Delocalization due to correlations in two-dimensional disordered systems

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Abstract. We study the spectral statistics of interacting spinless fermions in a two-dimensional disordered lattice. Within a full quantum treatment for small few-particle-systems, we compute the low-energy many-body states numerically. While at weak disorder the interactions reduce spectral correlations and lead to localization, for the case of strong disorder we find that a moderate Coulomb interaction has a delocalizing effect. In addition, we observe a non-universal structure in the level-spacing distribution which we attribute to a mechanism reinforcing spectral correlations taking place in small systems at strong disorder.

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1 Introduction

The ongoing miniaturization of electronic devices and the peculiar physics associated motivate the investigation of systems with reduced dimensionality. In such systems, the effect of Coulomb interactions is expected to be strong, and prominent experimental observations of the last decade are thought to be due to correlation effects.

One such experimental result concerns the magnitude of the persistent currents in disordered mesoscopic rings [1,2], which are much greater than theoretical predictions from approaches neglecting correlations [3]. The interaction effect seems to be beyond the perturbative regime, but a full treatment of the realistic situation is out of reach (for a review see [4]). Nevertheless, analytical [5] and numerical [6,7] calculations in 1D and in 2D have shown that a repulsive interaction can enhance the persistent currents.

As another important example, a metallic behaviour has been observed [8] (see [9] for a review) in 2D electron gases at low electronic density, where the ratio \( r_s \) of Coulomb to kinetic energy is large (\( > 10 \)). This cannot be explained by the standard scaling theory of localization which, neglecting electronic correlations, predicts an insulating behaviour in 2D for any finite disorder strength [10]. Since interactions become important when the electron density is low (large \( r_s \)), they have been suggested to be responsible for the observed metallic behaviour [7]. However, a perturbative introduction of the interaction leads to a reinforcement of the electron localization [11]. This points towards the necessity of treating the interactions beyond perturbation theory, and several approaches have been proposed in this direction.

Renormalization group techniques indicate that the interaction permits a metal-insulator transition in a weakly disordered two-dimensional electron gas [12,13]. However, despite some well reproduced properties (such as the effect of a magnetic field), a description of the transition is not possible and the metallic phase is based on the assumption of a Fermi liquid.

Alternatively, field theory based on the fact that the metallic phase is not a Fermi liquid (as argued in [14]) has shown that a perfect metal can be stable in 2D if the interaction is strong enough [15].

Furthermore, numerical calculation of the current-current correlation function using a quantum Monte Carlo approach has shown that interactions change the behaviour of the conductivity at low temperature from an insulating to a metallic one [16], as observed in the experiments.

All these approaches contain approximations. On the contrary, numerical studies of model systems allow for exact results, although they are limited to simplified models and small system sizes. Therefore, such studies are able to provide a complementary view of the mechanisms implied in the interplay between disorder and interaction.

In the present work, we numerically investigate interacting spinless fermions (spin-polarized electrons) in small two-dimensional lattices with disorder, performing a direct diagonalization of the Hamiltonian.

The limitation in size makes it difficult to vary directly the electronic density as in experiment. To change the interaction parameter \( r_s \), we vary instead the interaction strength \( U \) while keeping the system size \( L \) and the particle number \( N \) constant.
Table 1. Summary of the behaviour of the distribution $P(s)$ for different regimes of interaction $U$ and disorder in small two-dimensional systems. PWMS stands for Pinned Wigner Molecule Statistics (see text). The cross-over between the weak and strong interaction regimes represent the main result of the paper.

| $U$     | Weak disorder | Strong disorder |
|---------|---------------|-----------------|
| 0       | Wigner-Dyson  | Poisson         |
| $\infty$ | PWMS         | PWMS            |
| cross-over | monotonic  | non-monotonic   |

Within this approach, we explore the interaction effects on the ground state structure and the probability density $P(s)$ of the normalized level spacing $s = \Delta / \langle \Delta \rangle$, where $\Delta = E_1 - E_0$ is the energy spacing between the many-body ground-state and the first excited state. We denote by $\langle \ldots \rangle$ the average over the ensemble of disorder configurations.

