Absence of a Slater Transition in the Two-Dimensional Hubbard Model

S. Moukouri* and M. Jarrell

Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221

(Received 15 November 2000; revised manuscript received 14 May 2001; published 1 October 2001)

We present well-controlled results on the metal-to-insulator transition (MIT) within the paramagnetic solution of the dynamical cluster approximation in the two-dimensional Hubbard model at half filling. In the strong coupling regime, a local picture describes the properties of the model; there is a large charge gap $\Delta \approx U$. In the weak-coupling regime, we find that a symbiosis of short-range antiferromagnetic correlations and moment formation cause a gap to open at finite temperature as in one dimension. Hence, this excludes the mechanism of the MIT proposed by Slater long ago.

DOI: 10.1103/PhysRevLett.87.167010 PACS numbers: 71.27.+a, 71.30.+h

Introduction.—In this Letter we report the study of the metal-insulator transition (MIT) and its relation to antiferromagnetism (AFM) in the two-dimensional (2D) Hubbard model at half filling. Results from numerical simulations [1,2] have convincingly shown that the ground state of the model is an AF insulator, with the Néel temperature constrained to be $T_N = 0$ by the Mermin-Wagner theorem. However, the nature of the MIT is less clear, as there are two conflicting opinions concerning the MIT and its relation to AFM. The *first opinion* [3–5] is that the strong and weak coupling MI transitions are very different. When the local Coulomb repulsion parameter U is larger than the noninteracting bandwidth W, the ground state is an insulator with a large charge gap $\Delta \approx U$. The MIT occurs well before the onset of magnetism at the temperature $T_g \approx U$, and the spin and charge degrees of freedom are decoupled. The superexchange interaction couples the spins with the exchange constant $|J| \approx 4t^2/U$, and the spins govern the low-energy physics. This type of MIT, which is purely due to local correlations, is called a Mott transition. In weak coupling, a spin density wave (SDW) instability develops at $T = 0$ because of the nesting of the Fermi surface. The MIT is the direct consequence of the Brillouin zone folding generated by magnetic ordering. This type of MIT is referred to as a Slater transition. It is believed that this regime can be well described by the usual many-body weak-coupling approaches. The *second opinion* is due to Anderson [6] who has argued that the strong-coupling behavior presented above occurs for both strong and weak coupling so that a Mott gap is present for all $U > 0$ as in one dimension. As the temperature falls, local moments develop first because of the MIT and then they order so that AFM is the consequence of the MIT, not the converse. Because of this strong interaction, there is no adiabatic continuity between the noninteracting and interacting eigenstates. The conventional renormalizable many-body perturbation theory cannot describe this physics.

The nature of the MIT has been addressed in the Hubbard model in infinite dimensions [7–9] by applying the dynamical mean-field approximation (DMFA) [10]. The unfrustrated model is an example of the first scenario presented above with a Slater AF insulator in weak coupling, and a Mott MIT at strong coupling. The one-dimensional model is an example of the second scenario, since there is a gap in the charge excitation spectrum for all nonzero U [11], but no long-range magnetic order.

In 2D, the Mermin-Wagner theorem precludes any AFM transition at any finite temperature. Hence, if there is a MIT at finite T, it cannot be attributed to the Slater mechanism. Finite size simulations (FSS) employing the quantum Monte Carlo (QMC) technique have been applied to study this model quite extensively during the last decade [1–3,12]. But the difficulty with FSS is that at low temperatures, the correlation length is greater than the lattice size. Thus the effects of correlations are overestimated for smaller clusters because they are artificially closer to criticality than a system in the thermodynamic limit. This tendency is reduced only by increasing the cluster size, which moves the system in the direction of the thermodynamic limit. The spurious AFM gap that opens at finite T in the FSS renders the disentanglement of the MI and the AF transitions practically impossible. The situation is radically different in the dynamical cluster approximation (DCA), which is an extension of the DMFA. In the DCA, the system is already in the thermodynamic limit; however, the DCA restricts correlations to within the cluster length. As the cluster size increases, longer-range correlations are progressively included. The FSS and DCA results are complimentary in that the DCA (FSS) always underestimates (overestimates) the effects of nonlocal correlations [13,14]. Thus, the DCA will always systematically underestimate the gap formation inherent in the Anderson picture of the MIT. Therefore, if a gap is found in the DCA for a finite cluster, it will persist in the thermodynamic limit.

