Transition to an insulating phase induced by attractive interactions in the disordered three-dimensional Hubbard model

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We study numerically the interplay of disorder and attractive interactions for spin-1/2 fermions in the three-dimensional Hubbard model. The results obtained by projector quantum Monte Carlo simulations show that at moderate disorder, increasing the attractive interaction leads to a transition from delocalized superconducting states to the insulating phase of localized pairs. This transition takes place well within the metallic phase of the single-particle Anderson model.

Two limiting cases of the nontrivial problem of quantum transport in three dimensions (3D) in the presence of disorder and attractive interactions between particles were worked out by Anderson in the late 1950s.[1,2] In the limit of weak interactions, the increase of disorder leads to the Anderson transition from metallic transport to the localized insulating phase,[1] whereas, in the absence of disorder, attractive interactions between spin-1/2 fermions lead to the appearance of BCS superconductivity which is not affected by the introduction of weak disorder.[2] These limiting cases have been extensively investigated and detailed information is now available for the one-particle Anderson transition (see, e.g., Refs. 3–5) and the weakly disordered BCS superconductor (see, e.g., Refs. 6–8). However, a theoretical treatment of the intermediate regime, where both disorder and interactions are important, is difficult due to the absence of relevant small parameters. New results on the physical properties of transport in this regime are therefore of fundamental interest. Furthermore, an understanding of this realistic regime would contribute to the interpretation of recent experiments on 3D superconductor materials (InO in Ref. 9, α-Mo$_3$Si and α-Nb$_3$Ge in Ref. 10), where both disorder and interactions are naturally present. For example, an explanation of the unusual resistivity dependence on magnetic field observed in Ref. 9 requires a better understanding of the interplay between disorder and attractive interactions. In addition, recent breakthroughs in cold-atom experimental techniques have provided new possibilities for investigations of interacting atoms on 3D optical lattices, leading to the observation of a superfluid to Mott insulator quantum phase transition for ultracold atoms.[11] These extremely clean experiments open unprecedented possibilities for precise studies of lattice models with experimentally tunable interactions and provide new challenges for theoretical investigations of interacting bosons and fermions.[12]

Numerical simulations provide a valuable tool for the study of the nontrivial regime where both interactions and disorder play a relevant role. Among various numerical approaches, quantum Monte Carlo methods constitute the most promising possibility for the simulation of systems with a large number of particles.[13–17] These methods have several advantages compared to exact-diagonalization approaches

which are restricted to a relatively small number of particles.[18,19] In this work we use the projector quantum Monte Carlo (PQMC) method to perform numerical simulations of the 3D Anderson transition in the presence of attractive interactions. To the best of our knowledge, this approach allows us to study this interesting problem for the first time.

To investigate the interplay of disorder and attractive interactions, we study numerically the disordered 3D Hubbard model with N fermions on a cubic lattice with L^3 sites. The Hamiltonian is defined by

$$H = -t \sum_{\langle \mathbf{ij} \rangle \sigma} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} + \sum_{\mathbf{i}\sigma} \epsilon_{\mathbf{i}} n_{\mathbf{i}\sigma} + U \sum_{\mathbf{i}} n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}, \qquad (1)$$

where $c_{\mathbf{i}\sigma}^{\dagger}$ ($c_{\mathbf{i}\sigma}$) creates (destroys) a spin-1/2 fermion at site $\mathbf{i} = (i_x, i_y, i_z)$ with spin σ, and $n_{\mathbf{i}\sigma} = c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{i}\sigma}$ is the corresponding occupation number operator. The hopping term t between nearest-neighbor lattice sites parametrizes the kinetic energy and the random site energies $\epsilon_{\mathbf{i}}$ are homogeneously distributed in the interval $[-W/2, W/2]$, where W determines the disorder strength. The parameter U measures the strength of the short-range effective Hubbard attraction ($U < 0$) and periodic boundary conditions are taken in all directions. At $U = 0$, the Hamiltonian (1) reduces to the one-body Anderson model, which exhibits a metal-insulator transition in three dimensions.[3–5] We remind the reader that, contrary to the 3D case, all states are localized in 2D at $U = 0$ and $W \neq 0$.[3–5] For $W = 0$ the Hamiltonian corresponds to the clean attractive Hubbard model, with a superconducting ground state in 3D.

