Disorder and Interaction in 2D: Exact Diagonalization Study of the Anderson-Hubbard-Mott Model

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We investigate, by numerically calculating the charge stiffness, the effects of random diagonal disorder and electron-electron interaction on the nature of the ground state in the 2D Hubbard model through the finite-size exact diagonalization technique. By comparing with the corresponding 1D Hubbard model results and by using heuristic arguments we conclude that it is *unlikely* that there is a 2D metal-insulator quantum phase transition, although the effect of interaction in some range of parameters is to substantially enhance the noninteracting charge stiffness.

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A question of fundamental importance is whether the ground state of an interacting disordered electron system is a metal, an insulator, or some other state (e.g., superconductor). This question takes on particular significance in two-dimensional (2D) systems where it is generally accepted that (1) the disordered 2D system in the absence of any interaction is a localized (weakly localized for weak disorder) insulator, and (2) the interacting clean 2D system is a Fermi liquid metal at high electron densities (and a Wigner crystal at low electron densities). Little is known about the disordered interacting system when both disorder and interaction are strong and of comparable magnitudes so that neither may be treated as a perturbation. A notable attempt [1] by Finkel'stein to analytically explore the nature of the disordered interacting electron system remains inconclusive as the theory flows toward strong coupling. Recently renewed interest has developed [2] in this subject with much of the current motivation arising from a set of experimental measurements on the low temperature transport properties of low density 2D electron (or hole) systems confined in Si MOSFETs and GaAs heterostructures. These transport measurements (carried out as a function of carrier density) have been interpreted [2] by many (but *not* all) as exhibiting evidence for a 2D metal-insulator quantum phase transition (MIT) with the system being a metal at high density n ($>n_c$) and an insulator at low density ($n < n_c$) with n_c as the critical density separating the two phases. Much interest has naturally focused on this possible 2D MIT quantum phase transition, particularly because the corresponding noninteracting disordered 2D electron system is thought on rather firm grounds [3] to be always localized (Anderson localization) and therefore strictly an insulator at $T = 0$ in the thermodynamic limit. If such a 2D MIT exists it is of great interest because the metallic phase must be a non-Fermi liquid since it cannot be adiabatically connected to the corresponding insulating noninteracting 2D disordered system.

In this Letter we address the nature of the ground state of a disordered interacting 2D electron system numerically by exactly diagonalizing the few particle 2D interacting Hamiltonian and doing a disorder averaging. We use the extensively studied 2D Hubbard model [4] and its natural extensions for our exact diagonalization calculations. We study the effects of both on-site and longer range interactions whereas the disorder in our model is a random on-site disorder of strength W. Without interaction, our model is the 2D Anderson model, which has a localized insulating ground state, whereas without disorder our model is the Mott-Hubbard model which has an extended metallic ground state away from half filling. We restrict to low "metallic" filling factors (typically less than quarter filling). Our typical exact diagonalization study uses the Lanczos technique for $N = 6$ electrons (with spin) on a 4×4 2D lattice, corresponding to a filling of $\nu = 6/32 = 3/16$. This involves the diagonalization of matrices of $313\,600^2$ size. We typically average over 10 disorder realizations. Following standard notations [4] three parameters t (the hopping amplitude), U (the on-site interaction strength), and W (disorder strength) parametrize our minimal Anderson-Hubbard model. We carry out our exact diagonalization in the subspace of the total number of electrons N and the total spin component $S_z = [-(N - M)/2 + M/2]$ with M being the number of spin up electrons. We note that the Hilbert space grows exponentially with the system size, and the results presented in this work are the essential current limit on what can be achieved via the exact diagonalization technique for this problem.

