Phase separation in the Hubbard model

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We study the behavior of the mean number of particles $\langle n \rangle$ (density) as a function of the chemical potential μ in the two-dimensional Hubbard model, using a quantum Monte Carlo method. Working at $U/t=10$, 4, and -4 on lattices with 4×4, 6×6, and 8×8 sites, we do not find evidence of phase separation.

Following the discovery of high-T_c superconductivity in the cuprates,[1] the Hubbard model with positive Coulombic interaction has been suggested as the simplest Hamiltonian that may contain the basic ingredients to explain superconductivity[2] in these materials. Numerical studies have shown[3] that at half-filling this model has long-range antiferromagnetic (AF) order, as it occurs in the undoped cuprates. Other properties such as the optical conductivity[4] and short-range incommensurate order away from half-filling[5,6] are in good qualitative agreement with experimental results for the normal state. Moreover, Monte Carlo[7] and exact diagonalization results[8] have shown that there is a small binding of holes on 4×4 lattices when two holes are introduced in the half-filled background.[9]

The existence of hole attraction, an essential ingredient for superconductivity, leads us to two important questions. (1) Are the pairs stable or upon adding more holes does the system actually separate into two (hole-rich and hole-poor) phases? (2) If the pairs are stable, do they have long-range correlations? In this paper we will address the first question. The second one has been discussed in Ref. 10 and so far evidence for long-range pairing correlations has not been found in small lattices.

The Hubbard model is defined by the Hamiltonian

$$H=-t\sum_{\langle ij\rangle,\sigma}(c^{\dagger}_{i\sigma}c_{j,\sigma}+\text{H.c.})+U\sum_{i}(n_{i,\uparrow}-\tfrac{1}{2})(n_{i,\downarrow}-\tfrac{1}{2})-\mu\sum_{i,\sigma}n_{i,\sigma}\ , \tag{1}$$

where $c^{\dagger}_{i,\sigma}$ creates an electron at site i with spin projection σ, $n_{i,\sigma}$ is the number operator, and the sum $\langle ij\rangle$ is over pairs of nearest-neighbor lattice sites. t is the hopping parameter; U, the Coulombic interaction; and μ, the chemical potential.

When U increases, double occupancy is suppressed. An expansion in t/U maps the Hubbard model[11] for large U/t onto the t-J model at small J/t, with $J=4t^2/U$. The problem of clustering or phase separation in the t-J model has been previously discussed.[12,13] It is clear that in the limit of large J/t this model will have a phase separation because of the large cost in energy necessary to break AF bonds. The number of broken bonds can be minimized if the holes cluster together. In the limit of small J/t, where we expect similarities between the t-J and Hubbard models, the analytical argument indicating phase separation is based on the existence of a ferromagnetic instability to minimize the kinetic energy of the holes.[12] Exact diagonalization results of 4×4 clusters are claimed to support these results through the Maxwell construction.[12] This criterion is useful when one works in the *canonical* ensemble with a fixed number of particles. However, in the *grand-canonical* formalism where a chemical potential μ determines the number of particles $\langle n \rangle$ in average, it is simpler to study phase separation by monitoring the behavior of $\langle n \rangle$ as a function of μ. In fact, phase separation means that as we dope the half-filled system with holes, it will separate into two phases, one rich in holes with a density n_h and another without holes with $\langle n \rangle=1$ that will coexist at the same value of μ. This behavior translates into a first-order phase transition (discontinuous) in $\langle n \rangle$ as a function of μ showing clearly that some values of $\langle n \rangle$ are not allowed to the system, i.e., a dilute gas of holes with $\langle n \rangle \lesssim 1$ is not stable.

In Fig. 1(a) we show $\langle n \rangle$ versus μ for the Hubbard model with $U/t=4$ on 4×4, 6×6, and 8×8 lattices at $\beta t=8$. The value of $\beta t=8$ is already in the zero-temperature plateau for all the lattice sizes studied. This has been checked by monitoring the behavior of several magnitudes, e.g., energy, antiferromagnetic structure factor, etc., as a function of temperature. For small values of μ, the density $\langle n \rangle$ remains at the constant value of 1 due to the existence of the antiferromagnetic gap.[6] $\langle n \rangle$ starts to decrease when μ reaches the first state after the gap. However, notice that the change is very smooth and all the values of $\langle n \rangle$ are allowed. This behavior remains almost unchanged when we increase the lattice size, showing that we may be very close to bulk results. Another way of checking that there is no first-order phase transition is by looking at the temporal evolution of our numerical data close to the point where the "transition" may take place, i.e., in our case, when $\langle n \rangle$ starts moving away from 1. The existence of tunneling events from two different allowed values of $\langle n \rangle$ *and* the