We study this model by the PQMC method, which is an efficient method for investigation of the ground-state properties of interacting fermion systems. For attractive Hubbard interactions ($U < 0$), there is no sign problem and the method is exact up to discrete time steps and statistical errors, which can be well controlled.[14,20] We consider $N = 14$, 32, 62, and 108 particles on a cubic lattice of size $L = 3$, 4, 5, and 6, respectively, at an approximately constant filling factor $\nu = N/(2L^3) \approx 1/4$, $2 \leq W/t \leq 10$, and $U/t = -4$. For each disorder realization, we used a discrete Trotter decomposition with a time step $\Delta \tau = 0.1$ and projected through 60 time steps. In total we carried out 3000 Monte Carlo sweeps for each simulation, with approximately 1000 sweeps for equili-

bration. With these PQMC parameters we obtained good convergence of the computed physical quantities. The results are averaged over $N_R \geq 12$ disorder realizations, except for the most time-consuming simulations at $L=6$, where $N_R = 6$. The simulations are carried out in the sector with the total spin component $S_z=0$, which always contains the ground state.

A quantitative measure of the localization properties of the system can be obtained, even in the presence of interactions. It is based on the probability density distribution for an added pair at the Fermi edge. This distribution is approximately equal to the charge density difference $\delta\rho(\mathbf{i}) = \rho(\mathbf{i},N+2) - \rho(\mathbf{i},N)$, where $\rho(\mathbf{i})$ is the ground-state charge density at site $\mathbf{i}$ [$\Sigma_{\mathbf{i}}\delta\rho(\mathbf{i})=2$]. The values of $\rho(\mathbf{i},N)$, $\rho(\mathbf{i},N+2)$ are obtained from two independent PQMC simulations for the same disorder realization. For $U=0$, this difference is identical to the single-particle probability distribution for the eigenstate $\psi_F(\mathbf{i})$ of the Anderson model at the Fermi level, with $\delta\rho(\mathbf{i})/2 = |\psi_F(\mathbf{i})|^2$. From this distribution, we obtain the inverse participation ratio (IPR) for an added pair, $\xi = \{\Sigma_{\mathbf{i}}[\delta\rho(\mathbf{i})/2]^2\}^{-1}$, which determines the number of sites visited by this pair. At $U=0$, this quantity reduces to the usual one-particle IPR at the Fermi level. For $U \neq 0$, since the interaction is short ranged, ξ still determines the localization properties of pairs in the vicinity of the Fermi level.

A typical example of $\delta\rho(\mathbf{i})$ for an added pair is shown in Fig. 1 for a single disorder realization. For graphical representation $\delta\rho(\mathbf{i})$ is projected on the (x,y) plane, giving $\delta\rho_p(i_x,i_y) = \Sigma_{i_z}\delta\rho(i_x,i_y,i_z)$. The plots of Fig. 1 (left) refer to the weakly disordered regime ($W/t=2$). They clearly show delocalization of the added pair, both for free particles (top, $U=0$) and for the attractive Hubbard model (middle, $U/t=-4$). It should be noted that this disorder strength is much smaller than the critical disorder strength of the 3D Anderson transition which takes place at $W < W_c(U=0) \approx 16.5t$.[21] Therefore, these results confirm Anderson's theorem[2] according to which the Cooper pairs remain delocalized at weak disorder. Thus, the superconducting phase is not affected by weak disorder, since Cooper pairs can be formed by pairing the time-reversed eigenstates of the corresponding noninteracting disordered problem.