To characterize the nature of the ground state, i.e., its localization properties, we use the technique [5] suggested by Kohn a long time ago and calculate the charge stiffness D_c, sometimes also referred to as the Drude weight, of the finite system. We calculate charge stiffness for each individual disorder realization exactly through our finite-size diagonalization, and then obtain the root mean square average by averaging over a number of disorder realizations. The charge stiffness D_c, which is simply related to the persistent current [6], is the zero frequency weight of the long

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wavelength conductance (i.e., the Drude weight) in the system. As such, it is finite for a metal or a conductor and is zero for an insulator or a localized system in the thermodynamic limit [5]. Charge stiffness (or persistent current magnitude) has been extensively used in the literature in finite-size numerical localization studies [7] of disordered interacting systems, and it is empirically well known that the calculation of D_c in finite systems is an extremely effective way of numerically studying the localization problem in the presence of both interaction and disorder.

In Fig. 1 we show our calculated disorder-averaged charge stiffness for the 4×4 2D Hubbard cluster (with 6 electrons) as a function of the on-site repulsion U for various values of the disorder strength W. In the absence of any disorder ($W = 0$), the clean 2D Hubbard model away from half filling is expected to be a metal with a finite value of D_c, whereas the corresponding 2D Anderson model ($U = 0$, $W \neq 0$) is expected to be a weakly localized insulator for small W (crossing over to an exponentially strongly localized insulator for large W). The numerical results for these limiting cases ($W = 0$, $U \neq 0$ and $W \neq 0$, $U = 0$) are also shown in Fig. 1 for the sake of comparison and completeness.

The most important generic feature of the results shown in Fig. 1 is the peak in the charge stiffness at an intermediate value of $U \equiv U_c \sim W$ where the calculated charge stiffness for the finite 2D cluster has a maximum for a given disorder strength W. The charge stiffness D_c appears to decrease from this peak value (for a given W) for both $U \gtrless U_c$. Note that D_c increases sharply from $U = 0$ to $U = U_c$, and then decreases slowly for $U > U_c$. This peak or the maximum in D_c is rather manifest in Fig. 1 for $W/t = 5$ and 3 (i.e., for strong disorder) whereas for weak disorder (e.g., $W/t = 0.5$ in Fig. 1) the peak occurs at somewhat larger values of $U/W \gtrsim 2$ and is not so obvious from Fig. 1 (we have explicitly verified that the peak exists for $W/t = 0.5$ also). The actual value of U_c/t clearly depends on the disorder strength W, increasing with W/t from $U_c/t \simeq 0.95$ for $W/t = 0.5$ through $U_c/t \simeq 3.0$ for $W/t = 3$ to $U_c/t \simeq 3.5$ for $W/t = 5$. The qualitative behavior of our results is explained by the competition between U and W in the Anderson-Hubbard model. In a disordered system the random potential W favors a maximal occupation (double occupation for our spin 1/2 electrons) of the lowest energy sites. The on-site repulsion U, on the other hand, opposes double occupancy and favors configurations with a minimal number of double-occupied sites. This competition between W and U, where W tends to localize the charge density and U tends to homogenize the charge density, is a well-known feature [6] of the disordered Hubbard model. The results shown in Fig. 1, in particular the increase of D_c as U increases from zero for a fixed disorder strength W, is a direct result of the competition. Note that the actual crossover behavior of $D_c(U, W, t)$ shown in Fig. 1 cannot be parametrized by the single parameter; $U/W - D_c$ depends on both U/t and W/t. We have carried out similar calculations in an "extended" Anderson-Hubbard model with a long-range interaction (in addition to U) with results qualitatively similar to those shown in Fig. 1.