In the non-interacting case, $\Delta$ is equal to the one-body level spacing at the Fermi energy. The statistics of these one-body level spacings $P(s)$ has been extensively studied and found to be an indicator of the metal-insulator Anderson transition occurring in 3d as a function of the disorder strength [17,18]. In the diffusive regime, $P(s)$ corresponds to Wigner-Dyson statistics, while the Anderson insulating regime is characterized by Poisson statistics (table 1).

In the opposite limit, at $U = \infty$, the structure of the ground state is imposed by the Coulomb repulsion, which leads to a Wigner crystal pinned by the disorder. We show in section 4 that the resulting distribution $P_{U=\infty}(s)$ (which we call “Pinned-Wigner-Molecule Statistics”, PWMS) is non-universal for finite size systems.

For weak disorder, we found the dependence of $P(s)$ on $U$ to be consistent with previous studies: $P(s)$ crosses over smoothly from Wigner-Dyson statistics to its infinite interaction limit [19,20,21].

Within an approximative method (Configuration Interaction method, starting from Hartree-Fock orbitals), the strong disorder case has been studied by Benenti et al. for larger systems [22]. They obtain an interaction-induced transition of $P(s)$ from Poisson to Wigner-Dyson. Our findings of an increase of spectral correlations by moderate interaction show that this behaviour persists when electronic correlations are taken fully into account.

The non-trivial behaviour of the spectral statistics for strong disorder is discussed in section 3 after the presentation of the model we study (section 2). In section 2 we present results for the inverse participation ratio of the ground state in the many-body on-site basis, and we show that the increase of spectral correlations is related to a delocalizing effect. Our conclusions are discussed in section 5 and a small size effect modifying the shape of $P(s)$ is presented in the Appendix.

2 Disorder and Coulomb Interaction

We consider $N$ spinless fermions on a two-dimensional $L$ by $L$ lattice (in the following, we concentrate on $N = 4$ and $L = 6$). We note $M = L^2$ the number of sites.

The Hamiltonian of the system is $H = H_A + H_U$, where $H_A$ is the standard Anderson Hamiltonian

$$H_A = -t \sum_{<i,j>}(c_i^+ c_j + c_j^+ c_i) + \sum_{i=1}^{M} v_i c_i^+ c_i, \quad (1)$$

with $c_i^+$ ($c_i$) creating (destroying) an electron on the site $i$. The first term of $H_A$ allows for hopping between nearest neighbours $<i,j>$ on the lattice. We take $t = 1$, representing then the energy scale. Periodic boundary conditions are used, leading to a toroidal topology. The second term of $H_A$ models a disorder potential. The $v_i$ are independent random variables uniformly distributed in [$-W/2; W/2$], and $W$ is the disorder strength.

The interaction term is chosen to be of the Coulomb form:

$$H_U = \frac{U}{2} \sum_{i,j=1}^{M} \exp\left(-\frac{d_{ij}}{U}\right), \quad (2)$$

where $d_{ij}$ is the smallest distance on the torus between the sites $i$ and $j$ and $U$ is the interaction strength.

This model allows us to study qualitatively the effect of interactions in disordered systems. For the exact diagonalization of the Hamiltonian $H$, we have used a routine developed by Simon and Wu [23] based on the Lanczos algorithm [24].

3 Interaction induced many-body level-repulsion

In this section, we study in detail the probability distribution $P(s)$ of the first excitation energy whose behavior in different regimes is sketched in table 1.

In the absence of interactions, $P_{U=0}(s)$ corresponds to the Wigner-Dyson distribution $P_{WD}(s) = \frac{s}{\pi} \exp(-\frac{s^2}{2})$ for a diffusive (metallic) system. For a strongly disordered system (Anderson insulator), its limiting behavior for $L \to \infty$ is the Poisson distribution $P_{P}(s) = \exp(-s)^1$.

In the strong interaction limit ($U \to \infty$), the electrostatic energy dominates and the energetically lowest many-body states correspond to periodic distributions of the electrons (Wigner crystal) which are pinned even by a small amount of disorder. All Wigner crystals have the same electronic structure, thus the same Coulomb energy, but differ in their location on the lattice and therefore in their disorder energy.