A qualitatively new situation appears at a stronger disorder strength $W/t=7$ [Fig. 1 (right)]. Here, the two added particles are delocalized at $U=0$, since we are still inside the metallic single-particle phase $W < W_c(U=0)$. On the contrary, a pronounced peak appears for $\delta\rho(\mathbf{i})$ at $U/t=-4$, clearly showing the formation of localized pairs. This is borne out by the IPR which drops from $\xi=55$ at $U=0$ to $\xi=6.5$ at $U/t=-4$. This effect gives an indication that attractive interactions induce localization in the metallic regime of the noninteracting model, leading to the formation of a new phase of biparticle-localized states.

The results of the Bogoliubov–de Gennes (BdG) mean-field calculation[6,22] are shown in the two bottom plots of Fig. 1. We note that, within the BdG approach, at weak disorder strengths ($W/t=2$), interactions smooth out charge fluctuations, leading to an increase of the IPR, from $\xi=70$ at $U=0$ to $\xi=132$ at $U/t=-4$. On the contrary, at stronger
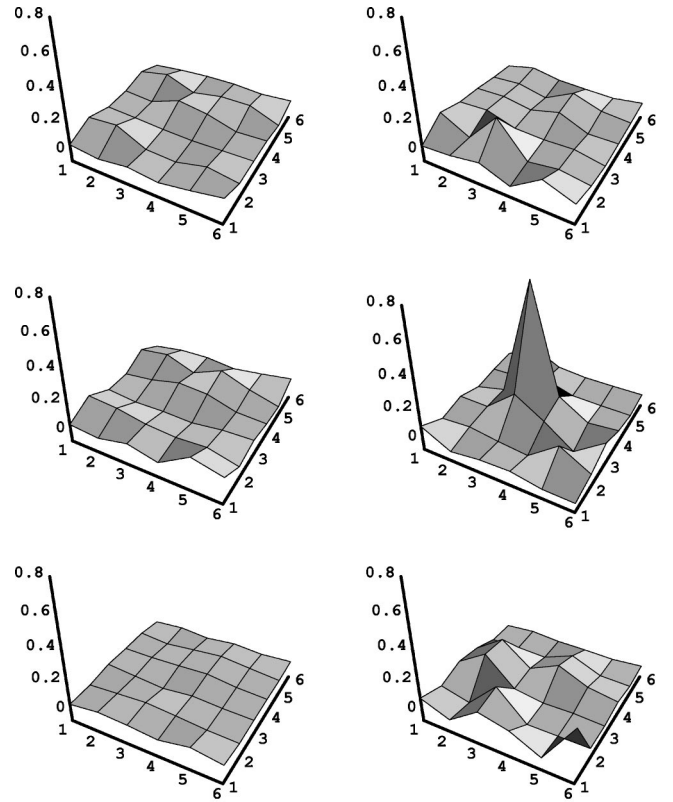

FIG. 1. Distribution of charge density difference for an added pair, $\delta\rho_p$, projected on the (x,y) plane for a $6 \times 6 \times 6$ lattice for the same single disorder realization, with $W/t=2$ (left) and $W/t=7$ (right), $N=108$. Top: exact computation for $U=0$, $\xi=70;55$ (left; right). Middle: PQMC calculation for $U/t=-4$, $\xi=48;6.5$ (left; right). Bottom: BdG mean-field calculation for $U/t=-4$, $\xi = 132;25$ (left; right). All quantities presented in all figures are in dimensionless units (see text).

disorder strengths ($W/t=7$) interactions slightly favor localization even within BdG approximation where the IPR drops from 55 to 25 when U/t goes from 0 to -4. This happens because the mean-field treatment of interactions introduces a site-dependent Hartree shift $U_H(\mathbf{i}) = |U|\rho(\mathbf{i})/2$.[22] At strong disorder, when the charge density $\rho(\mathbf{i})$ is highly inhomogeneous, this term acts as an additional disorder potential.[23] However, the main problem with the BdG approach is that many local minima appear and convergence is lost even at moderate disorder strengths and system sizes ($W/t>7, L \geq 6$). Furthermore, it is clear that important effects due to quantum phase fluctuations are beyond the mean-field approximation and thus localization of pairs cannot be reproduced within the BdG approach (see Fig. 1 at $W/t=7$).

