

Ground-state properties of the two-dimensional disordered Hubbard model

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(Received 6 April 2000; revised manuscript received 18 May 2000)

We study the ground state of the two-dimensional disordered Hubbard model by means of the projector quantum Monte Carlo method. This approach allows us to investigate the ground-state properties of this model for lattice sizes up to 10×10 , at quarter filling, for a broad range of interaction and disorder strengths. Our results show that the ground state of this system of spin- $\frac{1}{2}$ fermions remains localized in the presence of the short-ranged Hubbard interaction.

I. INTRODUCTION

The electronic transport properties of disordered systems have been the subject of much investigation in physics. From the pioneering work of Anderson (1958),¹ it is known that in three dimensions (3D) the eigenstates of a noninteracting electron gas in a random potential become localized at the Fermi energy above a critical value of the disorder strength W_c . In this regime, the eigenstates decay exponentially in space and hence cannot carry a current; thus the system is an insulator. For disorder strength, W lower than W_c , the eigenstates are extended and diffusive transport takes place in the system in accordance with Ohm's law. However, for two-dimensional (2D) systems, it was shown by the scaling theory of Abrahams *et al.*² that all states are localized for any disorder strength. Thus, it appears that there is no metal-insulator transition (MIT) for noninteracting electrons in 2D. The properties of noninteracting electrons in random potentials have since been studied systematically and the main physical effects have been understood.³ In this context, the experimental observation by Kravchenko *et al.*⁴ of a transition from insulating to metallic behavior, as seen in the resistivity as a function of temperature of the 2D electron gas, came as a great surprise to the community. The existence of this transition from insulating to metallic behavior as a function of density has been confirmed by other groups.^{5–8} The experiments were carried out on very high mobility, low electron density (n_s) samples which correspond to a regime where the electron-electron interactions (E_{ee}) are much stronger than the Fermi energy (E_F), such that the dimensionless parameter $r_s (\approx E_{ee}/E_F)$ lies in the range 5–50. This indicates the importance of electron-electron interactions in these systems. Further, it was shown experimentally that the application of an in-plane magnetic field (B_p) drives the system insulating.⁹ Since such a field can only couple to the spin, this experiment indicates the important role played by the spin degrees of freedom. While the early experiments have stimulated a spate of new experimental results, there has been no satisfactory theoretical explanation of the phenomenon of the 2D MIT, to date.

The effects of interactions in disordered systems have been studied from the metallic side in great detail, where the interactions are relatively weak.¹⁰ The study of interactions in the localized phase were mainly carried out within the

mean-field approximation, which led to a number of important results, for example the Efros-Shklovskii gap in the density of states near the Fermi level,¹¹ but could not take into account quantum interference effects, important in this many-body system. The investigation of a simple model of two interacting particles (TIP) in the localized phase showed that short-range attractive/repulsive interactions can lead to destruction of localization and propagation of pairs of particles on a length scale much larger than the one-particle localization length.¹² Thus, the effects of interaction on the localized phase are nontrivial and deserve a detailed study. This, however, is not an easy task. Indeed, even the analytical expressions for the matrix elements of the interaction in the localized phase are not known,¹³ hence numerical studies of the problem become important.

Recent numerical approaches to the question have included the studies of persistent currents by exact diagonalization of small 2D clusters¹⁴ and Hartree-Fock-based calculations without¹⁵ and with residual interaction.^{16,17} These approaches led to some interesting indications but did not allow the study of sufficiently large systems and/or sufficiently many particles. Other approaches based on level spacing statistics of many-body states made possible the study of larger systems and showed the existence of ergodic (delocalized) states for low-energy excitations, but not at the ground state.¹⁸ All these studies were carried out for spinless fermions. Recently, the properties of fermions with spin on a disordered 2D lattice were investigated using a finite-temperature quantum Monte Carlo (QMC) method.¹⁹ The temperature dependence of the resistivity obtained numerically indicated a transition from insulating to metallic behavior for sufficiently strong interactions and weak disorder strength. However, these calculations were carried out at finite albeit low temperatures ($T \geq E_F/24$), and technical problems ("fermion sign problem") did not permit the analysis of the ground state. This is not completely relevant to the experiments which were carried out at temperatures much below the Fermi energy²⁰ and thus require a better understanding of the properties of the ground state, as in the general scenario of quantum phase transitions.