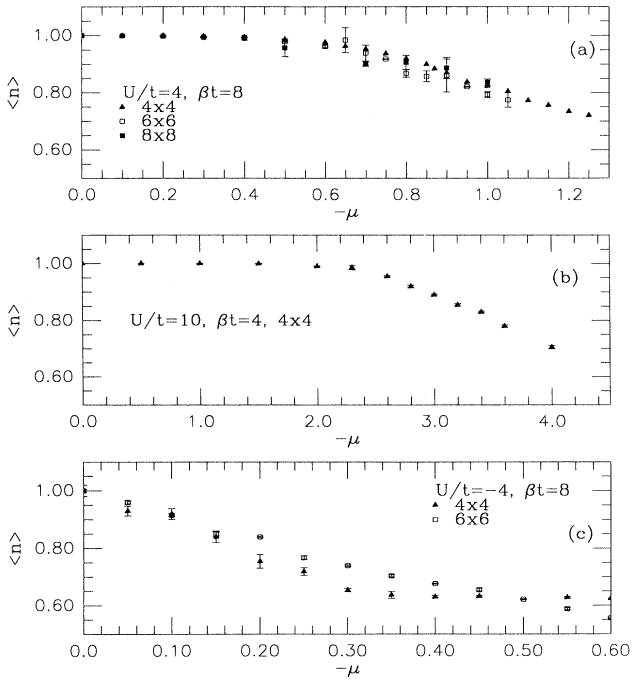

FIG. 1. (a) $\langle n \rangle$ vs μ for $U/t=4$ on different lattice sizes. (b) $\langle n \rangle$ vs μ for $U/t=10$ on a 4×4 lattice. (c) $\langle n \rangle$ vs μ for $U/t=-4$ on different lattice sizes.

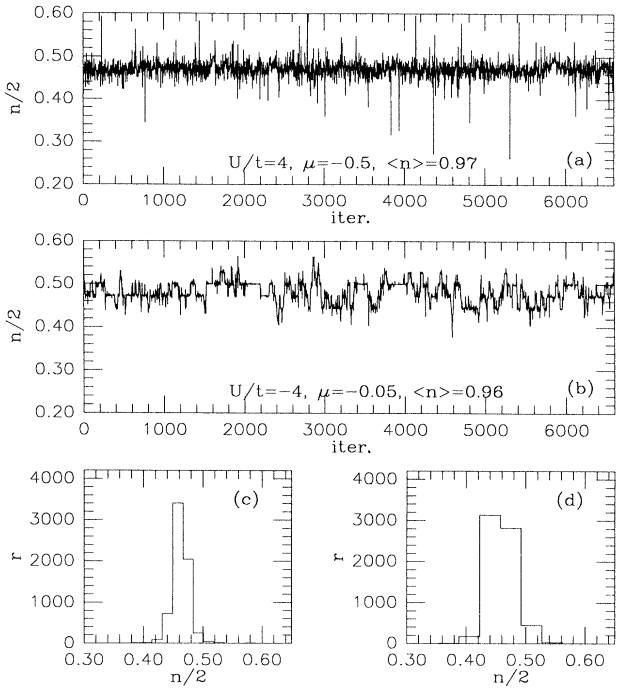

FIG. 2. (a) $n/2$ per sweep for $U/t=4$ on a 6×6 lattice at $\mu=-0.5$ and $\langle n \rangle=0.97$. (b) $n_\uparrow$ per sweep for $U/t=-4$ on a 6×6 lattice at $\mu=-0.05$ and $\langle n \rangle=0.96$. (c) Histogram for the data displayed in (a). r is the number of times an event was obtained. (d) Histogram for the data displayed in (b). r is the number of times an event was obtained.

avoidance of states in between should be a clear indication of a discontinuity (double-Gaussian-peak structure). This behavior can also be made more explicit by constructing histograms displaying the number of times that a certain value of n appears in a long simulation. In Fig. 2(a) we show the time evolution[14] of $n/2=(n_\uparrow+n_\downarrow)/2$ on a 6×6 lattice for $\mu=-0.5$, $\langle n \rangle=0.97$, and $\beta t=8$. We observe transitions among all the allowed levels very close to the average value $\langle n_\uparrow \rangle$, i.e., $n_h/N=\frac{19}{36}, \frac{18}{36}, \frac{17}{36}$, etc., but not among states having very different numbers of particles. In Fig. 2(c) we show the corresponding histogram where we clearly observe a single peak, instead of the two-peak behavior that would indicate a first-order phase transition.

We conclude that at $U/t=4$ the Hubbard model does not have phase separation. However, for this small value of U/t we do not expect a qualitative similarity with the t-J model. A convincing proof of this is shown in Fig. 3(a) where we compare the zero-temperature energy of the t-J model at $J/t=1.0$ obtained on a 4×4 lattice with the modified Lanczos method with the energy at $U/t=4$ for the Hubbard model also on a 4×4 lattice measured with the quantum Monte Carlo (QMC) method. At low doping the energy of both models differs considerably. For what value of U/t are the t-J and Hubbard models qualitatively similar? In Fig. 3(b) we again compare ground-state energies but for $U/t=4t/J=10$. We notice that now there is a better agreement and thus $J/t=0.4$ and $U/t=10$ is a point where the two models may have the same qualitative behavior.[15] It is remarkable that