In the limit of low densities, the ground state structure approaches the usual hexagonal Wigner crystal, the
number of possible positions on the lattice is large, and \( P_{U=\infty}(s) \) tends to Poisson. For higher densities we need to take into account commensurability effects. In the studied case, \( N \) and \( L \) are such that the nine energetically lowest \( U = \infty \) many-body states are square-shaped Wigner crystals (which we will refer to as “Wigner molecules”) differing only by their location on the lattice. These nine Wigner molecules have different disorder energy, and the first excitation energy is

\[
\Delta = E_1 - E_0 = \sum_{k=1}^{N} v_{j_k} - \sum_{k=1}^{N} v_{j_k},
\]  

where the \( j_k \) describe the sites occupied by a particle in the energetically lowest Wigner Molecule (the ground state) and the \( i_k \) the occupied sites in the second Wigner molecule (the first excited state). Since we only have nine configurations, \( P_{U=\infty}(s) \) is not exactly Poisson. Instead, it is a distribution which is intermediate between semi-Gaussian and Poisson, which we call pinned-Wigner-molecule statistics (PWMS).

Figure 1 shows \( P(s) \) with \( W = 5 \), for three values of \( U \). With this disorder strength, the single-particle localization length is larger than the system size, so that the motion of non-interacting particles through the sample is diffusive and \( P(s) \) follows Wigner-Dyson statistics at \( U = 0 \).

In this case, we find that the level repulsion decreases with increasing interaction strength. In this sense, this result is consistent with those of [19,20,21]. The difference is that the \( U = \infty \) limit of \( P(s) \) is in fact the PWMS and not Poisson for the investigated system sizes.

This behaviour is as expected: strong interactions drive the system out of the diffusive regime by setting up a Wigner Crystal which is pinned by disorder. Therefore spectral correlations disappear with increasing interaction strength.

Figure 1 shows our results for the case of stronger disorder (\( W = 20 \)). This disorder is not strong enough to have a Poissonian \( P(s) \) in the non-interacting case, and hence \( P_{U=0}(s) \) is intermediate between Poisson and Wigner-Dyson. Nevertheless, a single-particle state at the Fermi energy is localized over about three sites only, meaning that the system is far from the diffusive regime for \( U = 0 \).

The main feature is that at this disorder strength, the evolution of \( P(s) \) with the interaction strength is non-monotonic. Obviously, for stronger interactions the spectral correlations eventually decrease and \( P(s) \) approaches its infinite interaction limit (PWMS). For a moderate \( U \), however, the spectral correlations are increased relative to the non-interacting case (i.e. \( P(s) \) is more Wigner-Dyson-like). This is the main result of the present paper. The increase of spectral correlations could be the precursor of the transition towards universal correlations found in [22].

The non-monotonic behavior becomes less significant as \( W \) increases further. It is for this reason that we have presented our results for \( W = 20 \). Note that, with interaction, a peak appears in the \( P(s) \) curves. This peak is the manifestation of a mechanism enhancing spectral correlations in a non-universal way for small system size. We discuss this mechanism in detail in the appendix.

In order to characterize quantitatively the non-monotonic behaviour exhibited by \( P(s) \), we consider the evolution of the variance of \( s \) with \( U \). We show in figure 2 that this evolution in the cases of \( W = 5 \) and \( W = 20 \) is very different. At \( W = 5 \) there is a monotonous evolution towards smaller correlations, while at \( W = 20 \) the variance exhibits a minimum as a function of \( U \) (corresponding to an increase of the spectral correlations).

With a short range interaction, we have found similar results for \( P(s) \) at half filling. However, away from half filling, configurations not affected by interactions are connected by hopping matrix elements. Therefore, short range interactions cannot suppress the mobility of the electrons. As a consequence, the variance (or another parameter characterizing the distribution \( P(s) \)) does not reach its PWMS value at strong \( U \).
4 Delocalization in the many-body on-site basis