To investigate the properties of the ground state of the disordered interacting fermionic system, we choose the Hubbard model with site-diagonal disorder. This could be considered as an important first step on the way to investigations of more complicated models with Coulomb interactions, which might be more appropriate for experiments at low

densities. We study the ground state of our model on the square lattice by the projector QMC (PQMC) method. We use different characteristics to investigate the extent of the ground-state wave function for a broad range of model parameters: disorder strength (W), interaction strength (U), and filling factor (ν). The studies were carried out in the $S_z=0$ sector, with equal numbers of particles with up and down spins. This is thus the first numerical study to our knowledge of the ground state of a disordered, interacting system of fermions with spin.

This paper is organized as follows. In the next section, we describe the model and the method used. In the third section we present our results for the averaged Green function, the charge densities, and the inverse participation ratios, all of which we use to characterize the ground state. We present a summary of our conclusions in the final section.

II. MODEL AND METHOD

The two-dimensional disordered Hubbard model on a square lattice is given by

$$H = H_A + H_I$$

$$= \left(-t \sum_{\langle ij \rangle, \sigma} \hat{a}_{i, \sigma}^\dagger \hat{a}_{j, \sigma} + \sum_{i, \sigma} \epsilon_i \hat{a}_{i, \sigma}^\dagger \hat{a}_{i, \sigma} \right) + U \sum_i \hat{n}_{i \uparrow} \hat{n}_{i \downarrow}, \quad (1)$$

where the $\hat{a}_{i, \sigma}^\dagger$ ($\hat{a}_{i, \sigma}$) are the creation (annihilation) operators for a fermion of spin σ at site i with periodic boundary conditions, $\hat{n}_{i \sigma}$ is the number operator for spin σ at site i , t is the hopping parameter, the Hubbard parameter, U , measures the strength of the screened interaction, and ϵ_i , the energy of site i , is a random number drawn from a uniform distribution $[-W/2, W/2]$, which parametrizes the disorder. The first two terms represent the Anderson Hamiltonian and the last term represents the interaction H_I . In the limit $W=0$, this Hamiltonian reduces to the usual Hubbard model. The filling factor $\nu = N_p / (2 \times N^2)$, where N_p is the number of fermions (particles) and N is the linear dimension of the system; thus the total number of sites is N^2 .

We obtain the ground-state properties of this model by the PQMC method. The PQMC method was initially developed for the Hubbard model and has been used to obtain reliable results for large lattices.²¹ The method can be generalized in a straightforward manner to include random site energies. We now present some details of the calculation for completeness and refer the reader to the literature for more detailed accounts.

The PQMC method consists in obtaining the true ground state $|\psi_0\rangle$ of the Hamiltonian (1) by projection from a trial wave function $|\phi\rangle$ that is not orthogonal to the true ground state of the system,

$$|\psi_0\rangle = \lim_{\Theta \rightarrow \infty} \frac{e^{-\Theta \hat{H}} |\phi\rangle}{\sqrt{\langle \phi | e^{-2\Theta \hat{H}} | \phi \rangle}}. \quad (2)$$

The trial wave function is usually formed from the eigenstates of the noninteracting Hamiltonian (orbitals filled up to the Fermi level). In this case, we choose the eigenstates of the Hamiltonian H_A , thus including the random potential. To

carry out Monte Carlo (MC) simulations of this quantum Hamiltonian, it is first necessary to map it onto an effective classical Hamiltonian. Thus, the projection operator $\exp(-\Theta \hat{H})$ is first decomposed using the Trotter formula as $[\exp(-\Delta \tau \hat{H}_A) \exp(-\Delta \tau \hat{H}_I)]^L$ with $\Theta = \Delta \tau \times L$. This introduces a systematic error of order $(\Delta \tau)^2$ due to noncommutation of $\hat{H}_A$ and $\hat{H}_I$. The interaction is then decoupled by a discrete Hubbard-Stratonovich (HS) transformation, by the introduction of $N^2 \times L$ Ising-like fields. Since the complete summation over these degrees of freedom is too time-consuming to be practical, the method reduces to a MC sampling of physical properties, which is the second source of error, the statistical error. It is important to note that during the MC process, each configuration of Ising spins is assigned a weight, represented as a product of up- and down-spin determinants in this algorithm, which is interpreted as a probability. This quantity is positive definite only at half-filling for the uniform Hubbard model. The problems that arise from the nonpositive-definite nature of this quantity are referred to as the “fermion sign problem” in the literature and are known to be particularly severe slightly away from half-filling in finite temperature methods and restrict the lowest temperature that can be attained in the simulation (in the clean limit).