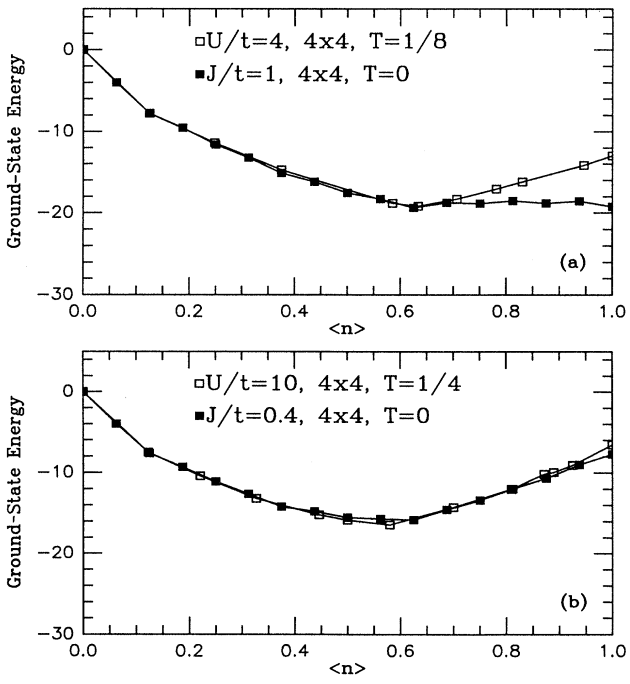

FIG. 3. (a) Comparison of ground-state energies for the t-J and Hubbard models as a function of $\langle n \rangle$ for $U/t=4t/J=4$. (b) Comparison of ground-state energies for the t-J and Hubbard models as a function of $\langle n \rangle$ for $U/t=4t/J=10$.

two different techniques applied in two different models show such a nice agreement. This opens the possibility of performing studies relevant to the t-J model using the QMC method. In Fig. 1(b) we present our Monte Carlo results for $\langle n \rangle$ versus μ for $U/t=10$ on a 4×4 lattice at an inverse temperature $\beta t=4$ which in spite of its apparent high value is already in the zero-temperature plateau for such a large value of U/t. We notice that $\langle n \rangle$ remains equal to 1 for larger values of $|\mu|$ due to the fact that the antiferromagnetic gap increases with U/t. After the gap, the change in $\langle n \rangle$ is very smooth. This fact suggests that even for U/t large the model does not have phase separation. Note that since at $U/t=4$ we did not find large differences between 4×4 and 8×8 lattices, there is no obvious reason to suspect that the same will not occur at $U/t=10$ where finite-size effects are usually milder. Numerically with the quantum Monte Carlo method it is extremely difficult to get accurate results away from half-filling for U/t larger than 10. This is due to the fact that away from half-filling, due to the sign problem, we have to make longer runs to get the statistical errors under control. Numerical instabilities and systematic errors increase with U, thus we are forced to reduce the time step[3] $\Delta\tau$ at the same time that we have to increase the size of our lattice in the temporal direction to keep βt constant. For larger values of U/t the statistical errors do not allow us to reach the zero-temperature plateau.

Finally, let us discuss the case of the Hubbard model with an attractive potential. This corresponds to replacing U by $-U$ in Eq. (1). This model has long-range pairing correlations in the ground state, i.e., a superconducting phase.[16,17] In Fig. 1(c) we show $\langle n \rangle$ versus μ for $U/t=-4$ on 4×4 and 6×6 lattices. Due to the absence of the antiferromagnetic gap, the density $\langle n \rangle$ starts changing from 1 immediately when μ becomes finite. The change is fast but note that the steepness of the curve does not increase when we change the lattice size. On the other hand, the behavior of $n_\uparrow=n/2$ shown in Fig. 2(b) for $\mu=-0.05$ and $\langle n \rangle=0.96$ shows transitions among all the allowed values for n near its mean value. The Hubbard-Stratonovich decoupling for this model treats equally spins up and down. That is the reason we do not have sign problems in this case and why $n_\uparrow$ is equal to $n_\downarrow$ iteration by iteration. Using the data from Fig. 2(b), we constructed the histogram for the distribution of $n/2$ [Fig. 2(d)] observing the existence of a single peak. Thus we believe that the attractive Hubbard model in two dimensions does not phase separate.

In summary, studying the behavior of the density of particles as a function of the chemical potential for the two-dimensional Hubbard model with both positive and negative U, we find that, in the parameter regime for which we have carried out numerical simulations, there is no evidence for phase separation.

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[14]Notice that since the Hubbard-Stratonovich decoupling that we use in our quantum Monte Carlo method treats differently spin up and spin down, these two magnitudes are equal on average but they do not take the same value from iteration to iteration. Then, as we noticed in the data shown in Fig. 2(a) and its corresponding histogram [Fig. 2(c)], at a given iteration an odd number of particles on the system can be allowed.

[15]It is important to be aware of the fact that the values of U/t and J/t for which the Hubbard and t-J models are equivalent may depend on the magnitude studied, i.e., whether it is the ground-state energy, correlation functions, etc.

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