Using the DCA, we show that a MIT occurs in the 2D Hubbard model at half filling and finite temperature at both weak- and strong-coupling regimes. This result is to be contrasted with the weak-coupling approaches which predict that a gap will exist only at $T = 0$ as a consequence of AFM. We argue that at weak couplings the symbiosis of short-range AFM correlations and local moment formation is the key mechanism for the opening of a gap. The local moments form at a relatively high T leading to a short-range AFM order, that in turn enhances the moments which

enhance the AF order, etc. This leads to the destruction of the Fermi liquid state found in the DMFA studies [15]. We discuss the validity of our conclusions drawn from finite clusters at the thermodynamic limit.

Method.—A detailed discussion of the DCA formalism was given in previous publications [14,16,17]. The compact part of the free energy is coarse grained in reciprocal space, projecting the problem onto a finite-sized cluster of N_c points embedded in a self-consistently determined host. When $N_c = 1$, the DCA recovers the DMFA, and when $N_c \to \infty$, it becomes exact. The cluster problem is solved with a generalized version of the Hirsch-Fye QMC algorithm [18], and the spectra are analytically continued with the maximum entropy method [19]. We use the DCA to study the single band Hubbard model in a two-dimensional square lattice at half filling. The model is characterized by W and U. We set $W = 2$ and we vary U from $U = W/4$ to $U = 2W$.

Results.—Jarrell [7], Georges and Krauth [8], and Rozenberg *et al.* [9] originally obtained a numerically exact solution from the DMFA in the limit of infinite dimensions using QMC. The analysis of these mean-field equations revealed the existence of a transition between a paramagnetic state and an AFM state. The paramagnetic solution was shown to be a Fermi liquid for small values of the interaction U and an insulator for large U [20]. Georges and Krauth identified this transition by observing the behavior of the double occupancy which is given by $\langle D\rangle = \langle n_\uparrow n_\downarrow\rangle$, where n_σ is the density of spin σ, and of the single-particle Green's function $G(\tau)$. $\langle D\rangle(T)$ displays a minimum in the Fermi liquid regime. But when the system is an insulator for $U > U_c$, $\langle D\rangle$ always increases with T. We observe the same qualitative behavior as in [8] when $N_c = 1$.

We perform the same kind of analysis to study the effect of short-range AFM correlations that are absent in the DMFA. The behavior of $\langle D\rangle$ as a function of N_c depends strongly upon U. In the strong-coupling regime, $\langle D\rangle(T)$ is essentially independent of N_c (Fig. 1). This was expected, since for large U, local fluctuations dominate; they are already captured in $N_c = 1$. In the weak-coupling regime, the minimum found for $N_c = 1$ flattens progressively as N_c increases from 8 to 16. At $N_c = 36$, there is a downturn in $\langle D\rangle$ at low T. By localizing the moments at low temperatures, the system gains free energy by taking advantage of the short-range magnetic order. There is a similarity between the curves of $U = 1$ and $U = 0.5$ which are in the weak-coupling regime. Hence, we expect this behavior to be generic in this region. This finding is in agreement with a recent finite system QMC simulation [21].

The density of states (DOS) $\rho(\omega)$ (shown in Fig. 2) confirms the destruction of the Fermi liquid quasiparticle peak by short-range AFM correlations. With increasing N_c, the gap opens fully, and the Hubbard sidebands become more pronounced, consistent with the suppression of $\langle D\rangle$ shown in Fig. 1. Since we work within the paramagnetic equations, the opening of the gap in the weak-coupling regime cannot be attributed to the Slater mechanism.