We have studied system sizes of up to 10×10 at quarter and one-eighth fillings (50 and 25 particles). We carried out extensive checks on the MC parameters to assure ourselves of convergence, as described in Ref. 22, but in the presence of disorder. Thus, we chose $\Theta = 3.0$, with $L = 30$, to have $\Delta \tau = 0.1$. The symmetric Trotter decomposition then reduces the systematic error to $(\Delta \tau)^3 \approx 0.001$. We checked for statistical convergence of our data in several ways. By varying the number of sweeps after equilibration, we determined that 1000 MC sweeps are sufficient for equilibration and 2000 further sweeps for property estimates. We carried out measurements until the standard deviations on our values were of the order of the systematic error. We also tested our results against results obtained from exact diagonalizations for small system sizes, and the results for the charge density, $n_i = n_{i \uparrow} + n_{i \downarrow} = \sum_\sigma \langle \hat{n}_{i \sigma} \rangle$, presented in Fig. 1 show good agreement with the exact results. Convergence is of course the best for the ground-state energy as compared to other physical quantities, and we have a relative accuracy of 10^{-3} when compared to exact calculations. As for the effect of disorder on the sign problem, it was possible to study the 10×10 lattice for $U/t = 6$ for disorder strengths W/t of up to 7–10. Our measure of the severity of the sign problem is to consider the quantity $f = 1 - (\text{number of negative determinants}) / (\text{total number of determinants})$. In all the cases considered, we have $f = 0.999$, which indicates that the sign problem is under control.

From the simulations, it is possible to obtain ground-state expectation values of the single-particle Green function, $G_{ij} = \sum_\sigma \langle \hat{a}_{i, \sigma}^\dagger \hat{a}_{j, \sigma} \rangle$, where the average is a MC average. Further, we can obtain ground-state expectation values of other one- and two-body operators, such as the charge density and the charge-charge correlation functions. Each disorder realization constitutes a full PQMC calculation. The properties are averaged over 16 disorder realizations. Thus, we have obtained the evolution of the Green function with distance,

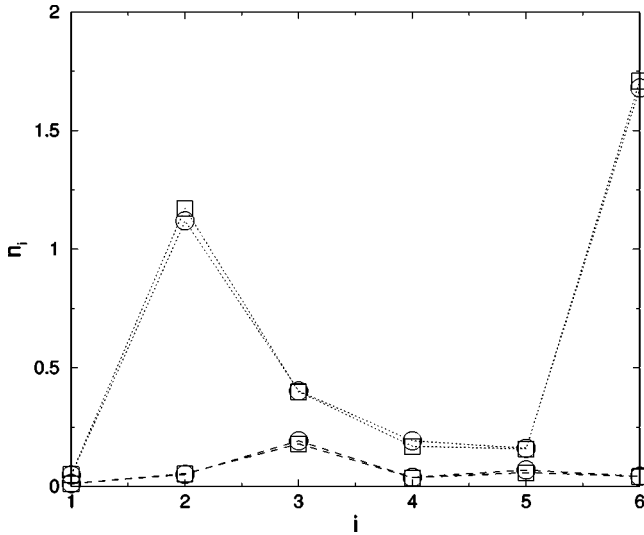


FIG. 1. Comparison of exact diagonalization (circles) and PQMC (squares) results for the charge density (n_i) per site (i) for a two-chain Hubbard model, dotted lines correspond to the upper chain and dashed lines to the lower chain, with system size 6×2 , $U/t=2$, $W/t=10$, and filling at four particles. The site energies used ϵ_i/t are $(4.28, -3.39, -0.45, -1.03, 0.99, -4.35)$ for the upper chain and $(1.47, 3.61, -0.78, 1.99, -0.56, 4.58)$ for the lower chain, which account for the low charge densities on the lower chain.

the charge densities, and the inverse participation ratios. Our results will be described in the following section.

III. RESULTS AND DISCUSSION

To characterize the properties of the ground state, we study the correlation function defined as

$$C(\mathbf{r}) = \frac{1}{N^2} \left\langle \sum_{i,j} |\langle \hat{a}_{i,\uparrow}^\dagger \hat{a}_{j,\uparrow} \rangle + \langle \hat{a}_{i,\downarrow}^\dagger \hat{a}_{j,\downarrow} \rangle|^2 \delta_{i-j,\mathbf{r}} \right\rangle, \quad (3)$$