A more quantitative description of the localization effect induced by attractive interactions can be seen from the dependence of IPR $\langle\xi\rangle$ on disorder strength, W, shown in Fig. 2, with $\langle\xi\rangle$ averaged over realizations of disorder. The data clearly show that interactions lead to a significant reduction of $\langle\xi\rangle$. For $U=0$, the dependence of $\langle\xi\rangle$ on W is characterized by two distinct regions: a relatively flat region for large W where $\langle\xi\rangle$ slowly approaches the asymptotic value of 1 and another region in which $\langle\xi\rangle$ grows with decreasing W. At very weak disorder $\langle\xi\rangle$ remains bounded by the total number
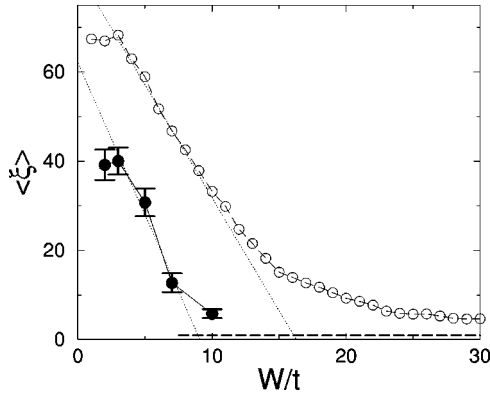
FIG. 2. Inverse participation ratio $\langle \xi \rangle$ averaged over disorder realizations, as a function of disorder strength W for a $6 \times 6 \times 6$ lattice, at $U=0$ (open circles) and $U/t=-4$ (solid circles). Dotted lines show linear fits to the data, the dashed line represents $\xi=1$ (see text), and error bars indicate statistical errors.

of lattice sites. The linear fit of the $\langle \xi \rangle$ data in the second region crosses the $\langle \xi \rangle = 1$ line at $W_c(U=0) \approx 16t$ which is very close to the exact value of W for the Anderson transition for noninteracting particles, $W_c \approx 16.5t$.[21] A similar analysis carried out for the $\langle \xi \rangle$ data in the presence of interactions gives transition from delocalized to localized pairs at $W_c(U=-4t) \approx 9t$. This can be considered as a new phase of bi-particle localized states (BLS phase).

Further evidence for the interaction-induced transition comes from a finite-size scaling analysis. The relevant dimensionless quantity for such an analysis is the system conductance $g(L)$.[3,24] For large $g(L)$, the macroscopic transport theory in the 3D delocalized phase gives $g(L) \propto L \propto \xi/L^2$ since $\xi \propto L^3$ for delocalized wave functions. For the localized phase, ξ is determined by the localization length l and is independent of the system size L, with $\xi \sim l^3$. Hence, the ratio ξ/L^2 falls off as $1/L^2$ in this regime. Therefore the transition point $g(L) \approx 1$ can be located from the condition $\xi(L)/L^2 = $ const. The results of the finite-size scaling analysis for the scaled ratio ξ/L^2 are shown in Fig. 3 for $3 \leqslant L \leqslant 6$. The range of disorder values studied ($3t \leqslant W \leqslant 10t$) corresponds to the metallic side of the single-particle Anderson transition. Therefore the scaling analysis at $U=0$ shows an increase of ξ/L^2 with system size. A strikingly different situation appears at $U=-4t$: at $W/t=3$ and 5 the scaling ratio ξ/L^2 still grows with system size, while at $W/t=7$ and 10 this quantity drops with L. This suggests the appearance of a superconductor-to-insulator transition induced by attractive interactions, with the transition point $W_c(U=-4t) \approx 6t$ at the thermodynamic limit. This value is in reasonable agreement with the value obtained for a single system size in Fig. 2. A precise location of the transition point would require a significant increase of the system sizes and a larger number of disorder realizations. However, the results obtained in the present study clearly show the transition to an insulating phase at disorder strengths, being less than half the value of the critical disorder strength for the single-particle Anderson transition. Hence, in the presence of attractive interactions, the insulating phase penetrates inside the metallic noninteracting phase. This unexpected result can be understood on
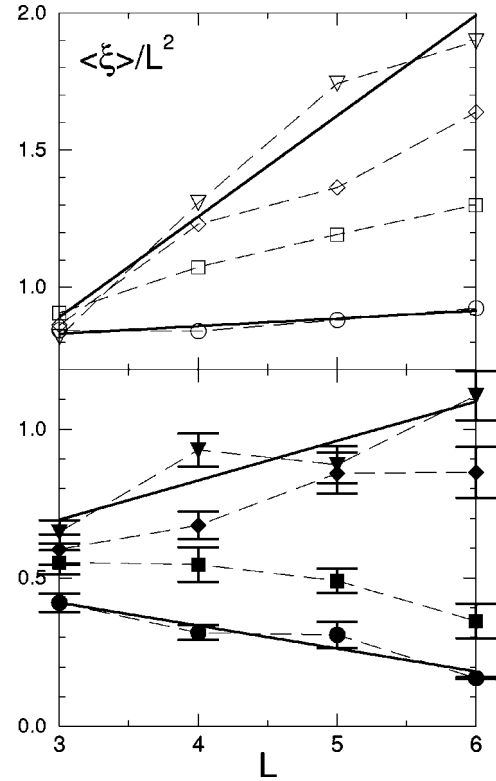