The fact that $P(s)$ approaches the Wigner-Dyson distribution in the presence of a moderate interaction could be interpreted as a signature of a delocalization of the electrons. Whereas the link between spectral correlations and localization is clear for one-particle level statistics ($U = 0$), it is less obvious in the interacting regime. To clarify this interpretation, we have studied the localization of the ground-state

$$\langle \Psi \rangle = \sum_n \langle n \rangle$$

in the many-body on-site basis $\left\{ \langle n \rangle \right\}$, via its inverse participation ratio

$$\mathcal{R}^{-1} = \sum_n |\langle n \rangle|^4.$$  \hspace{1cm} (5)

Contrary to $P(s)$, the inverse participation ratio $\mathcal{R}^{-1}$ depends on the choice of the basis in which it is calculated. To be allowed to interpret the inverse participation ratio as a measurement of the electron localization, we have chosen for $\left\{ \langle n \rangle \right\}$ the Slater determinants

$$c_{i_1}^+ c_{i_2}^+ c_{i_3}^+ c_{i_4}^+ |0\rangle$$

which correspond to the four particles being localized on the lattice sites $i_1$, $i_2$, $i_3$, and $i_4$ and where $|0\rangle$ is the empty lattice state.

If $|\langle n \rangle|$ is given by one of these basis states $|n\rangle$, then $\Psi_n = \delta_{n,m}$, and $\mathcal{R}^{-1} = 1$. If, on the other hand, $|\langle n \rangle|$ is a superposition of many elements of $\left\{ \langle n \rangle \right\}$, then $\mathcal{R}^{-1}$ is very small compared to unity. Since the basis is built with completely localized electrons, $\mathcal{R}^{-1}$ can be interpreted as a measurement of the localization of electrons in the many-body state $|\langle n \rangle\rangle$.

Figure 3 shows numerical results for the inverse of the average of $\mathcal{R}^{-1}$. In the case of weak disorder ($W = 5$, in the inset), this quantity is monotonically decreasing with $U$, as expected. The $U = 0$ diffusive situation with delocalized particles is perturbed by moderate interactions which increase the scattering, reducing both the mobility and $1/\langle \mathcal{R}^{-1} \rangle$. In the regime of strong interactions, the electrons form a Wigner crystal to minimize electrostatic energy. Since this corresponds to one particular state of the chosen basis, $\mathcal{R}^{-1}$ decreases to one.

In the regime of strong disorder, the behaviour is very different. At weak interaction, $1/\langle \mathcal{R}^{-1} \rangle$ increases with $U$, which means that interaction has a delocalizing effect. This can be understood within the following scenario.

At $U = 0$, we have localized one-body wave functions, the disorder being strong enough to dictate the electronic configuration. For finite $U$, the effect of the interaction depends on this particular sample-dependent configuration. In some samples, this electronic structure is close to the one adapted to interaction (Wigner molecule), therefore the interaction strengthens the localization. On the other hand, in most samples, the disorder-adapted electronic configuration is rather different from the Wigner molecule structure. Therefore, increasing interaction strength induces charge reorganizations (as proposed in \cite{25} in the context of one-dimensional rings) at particular sample-dependent values of the interaction strength $U_c$. When $U \simeq U_c$, the competition between interaction and disorder leads to a ground state which is a superposition of a state adapted to disorder and another one adapted to interaction. This results in a pronounced delocalization.

Since $U_c$ is strongly sample-dependent, these delocalizations are smoothed by the disorder average. Furthermore, we expect that as $W$ increases, the mean value of $U_c$ also increases and its distribution spreads, consistent with the behaviour observed in figure 3.

To illustrate these considerations, we can define for each sample the increase

$$\delta = \mathcal{R}^{-1}(U) - \mathcal{R}_0^{-1}$$

(7)
of $R^{-1}$ with respect to the non-interacting value $R_{n}^{-1}$. Figure 4 depicts the distribution of this quantity at $W = 20$, for two different values of $U$. We can see that the most probable value of $\delta$ is close to zero. Nevertheless, for $U = 2.5$ the negative tail of the distribution, corresponding to strong delocalizations, is more pronounced than the positive one, which corresponds to strong localizations, resulting in a negative average of $\delta$. This is not the case when the interaction is strong ($U = 9$). We can conclude that for $W = 20, U_c$ is more probable to be close to 2.5 than 9.