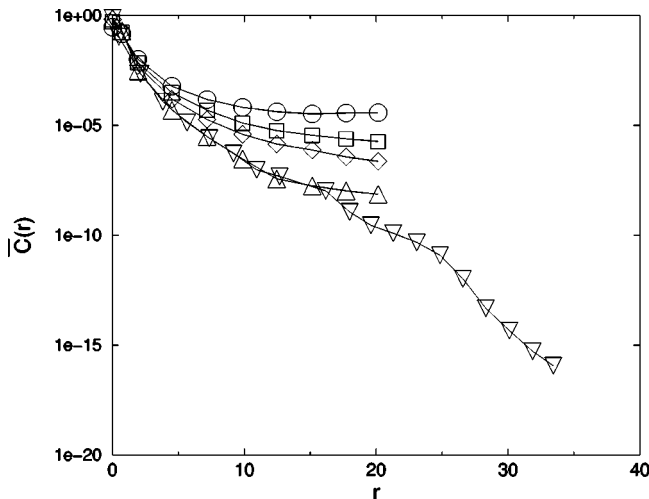
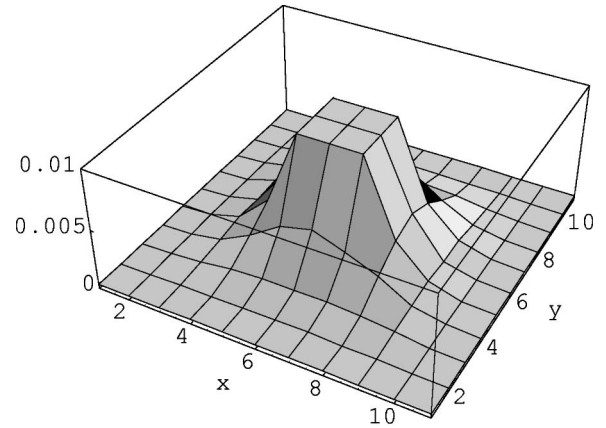
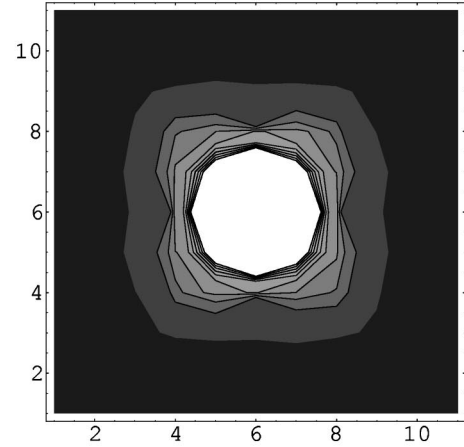


FIG. 2. The decay of the direction averaged correlation function $\bar{C}(r)$ vs r for a 30×30 system for $U/t=0$, with $W/t=2$ (circles), 7 (squares), 10 (diamonds), 15 (up-triangles), and a 50×50 system at $W/t=15$ (down-triangles), averaged over 16 disorder realizations, at quarter filling.



(a)

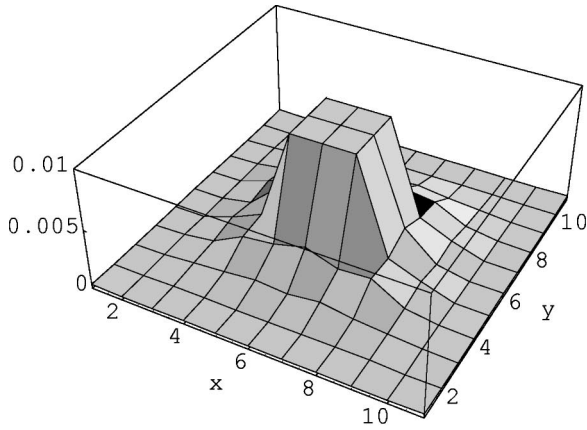


(b)

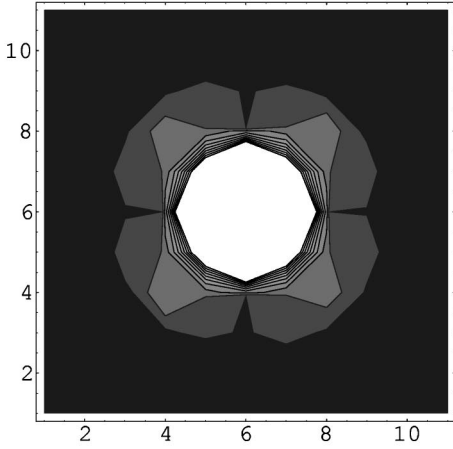
FIG. 3. Decay of $C(\mathbf{r})$ for Hamiltonian (1) with $U/t=0$, $W/t=7$, $N=10$, and $\nu=1/4$ (50 fermions on a 10×10 lattice), averaged over 16 disorder realizations. The upper part (a) shows the decay in 3D form for the interval $0 \leq C(\mathbf{r}) \leq 0.01$, the lower part (b) is a contour plot of the same data.

