an artificial soft gap at the Fermi energy since screening is not treated properly. Although this artificial gap is much narrower \( g \sim 1/\ln |\varepsilon - \varepsilon_F| \) than the Coulomb anomaly and thus difficult to observe the results for the DOS on the metallic side of the MIT may be influenced and more sophisticated investigations will have to be carried out. Second, we want to comment on the relation between Coulomb gap in the insulating phase and Coulomb anomaly in the metallic phase. It has been suggested that both are different manifestations of the same physical phenomenon. However, the Coulomb gap is a result of the Hartree part of the interaction and its existence is tied to the long-range nature of the Coulomb interaction. In contrast, the Coulomb anomaly is produced by the exchange interaction and arises independently of the range even for point-like interactions. Therefore a system with a short-range model interaction will display a Coulomb anomaly but not a Coulomb gap. Further work is necessary to clarify how the Coulomb anomaly changes to the Coulomb gap at the MIT (in the case of long-range interactions) or how it vanishes on the insulating side for short-range interactions.

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