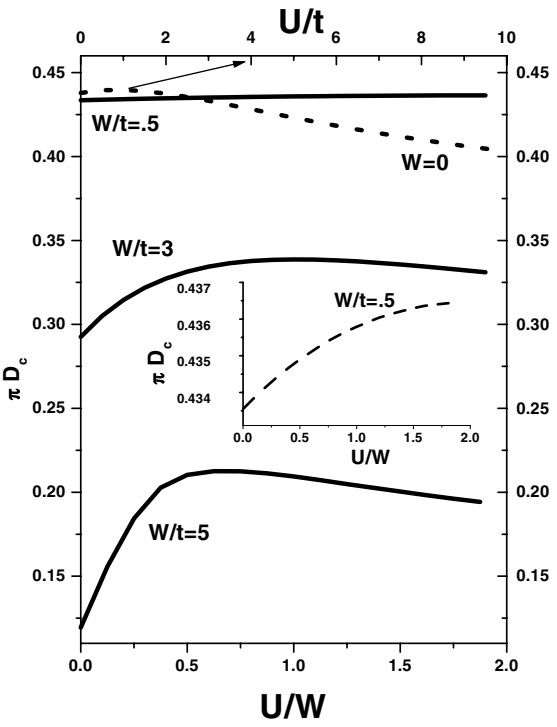

FIG. 1. The rms (averaged over 10 disorder realizations) charge stiffness D_c as a function of onsite repulsion U in the 2D 4×4 disordered Hubbard cluster for 6 electrons. Results for four values of disorder ($W/t = 5$, 3, 0.5, 0) are shown with the abscissa for the clean ($W = 0$) system in the top. The inset shows D_c for $W/t = 0.5$ in an expanded scale.

The direct interpretation of our exact finite-size results shown in Fig. 1 is that the conductance of a finite disordered 2D system increases when the interaction is turned on (at a fixed disorder), reaching a maximum for $U = U_c \sim W$, and then it decreases slowly with still increasing U. The issue of applying these numerical results based on 4×4 2D clusters to address the fundamental question of 2D MIT is, however, extremely tricky. For example, one popular recent line of thinking, based mostly on numerical work involving spinless electrons in finite 2D systems [7], has been to interpret equivalent results on interaction-enhanced conductance as evidence in favor of a 2D MIT, with the peak in D_c at $U \sim U_c$ being interpreted as an intermediate metallic phase. We disagree with this interpretation for reasons to be discussed below.

Our conclusion that the charge stiffness results depicted in Fig. 1 do not indicate the existence of a true 2D MIT, but instead show a crossover from an Anderson insulator at small U/W to a disordered Mott insulator (a "Wigner glass" phase) at large U/W with an intermediate crossover regime (around $U = U_c \sim W$) of interaction-enhanced finite size conductance (or equivalently, an enhanced localization length), which is *not* a thermodynamic "metallic phase," is based on two complementary sets of arguments:

(1) Comparison with the corresponding one dimensional (1D) results; and (2) strong circumstantial evidence based on heuristic theoretical arguments.

To better understand the nature of the 2D disordered Hubbard model we have carried out an identical finite system charge stiffness calculation on the corresponding 1D disordered Hubbard model (1D Hubbard rings). We show the corresponding 1D Anderson-Hubbard model results in Fig. 2 for 6 electrons on a 12 site ring (corresponding to quarter filling). The 1D results of Fig. 2 are qualitatively identical to the 2D results of Fig. 1: D_c in the disordered 1D Hubbard model initially increases as a function of U/W for a fixed W, showing a maximum at $U = U_c \sim W$, and then it decreases slowly for large $U > U_c$, exactly as in 2D system. The "critical" U_c/t for the charge stiffness peak in the 1D system is $U_c/t \simeq 0.7$, 3.3, 4.5 for $W/t = 0.5$, 3, 5, respectively (which are not that different from the corresponding 2D results at $3/16$ filling).

Noting that the charge stiffness results shown in Figs. 1 and 2 in the 2D and 1D disordered Hubbard models, respectively, are essentially indistinguishable (i.e., just by looking at the results of Figs. 1 and 2 one does not know which one corresponds to 1D and which to 2D since the results are qualitatively identical) one is forced to conclude that if the results of Fig. 1 are interpreted as exhibiting evidence for a 2D MIT then one must, based on the results of Fig. 2, infer that there is also a 1D MIT in the disordered 1D Hubbard model as a function of the interaction strength. We mention in this context that we have verified that the 1D disordered *extended* Hubbard model (with additional long range interaction) produces results qualitatively similar to those in the corresponding 2D system—thus the equivalence between 1D and 2D charge stiffness results is valid for finite and long range interactions also.