where $\mathbf{r}=\mathbf{i}-\mathbf{j}$ is the vector in the plane between the sites labeled i and j , and the averages are carried out over the ground-state eigenfunction and the different disorder realizations for all possible initial positions of $\mathbf{r}$, i.e., all corresponding i and j . $C(\mathbf{r})$ can be calculated from the Green function, $G_{ij} = \sum_{\sigma} \langle \hat{a}_{i,\sigma}^\dagger \hat{a}_{j,\sigma} \rangle$, already defined in Sec. II. Our present work is restricted to the study of equal-time characteristics. Thus, our study is complementary to the other finite-temperature QMC calculation¹⁹ that concentrated on approximate dynamical quantities and not on the structure of the ground-state wave function itself. We note that $C(0) = N^{-2} \langle \sum_i (n_{i\uparrow} + n_{i\downarrow})^2 \rangle \sim 4\nu^2$ in the limit of weak disorder and $C(0) \sim 4\nu$ in the strongly localized limit. The dependence of $C(r)$ on distance r is related to the localization of the eigenstate, i.e., we expect exponential decay of this quantity for localized states and slow decay at long distances for extended states, as discussed in greater detail in the next paragraph. We also study the direction-averaged correlation function $\bar{C}(r)$ which now depends only on the distance $r = |\mathbf{r}|$.

In Fig. 2, we show the decay of $\bar{C}(r)$ with r , for the 2D Anderson model, system (1) at $U/t=0$, for various disorder strengths. The change from flat behavior with r at weak dis-



(a)



(b)

FIG. 4. Same as in Figs. 3(a) and 3(b) with $U/t=6$ and the same disorder realizations.

order, when the eigenfunctions are delocalized in the finite-sized system ($W/t=2$), to asymptotic exponential decay for stronger disorder, $W/t \geq 10$ (when the localization length is smaller than the system size), is evident. We note that the initial nonexponential decay in the localized case is due to the fact that the ground-state eigenfunction is a superposition of one-particle eigenstates of different energies. In fact, the one-particle localization length l_1 of a state depends on its energy and therefore the many-body state, which is the Slater determinant of the one-particle states up to the Fermi level, initially decays more rapidly. This is due to the low-lying states of smaller localization lengths and it is only in the asymptotic limit that the decay of the many-body ground state is determined by the maximum l_1 at E_F . This physical structure of many-body states complicates the observation of asymptotic exponential decay corresponding to the one-particle localization length $l_1(E_F)$ at the Fermi level. Despite these complications, the asymptotic slope is seen to depend strongly on W (Fig. 2), which is consistent with the exponential growth of l_1 with decreasing W in 2D.³ Nevertheless, the equal-time characteristic $\bar{C}(r)$ does reflect the change from localized to delocalized eigenstates. In view of this, the investigation of the correlation function $\bar{C}(r)$ in the presence of interactions should tell us the impact of interactions on the localization properties of eigenstates.

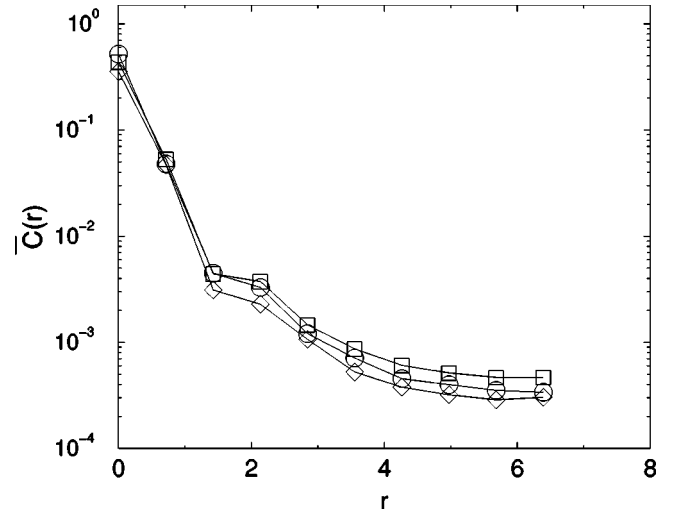


FIG. 5. The decay of the direction averaged correlation function $\bar{C}(r)$ vs r for the Hamiltonian (1) with $U/t=0$ (circles), 2 (squares), 6 (diamonds) for $W/t=7$, $N=10$, and filling $\nu=\frac{1}{4}$ (50 fermions on a 10×10 lattice), averaged over the same 16 disorder realizations.