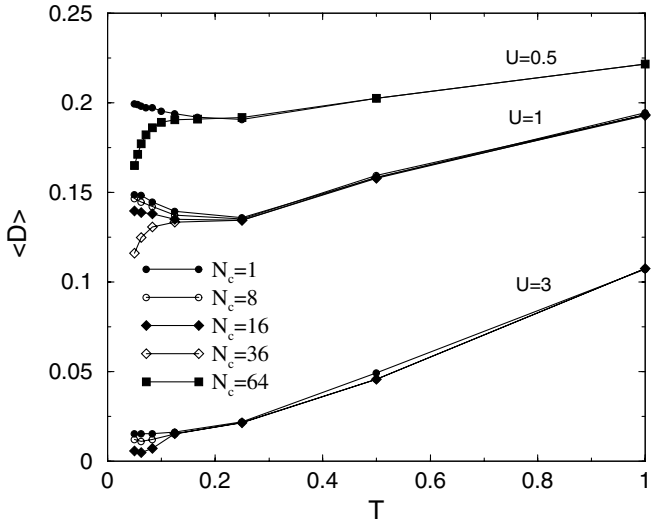

FIG. 1. The double occupancy D for $U = 0.5$, $U = 1$, and $U = 3$ for various N_c.

In Fig. 3 we show a tentative phase diagram obtained with $N_c = 1, 8, 16, 64$. The boundary line between the metallic and the insulating phases is defined as the point where a true gap opens to the system within our numerical accuracy; the criterion for the gap opening is roughly $\rho(\omega = 0) < 1 \times 10^{-2}$. Hence for temperatures just above this line, $\rho(\omega)$ displays a pseudogap. As expected, for $U > W$, the boundary line is almost independent of the cluster size. For $U < W$, however, the $N_c = 1$ line ends at $U = U_c \approx W$. For $U < U_c$, a Fermi liquid is stable at low T. For larger clusters, we do not find a quasiparticle peak, except when $U \lesssim U_c$, and U_c strongly decreases as N_c increases. This seems to be compatible with *the absence of a weak-coupling fixed point in the two-dimensional Hubbard model at half filling*. However, since an exponential behavior of the gap is expected in this limit, the numerical cost becomes too high at very

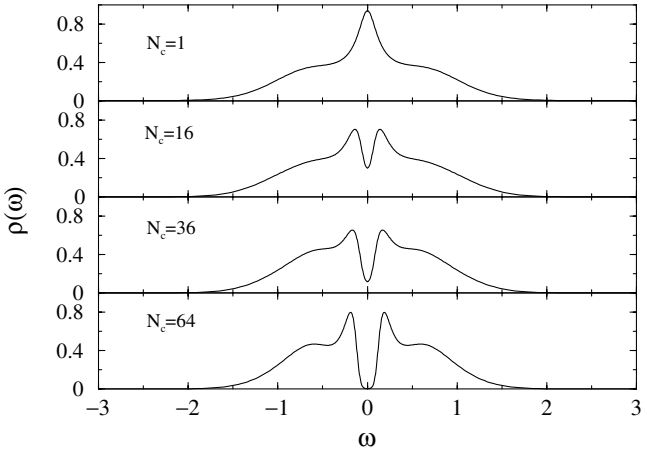

FIG. 2. The DOS $\rho(\omega)$ at $\beta = 32$ and $U = 1$.