5 Conclusion

We have studied the spectral statistics of interacting spinless fermions in a two-dimensional disordered system, using exact diagonalization.

We have found that correlations in the statistics of the level spacing between the many-body ground state and the first excited state are increased by a moderate interaction when the disorder is strong enough to localize the one-particle wave functions. The interpretation of this effect as a delocalization of the electrons has been supported by the study of the inverse participation ratio for the ground state.

The delocalization effect can be understood as a consequence of a competition between disorder and interaction for the structure of the ground-state, taking place at some sample-dependent value of the interaction strength. This competition results in charge reorganization caused by increasing interaction from a configuration minimizing the disorder energy to a configuration more adapted to the interaction.

A Appendix: Non-universal level statistics in small systems

The peak appearing in the $P(s)$ curve of figure 1b for $U = 20$ is the manifestation of a mechanism enhancing spectral correlations in a non-universal way. Since its major ingredient is a competition between disorder and interaction, this mechanism could be the precursor of what happens in bigger systems, where other mechanisms could take place at higher order, resulting in enhanced spectral correlations even in the thermodynamic limit.

The mechanism we want to describe takes place in very small systems when the mean level spacing $\langle \Delta \rangle$ is not much smaller than the hopping $t$. In order to explain this mechanism, we start by considering the simpler non-interacting situation, before treating the interacting case.

A.1 Non-interacting case

Without the hopping $t$, the eigenstates of the system are Slater determinants of particles localized on single sites, and the distribution of their energies is Poisson. In the limit of strong disorder, $W \gg t$, the coupling $t$ of neighbouring sites is typically much smaller than their difference in on-site energy. Therefore, particles remain localized on single sites, except in samples for which the energy of the highest occupied site $i$ is almost degenerate with that of the lowest unoccupied site $j$, and with these two sites being nearest neighbours.

In those samples, the hopping couples two almost degenerate levels, resulting in a delocalization of one electron over these two sites (as pointed out in [20]).

If the mean spacing $\langle \Delta \rangle$ is bigger than $t$ (small size or very big $W$), the two coupled levels can be considered as a two-level system. Therefore the level spacing is

$$\Delta = \sqrt{(v_j - v_i)^2 + 4t^2}. \quad (8)$$

In the case where the sites $i$ and $j$ are not nearest neighbours $\Delta = v_j - v_i \simeq 0$. As a consequence, the special samples are responsible for the appearance of a dip and a peak in $P(s)$ at $s = 0$ and $s = 2t/\langle \Delta \rangle$, respectively.

On the other hand, if the mean spacing $\langle \Delta \rangle$ is smaller than $t$ (greater size and not too big $W$), typically more than two levels are coupled and eventually universal random-matrix-theory-like correlations can arise. Even though at intermediate sizes the spectral correlations are still greater in the special samples, their weight in the ensemble rapidly decreases with $L$. In the thermodynamic limit, the anomaly therefore disappears.

A.2 Interacting case

In the absence of hopping ($t = 0$), given a quite strong disorder $W$, it is always possible to find values of $U$ such that the two energetically lowest many-body states of a given sample are almost degenerate. For example, one can

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minimize the interaction energy (with a Wigner crystal) and the other one can be slightly different, increasing the interaction energy while reducing disorder energy.

Now, the first two many-body states can in certain samples be connected by only a single hop of one particle. The probability for such a situation is quite large since one many-body state is coupled to many others by the hopping of one of the particles.

In those samples, the introduction of the hopping couples directly two almost degenerate levels. If the values of $U$ and $W$ are strong enough, the particles remain localized on individual sites except the one implied in the connection of the two states. This results in a delocalization of the ground state in the on-site basis ($R = 2$).

For $\langle \Delta \rangle > t$ (small size or very big $W$), the two coupled levels can again be considered as a two-level system, and the non-universal correlations appear as explained previously.

For $\langle \Delta \rangle < t$ (greater size and not too big $W$), typically more levels are coupled and the two-level system approximation breaks down. As for the non-interacting case, this mechanism disappears in the thermodynamic limit. However, other mechanisms involving more hoppings can take place, and the competition between disorder and interaction might still induce delocalization and eventually stem the spectral correlations seen in [22].

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