The dependence of $C(r)$ on r , shown in Figs. 3(a) and 3(b) for the 2D disordered, noninteracting Hubbard model ($U/t=0$), also clearly shows localization of the ground-state eigenfunction. The decay [as seen from the contour plot Fig. 3(b)] is approximately symmetric in r , which is due to averaging over different disorder realizations. Hence, it should be useful to study this quantity also in the interacting case, to clarify the ground-state properties.

The behavior of $C(r)$ as a function of r , for relatively strong interaction strength ($U=6t$), is shown in Figs. 4(a) and 4(b). The comparison with the noninteracting case [Figs. 3(a) and 3(b)] clearly shows that even such a strong interaction produces only a slight change in the correlation function. We observe similar behavior for other disorder and interaction strengths ($5 \leq W/t \leq 10, 0 < U/t \leq 6, \nu = \frac{1}{4}, \frac{1}{8}$, results not presented here). This, in our opinion, provides direct

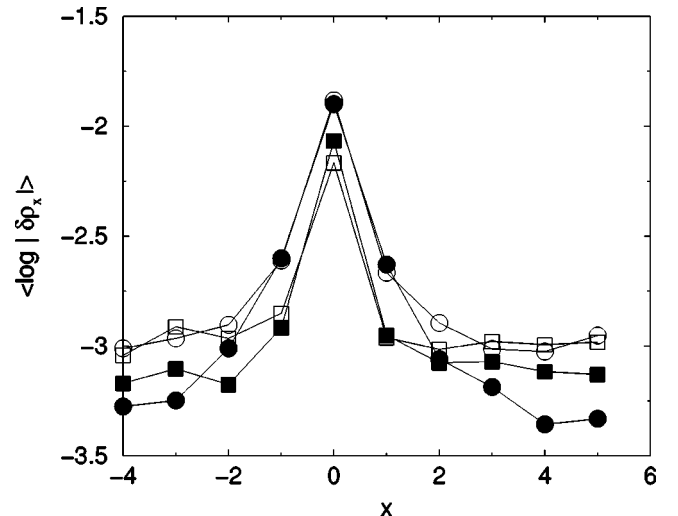


FIG. 6. Behavior of $\langle \ln |\delta \rho_x| \rangle$ with x for $U/t=0$ (filled symbols), 2 (open symbols) and $W/t=2$ (squares), 7 (circles) with $N=10$, $\nu=\frac{1}{4}$, and $a=1.1$, averaged over the same 16 realizations.

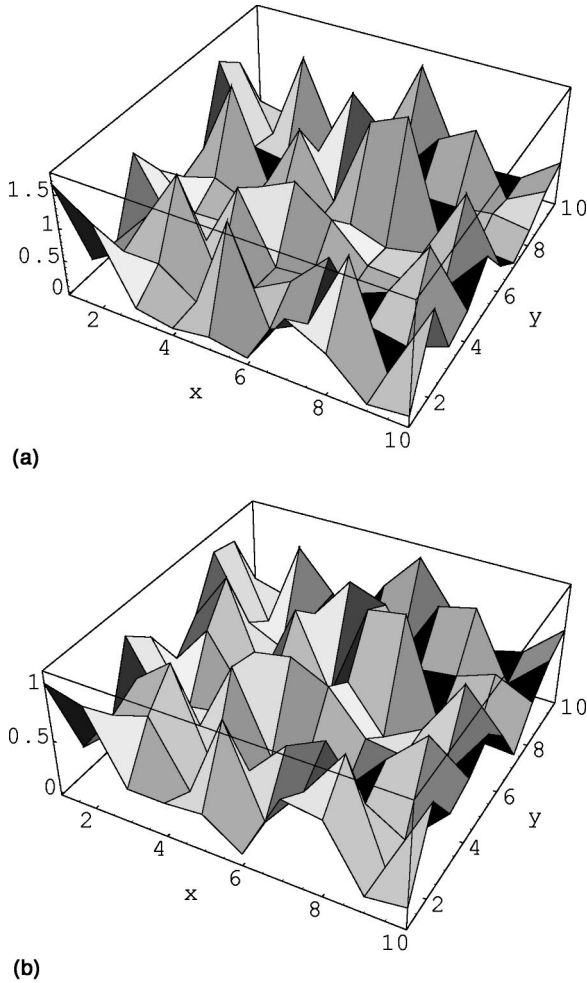


FIG. 7. Charge density (n_i) at site i for $U/t=0$ [upper figure (a)] and 6 [lower figure (b)] for a 10×10 lattice, $W/t=7$, $\nu=\frac{1}{4}$ for one realization of disorder.