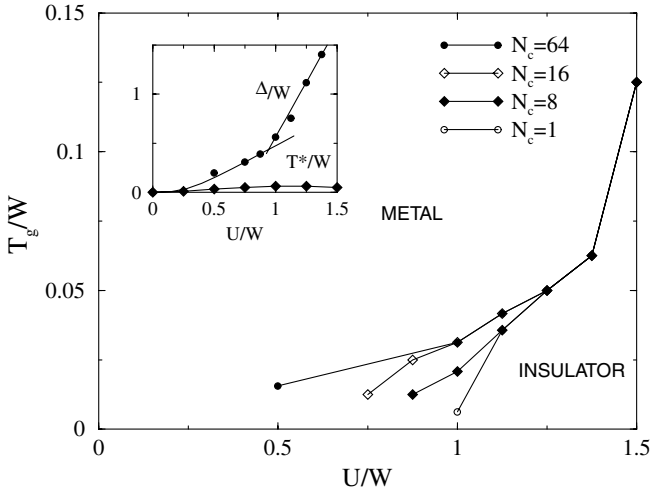

FIG. 3. The temperature T_g the gap opens in $\rho(\omega)$ $N_c = 1$, 8, 16, and 64 as functions of U. In the inset the mean-field transition temperature T^* and the gap Δ as functions of U; the linear ($U > W$) and exponential ($U < W$) fits for Δ serve as guide to eyes.

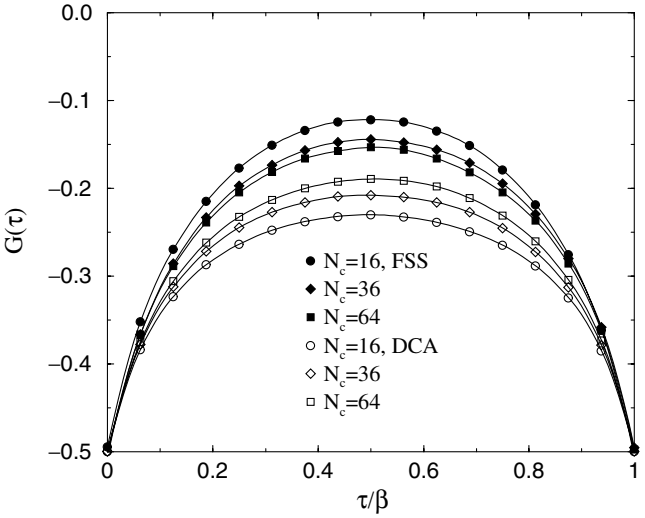

FIG. 4. The imaginary-time Green's function at the Fermi point $X = (\pi, 0)$ calculated with finite size QMC (filled symbols) and with the DCA (empty symbols) when $U = 1.1$, $\beta = 16$.

small couplings; the smallest value of U we were able to observe a pseudogap is $U = 0.5$. For instance, it was necessary that $N_c > 36$ in order to see a gap at $U = 1$ (as shown in Fig. 2). We believe that this gap is due to a synergism between short-ranged order and moment formation as evidenced by the suppression of $\langle D \rangle$ (Fig. 1) and the enhancement of the Hubbard sidebands (Fig. 2) seen when the gap opens.

It has been argued that the SDW picture might capture the description of the insulating state of the cuprates in the weak to intermediate coupling regime [22]. We show in the inset in Fig. 3 the gap Δ and the mean-field transition temperature, which to a very good approximation is also the pseudogap temperature T^* characterized by a peak in the bulk susceptibility and the onset of the pseudogap in the DOS. T^* defines the temperature where short-ranged AF correlations emerge. If the gap were due only to these correlations, then we expect $\Delta \approx T^*$. For example, in the SDW approximation $\Delta/T^* = 1.76$ [23]. We find that Δ/T^* strongly deviates from this prediction. In fact, we find that $\Delta \gg T^* > T_g$; hence, SDW ordering is not the mechanism that leads to the gap formation.