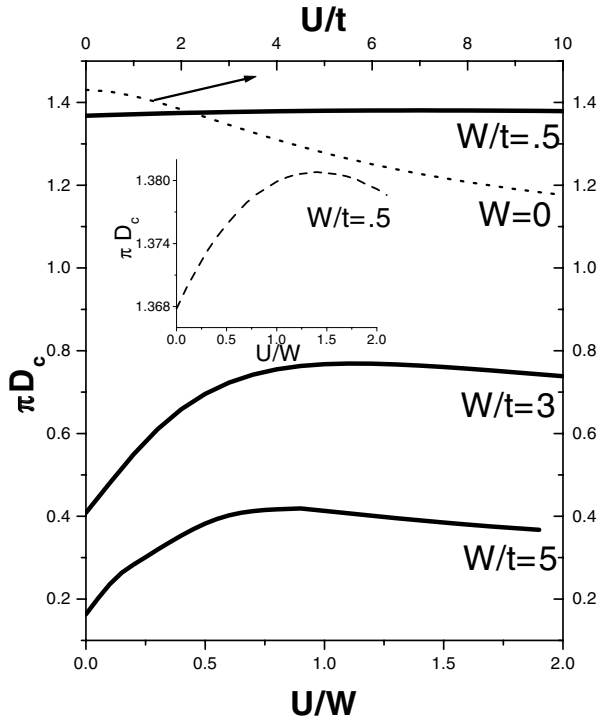

FIG. 2. The same as in Fig. 1 for the 1D disordered Hubbard ring of 12 sites and 6 electrons.

There are, however, very compelling theoretical grounds [8] to believe that 1D disordered systems are localized even in the presence of interaction. Thus, the results of Fig. 2 cannot be interpreted as evidence for a 1D MIT—instead the maximum in D_c as a function of U indicates only the interaction-induced enhancement of the localization length (or, equivalently the persistent current [6]), which in a finite system increases the Drude conductance or the charge stiffness. Based on the striking qualitative similarity between the 1D (Fig. 2) and the 2D (Fig. 1) results and the fact that both systems have strictly localized or insulating ground states in the disordered, $W \neq 0$, noninteracting, $U = 0$, system, we therefore conclude that the 2D results of Fig. 1 do not indicate a 2D MIT; it indicates only an interaction-induced enhancement of the 2D localization length for intermediate interaction strengths $U \sim U_c$. Note that while the intermediate-interaction crossover regime ($U \sim U_c$) is *not* a new quantum phase (it is still an insulator), the interaction-induced enhancement of the 2D localization length may be extremely large, and even the experimental 2D systems [2] showing the so-called 2D MIT may actually be "effective" metals since the enhanced localization lengths may be larger than the actual system size (or, the phase breaking length at finite temperatures).

In addition to the above empirical argument for the nonexistence of a 2D MIT based on the comparison between 1D and 2D exact diagonalization results we have a heuristic theoretical argument which points to the same conclusion. The small U ($\rightarrow 0$) and the large U ($\rightarrow \infty$) interaction limits of the disordered 2D Hubbard model are believed to be insulating or localized on theoretical grounds. The noninteracting ($U \rightarrow 0$) disordered 2D system is known to be localized for any finite disorder (the localization length is exponentially large, the so-called weak localization regime, for small disorder) by virtue of the scaling theory of localization [3]. The localized large U ($\rightarrow \infty$) regime arises from the fact that the pure Hubbard ground state (in the absence of disorder) must have strong ferromagnetic correlations in the large-U limit in order to minimize the interaction energy. In fact, it is known [9] that the large U ground state of a Hubbard-type model with an additional next-nearest neighbor hopping term is ferromagnetic (the same is true for the pure Hubbard model at fillings close to half). In this limit, therefore, interaction tends to become less relevant since the electrons being spin polarized avoid each other. The system in this large-U limit may thus be approximately equivalent to a noninteracting or weakly interacting system (albeit a spin-polarized one), and the introduction of any disorder ($W \neq 0$) necessarily localizes this 2D "effectively noninteracting" Hubbard system. The weakly