evidence that even in the presence of strong interactions, the ground state of the system remains localized. This conclusion is further supported by the data for the direction-averaged correlation function, $\bar{C}(r)$, presented in Fig. 5. In fact, this direction average further smoothes fluctuations due to disorder. Indeed, even the introduction of relatively strong interactions ($U/t=6$) affects this function very weakly. Evidently, it would be desirable to study much larger system sizes and stronger disorder and interaction strengths (larger values of W/t and U/t) to see better asymptotic exponential decay. However, technical limitations prevent us from studying larger system sizes and more extreme parameter values. However, the very weak changes induced in $\bar{C}(r)$ by the interaction indicate the localized properties of the ground state.

As an alternative test for localization, we use another, more indirect method, similar to the approach presented in Ref. 23. As discussed in Ref. 23, we vary the amplitude of on-site disorder ϵ_i for sites i along one vertical line of the square lattice, as $\epsilon_i \rightarrow a \times \epsilon_i$ with $a=1.1$ and 1.3 , corresponding to 10% and 30% change in disorder. We then study the charge-density difference $\delta\rho_x$ produced by this perturbation, as a function of distance x from the original line. We average over all sites with the same x and additionally average $\ln|\delta\rho_x|$

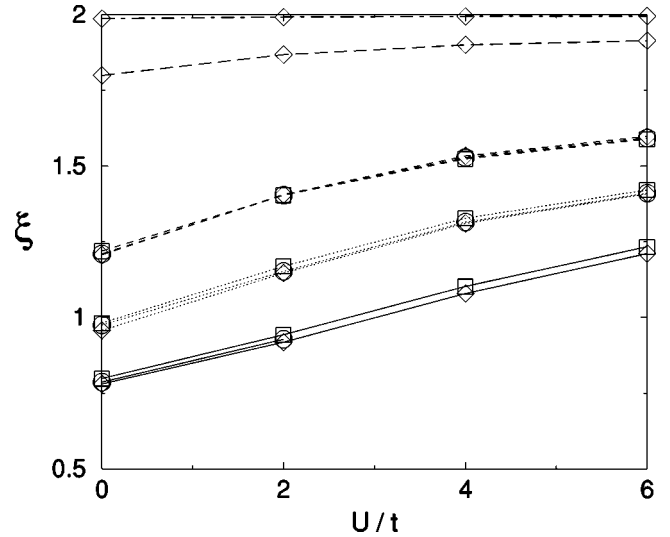


FIG. 8. IPR (ξ) vs U/t for system sizes 10×10 (circles), 8×8 (squares), and 6×6 (diamonds) and increasing disorder strength from top to bottom, $W/t=0.5$ (dot-dashed), 2 (long-dashed), 5 (dashed), 7 (dotted), and 10 (solid) lines, at quarter filling, averaged over the same 16 disorder realizations.

over 16 disorder realizations. The comparison of data for 10% and 30% variation shows that we are in the linear-response regime. The results are presented in Fig. 6. For $U/t=0$, the response function shows a sharp drop from the initial peak followed by a slower decay at longer distances. This behavior is qualitatively similar to the decay of the correlation function (Fig. 2, Fig. 5), for the same physical reasons as analyzed above. Introducing interactions does not affect the main structure of the curve at all, which drops very quickly from the center by more than one order of magnitude. We interpret this as a sign of a localized ground state. At the same time, we note that there is a slight difference introduced by interactions at the tails of the response functions. However, this corresponds to a density variation less than 0.1%, which is at the limit of the accuracy of our calculation. In light of the ensemble of data, we conclude that the ground state in the presence of interactions remains localized.