FIG. 3. Dependence of the scaled inverse participation ratio $\langle \xi \rangle / L^2$ on the linear dimension of the system, L, for $U=0$ (top) and $U/t=-4$ (bottom), with $W/t=3$ (triangles), 5 (diamonds), 7 (squares), and 10 (circles). Error bars show statistical errors. The straight line fits show the average dependence on L for the extremal values of W studied, designating the transition from superconducting to insulating behavior for $U/t=-4$.

the basis of the following physical argument.[25] The attractive interaction creates pairs of effective mass $m^\star$ twice as large as the single-fermion mass m. This halves the effective hopping term $t^\star \propto 1/m^\star = 1/2m$ which induces an increased effective disorder $W/t^\star = 2W/t$ and thus enhances localization effects. Such an argument predicts a decrease in critical disorder strength by a factor of 2, which is in reasonable agreement with our results. However, we note that at values of the attractive interaction $|U| \gg W, t$, it would be necessary to modify the argument given above. When $|U| \gg W, t$, the attractive Hubbard model can be mapped onto a model of hard-core bosons, with effective hopping $t^\star = 2t^2/|U|$ and with effective disorder $W^\star = 2W$. In this limit, the effective disorder strength $W^\star/t^\star = W|U|/t^2$. However, in the present study at $|U|=4t$, $2t \leqslant W \leqslant 10t$, we are rather far away from the preceding limit. We note that the appearance of a bound pairs phase has been recently discussed in the framework of dynamical mean-field theory for attractive interactions at $W=0$.[26]

In conclusion we show that in disordered systems, attractive interactions that lead to superconductivity at weak disorder also lead to the insulating phase of localized pairs at moderate disorder strengths, well within the metallic phase of noninteracting fermions. Thus, by increasing the attraction

strength, one can go from superconducting to insulating behavior. This is also possible by increasing disorder. Of course, experimentally, it is not easy to vary the interaction and disorder strengths. However, indirectly, this can be achieved by introducing a relatively strong magnetic field. This magnetic field can increase the effective disorder strengths since it forces an electron to return to the impurity.[27] At the same time, it also effectively decreases attraction by pair breaking. Thus, the increase of magnetic field may first increase the disorder and drive the system from superconductor to insulator with localized pairs as seen experimentally in InO films.[9] Further increase of magnetic field breaks pairs and leads to a transition from the insulating phase of localized pairs to a metallic phase of almost noninteracting fermions. Such a scenario leads to a transition from superconductor to insulator, followed by an insulator-to-metal transition with increasing magnetic field, in qualitative agreement with experimental observations.[9]

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