We now show that the conclusions drawn from finite clusters are valid in the thermodynamic limit. For this, we exploit the complementarity between the DCA and FSS [13,14]. In Fig. 4, we show the imaginary-time Green's function $G(\tau)$ at the Fermi point $X = (\pi, 0)$. This quantity has a more rapid decay from its maximum at $G(\beta/2)$ when the effects of the correlations are stronger so that the gap is more pronounced. In finite systems, the decay is sharper for smaller lattices, while in the DCA the opposite occurs. This behavior marks the fundamental difference between the FSS and the DCA. At low temperatures, in FSS, the correlation length is greater than the lattice size. Thus the effect of correlations is overestimated for smaller clusters because these systems are artificially closer to criticality than a system in the thermodynamic limit. This tendency is reduced by increasing the cluster size. The situation is radically different in the DCA where the system is already in the thermodynamic limit. The DCA restricts correlations to within the cluster length. As the cluster size increases, long-range correlations are progressively included. Thus, the effects of the correlations increase with cluster size. Since the two techniques must become identical in the thermodynamic limit, the $G(\tau)$ curve in the limit is bracketed by the FSS and DCA curves.

This complementarity is also seen in the spectra. In the weak-coupling regime, the FSS and the DCA start from two different physical limits. A finite system is always an insulator as soon as T is less than the energy separation between the ground state and the first excited state. Hence finite systems always show gaps or pseudogaps if T is sufficiently low. On the contrary, for $N_c = 1$, the DCA is identical to the DMFA which at weak couplings yields a local Fermi metal. As the cluster size increases, one expects the two techniques, which become identical in the thermodynamic limit, to converge towards this limit from complementary directions. In the strong-coupling regime, the DMFA has a gap, too. But this is always smaller than the one found in the FSS for the same set of parameters. Hence the convergence towards the thermodynamic limit in the DCA will be from smaller gaps to larger, while the converse occurs in FSS. The DOS shown in Fig. 5 supports these conclusions. The finite size gap in the FSS decreases when the cluster size goes from $N_c = 16$ to 64. In the DCA, there is a pseudogap for $N_c = 16$ that turns into a true gap when the cluster size is increased to 64. Since by construction the DCA underestimates the gap,

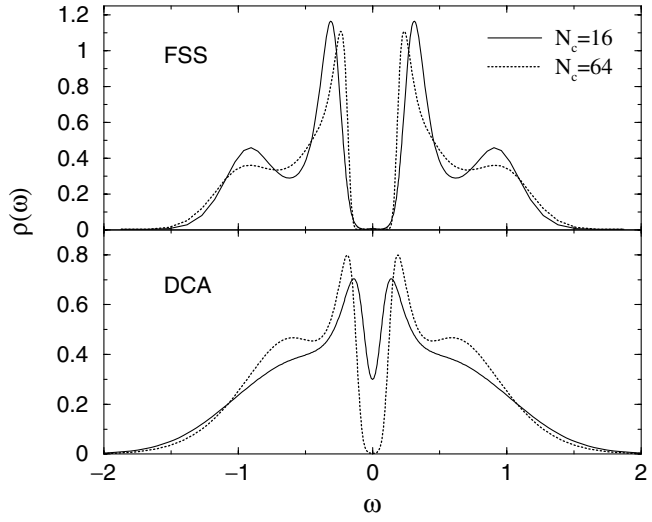

FIG. 5. The DOS $\rho(\omega)$ from finite size QMC (top) and from DCA (bottom) at $U = 1$, $\beta = 32$, and $N_c = 16$ and 64.

we can affirm that at this temperature, the gap exists in the thermodynamic limit. Its actual value is bracketed by the FSS and the DCA.