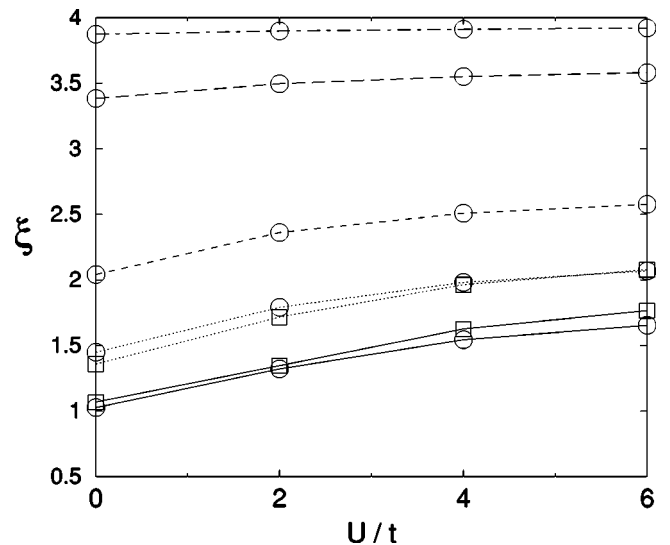


FIG. 9. Same as in Fig. 8 for system sizes 8×8 (circles) and 4×4 (squares) at $\frac{1}{8}$ filling.

In a sense the Hubbard repulsion leads to local rearrangements of charge and does not seem to influence the long-distance properties of the system. This is clearly illustrated in Figs. 7(a) and 7(b), where the interaction leads to a more homogeneous charge distribution (note the change in the vertical scale) but does not drastically change the global profile. At the same time, it is known that there exist situations where the short-range Hubbard interaction can qualitatively change the situation and introduce long-range order. However, our data show that this is not the case in the present situation, with disorder.

This point of view is further borne out by the data for the inverse participation ratio (IPR), ξ , presented in Fig. 8. The IPR, defined as $\xi = (\sum_i n_i)^2 / (N \sum_i n_i^2)$, gives the average number of sites visited per particle. While initially developed for noninteracting systems, the same characteristic has been used as well for many-body systems.^{14,17} The value of ξ is bounded from above at fixed filling, with $\xi \leq \xi_{\max} = (2\nu)^{-1}$, corresponding to the weak disorder limit and from below with $\xi \geq \xi_{\min} = 0.5$ in the strongly localized limit. We note that $C(0) \times \xi = 2\nu$. We have studied the IPR as a function of system size and interaction strength at $\frac{1}{4}$ (Fig. 8) and $\frac{1}{8}$ (Fig. 9) filling. At $U/t = 0$, the IPR naturally increases with decreasing disorder as states become more extended. At strong disorder ($W/t \geq 5$), ξ is not sensitive to the system size since the states are localized and at fixed filling the IPR is counted per particle. The Hubbard interaction smoothly increases the IPR but does not introduce a qualitative change. This corresponds to the local reorganization of charge introduced by U leading to a more homogeneous charge-density distribution, as discussed above. The data presented for $\frac{1}{8}$ filling in Fig. 9 show qualitatively similar behavior. However, the size variation is more restricted in this case ($N \leq 10$ in our studies).

At this point, it is interesting to compare our studies with a recent finite-temperature QMC study of a similar model.¹⁹ These authors considered the Hubbard model on a square lattice, with off-diagonal disorder, in contrast to our study. This is due to the fact that the method used, a finite-temperature QMC method, suffers from a severe sign problem in the presence of diagonal disorder. For off-diagonal

disorder, the situation becomes better, but the problem persists, restricting the lowest accessible temperatures. Their studies of several physical characteristics, including the conductivity (obtained by approximate analytic continuation of the imaginary time Green function), indicate the presence of an interaction-induced metal-insulator transition in their model. However, this method is not adapted to analysis of the ground-state properties. Our results are not in direct contradiction with this study, since it is fully possible that the ground state remains localized, while the low-lying excited states become delocalized. Such a situation has been observed in numerical studies of spinless fermions with Coulomb interactions on a 2D lattice with disorder.¹⁸ Our result directly demonstrates the localized nature of the ground state even in the presence of strong interactions. This is important in the framework of general studies of zero-temperature quantum phase transitions.

IV. CONCLUSIONS

We have used the projector quantum Monte Carlo (PQMC) method to study the ground state of the 2D disordered Hubbard model. This method allows us to study systems of up to 50 spin- $\frac{1}{2}$ fermions on a 10×10 lattice, for interaction strengths U/t up to 6 and a broad interval of disorder strengths. The comparison of several properties in the absence and presence of the Hubbard interaction allows us to conclude that interactions lead to local rearrangements of charge but do not destroy the localized structure of the ground state, within the range of parameter values studied.

These results indicate that short-range interactions are probably insufficient to bring about a quantum phase transition in the ground state of this system. Thus, it becomes important to consider the effect of long-range Coulomb interactions for electrons on a disordered lattice.

ACKNOWLEDGMENTS

We thank M.-B. Lepetit for useful discussions and the IDRIS, Orsay, for allocation of resources on their supercomputers.

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