localized (for small disorder) large $U(\rightarrow \infty)$ 2D system has, however, an exponentially longer localization length (which explains the enhanced D_c for large U in Fig. 1) than the usual noninteracting ($U \rightarrow 0$) disordered limit because the ferromagnetic spin-polarized phase ($U \rightarrow \infty$) has a larger Fermi energy, which would exponentially enhance the localization lengths. Thus, both the small U and the large U regimes are necessarily localized, and the enhancement of D_c in the intermediate-$U(\sim U_c)$ regime must either indicate a crossover between an Anderson insulator ($U \sim 0$) and a disordered Mott insulator (equivalently a Mott glass, "Wigner glass" in the corresponding continuum system) for $1/U \sim 0$ or involve *two* quantum phase transitions—one from the low-U Anderson insulator phase to the intermediate ($U \sim U_c$) metallic phase with enhanced D_c and then again from this intermediate metallic phase to the large-U Mott glass phase. We see absolutely no features in our 2D or 1D numerical results which could be indicative of such a double or re-entrant insulator ($U \sim 0$)-"metal" ($U \sim U_c$)-insulator ($1/U \sim 0$) quantum phase transition.

We conclude with a critical discussion of the recent low temperature experimental results in low density, high mobility 2D systems which have motivated the current resurgence in the issue of 2D MIT in disordered and interacting electron systems. Experimentally one finds [2] that the high density regime ($n > n_c$) is metallic in the sense of having a positive temperature coefficient ($\frac{d\rho}{dT} > 0$) of the resistivity ρ, and the low density ($n < n_c$) is insulating with $\frac{d\rho}{dT} < 0$. This has been interpreted by many [2] (but not all [10,11]) as clear evidence of an interaction-driven MIT occurring at a critical density n_c. The standard interpretation of these experimental observations as a 2D MIT is, however, problematic because the high density phase (i.e., the *less* interacting phase) is the nominal metallic phase according to this interpretation. This makes little sense since the noninteracting or the weakly interacting very-high density phase must be a weakly localized 2D insulator based on the scaling theory [3]. Thus, very similar to the conclusion we reached for our exact diagonalization numerical results, the experimental situation must correspond to either a double quantum phase transition (the very high density phase is a weakly localized insulator, with the intermediate regime, corresponding to our peak in D_c around $U \sim U_c$, being a novel interaction-induced metallic phase) or just a sharp crossover from a high density weakly localized insulator to a low density strongly localized insulator occurring around $n \sim n_c$. Experimentally, there is little evidence for *two* quantum phase transitions (note that there must be two quantum phase transitions or none; it cannot be one quantum phase transition and one crossover). Therefore we believe, based on arguments similar to what we use to interpret our theoretical results presented in this paper, that the experimental observations are indicating a very sharp crossover (around $n \sim n_c$) from a weakly to a strongly localized 2D insulator as n decreases, and the high density regime ($n > n_c$) is only an effective metal because the effective system size (the phase breaking length at finite T) is smaller than the localization length which may have been substantially enhanced by interaction effects as we show in this paper. There is some very recent experimental support [10] for this scenario.

We emphasize that the interaction induced enhancement of D_c for $0 < U/W \lesssim 1$ in Fig. 1 should not be considered as evidence in favor of a 2D MIT (as was recently done in Ref. [7] based on finite system studies of *spinless* electrons using smaller system sizes), particularly since (1) the interaction enhancement is only effective for very large disorder strength ($W/t > 1$) where the system is likely to be localized any way (note that for weak disorder, $W/t < 1$, there is essentially no interaction induced D_c enhancement—if there is indeed an interaction-driven 2D metallic phase it is likely to be in the *low* disorder regime where Fig. 1 indicates little interaction enhancement), and (2) the actual interaction-enhanced D_c values in the strong disorder regime in Fig. 1 are still extremely small in magnitude (and are much smaller than the corresponding D_c values for noninteracting weak disorder system, which is still known to be weakly localized by virtue of scaling localization). We therefore conclude that the interaction enhancement of D_c seen in Fig. 1 (and Fig. 2) indicates an interaction-driven enhancement of the localization length in the strong disorder regime, and *not* a 2D MIT.

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