Conclusion.—We have presented well-controlled results on the MIT in the 2D Hubbard model obtained by the DCA. We find that the double occupancy and the single-particle DOS show evidence of a gap for both small and large values of U at finite T. Since a finite-temperature gap persists well into the weak-coupling regime, and there is no long-range order until $T = 0$, the Slater mechanism is likely not responsible for the metal-insulator transition in the two-dimensional Hubbard model. Instead, the gap is due to a synergism between short-ranged order and moment formation, as evidenced by the concomitant opening of the gap and the suppression of the double occupancy. Since the charge fluctuations are suppressed at finite T by the MIT and the spins do not order until $T = 0$, spin-charge separation also persists into the weak-coupling regime. As the DCA systematically underestimates the gap formation, these conclusions are valid in the thermodynamic limit. The resulting phase diagram is consistent with Anderson's view that the effective Hamiltonian for the 2D Hubbard model at half filling for all $U > 0$ and $\Delta \gg T$ is the 2D Heisenberg Hamiltonian [6]. Finally, our results put some constraints on theories of high temperature superconductivity. Since theories based on weak-coupling expansions are unable to describe these results, their prediction in the doped case is questionable.

Part of this work was performed during the visit of S. M. to the University of Southern California; we thank G. Bickers for the warm hospitality and for useful conversations. We gratefully acknowledge discussions with G. Baskaran which motivated this work, we thank C. Huscroft for his help on parallel programming, and we thank M. Ma for helpful discussions. This work was supported by the National Science Foundation Grants No. DMR-0073308 and No. PHY94-07194 and the Ohio Supercomputing Center.

*Present address: Department of Physics, University of Michigan, Ann Arbor, MI 48109.

[1] J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).
[2] S. R. White *et al.,* Phys. Rev. B **40**, 506 (1989).
[3] M. Vekic and S. R. White, Phys. Rev. B **47**, 1160 (1993).
[4] P. Nozières, Eur. Phys. J. B **6**, 447 (1998).
[5] J. R. Schrieffer *et al.,* Phys. Rev. B **39**, 11 663 (1989).
[6] P. W. Anderson, Adv. Phys. **46**, 3 (1997); in *The Theory of Superconductivity in the High-T_c Cuprates,* Princeton Series in Physics (Princeton University Press, Princeton, 1997), pp. 291–294.
[7] M. Jarrell, Phys. Rev. Lett. **69**, 168 (1992).
[8] A. Georges and W. Krauth, Phys. Rev. Lett. **69**, 1240 (1992).
[9] M. J. Rozenberg *et al.,* Phys. Rev. Lett. **69**, 1236 (1992).
[10] W. Metzner and D. Vollhardt, Phys. Rev. Lett. **62**, 324 (1989); E. Müller-Hartmann, Z. Phys. B **74**, 507–512 (1989).
[11] E. H. Lieb and F. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[12] S. Moukouri *et al.,* Phys. Rev. B **61**, 7887 (2000).
[13] C. Huscroft *et al.,* Phys. Rev. Lett. (to be published); cond-mat/9910226.
[14] S. Moukouri *et al.,* e-print cond-mat/0004279.
[15] A. Georges *et al.,* Rev. Mod. Phys. **68**, 13 (1996).
[16] M. H. Hettler *et al.,* Phys. Rev. B **58**, 7475 (1998); M. H. Hettler *et al.,* Phys. Rev. B **61**, 12 739 (2000).
[17] Th. Maier *et al.,* Eur. Phys. J. B **13**, 613 (2000).
[18] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[19] M. Jarrell and J. E. Gubernatis, Phys. Rep. **269**, 135 (1996).
[20] The authors of [8] and [9] later found hysteresis at very low temperatures from which they infer a first order transition (see [15]). However, all of the calculations presented here occur at higher temperatures, and for $N_c \gg 1$, we do not observe a Kondo peak which was prerequisite for their scenario at the MIT.
[21] T. Paiva *et al.,* e-print cond-mat/0008044.
[22] N. Bulut, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. **73**, 748 (1994).
[23] P. Fazekas, in *Lecture Notes on Electron Correlation and Magnetism,* Series in Modern Condensed Matter Physics Vol. 5, edited by I. Dzyaloshinski, S. Lundqvist, and Yu Lu (World Scientific, Singapore, 1999), p. 371.