Phase diagrams of the two-dimensional Hubbard and t-J models by a variational Monte Carlo method

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We use a variational Monte Carlo technique to study the ground state of the two-dimensional Hubbard and t-J models on a square lattice. We use a trial wave function that allows a continuous description of the paramagnetic, antiferromagnetic, and superconducting phases, as well as the coexistence of these phases, with no *a priori* constraint on double occupancy. The phase diagram of both models is given for intermediate coupling ($U = 10t$). We show that the apparent discrepancies between the two models, that appeared in previous variational Monte Carlo studies, are not present when this sufficiently good variational wave function is used. The two models are in good qualitative agreement. We find that except at half filling a pure antiferromagnetic phase does not exist but is always in coexistence with a d-wave superconducting phase, and is followed by a pure d-wave superconducting phase at doping up to $\delta \sim 0.3$. The staggered magnetization and the superconducting gap are measured, and a comparison with other analytical or numerical results is made.

I. INTRODUCTION

The discovery of high-T_c superconductivity,[1] and the observation by Anderson that the two-dimensional Hubbard model can be of some relevance to these compounds[2] has led to a renewal of interest in understanding the nature of the ground state of this model. Another model that was also proposed was the so-called t-J model, first introduced as the strong-coupling limit of the Hubbard model,[3] and that later proved also to be able to describe the two-band structure of the high-T_c compounds.[4,5] One question of crucial interest is the interplay of superconductivity and antiferromagnetism and whether these two phenomena appear in these models under their standard form or under more subtle arrangements (spin liquids, flux phases, or others).

All the approaches of these strong-coupling problems involve approximations, and it is sometimes difficult to sort the artefacts due to the approximations from the true features of the model. In this paper we try to ascertain the conclusions obtained by various authors (Yokoyama and Shiba, Gros, Lee, and Feng, and ourselves) within the framework of a variational Monte Carlo[6–11] (VMC). The VMC method provides variational upper bounds for the ground-state energy, which can be considered exact up to the eventually residual bias due to finite-size effects. Beyond the conclusions on the energy of the ground-state, other conclusions on the nature of this state (short- and long-range correlations and order) are much more difficult to draw and can only be the result of a whole set of presumptions.

Using the VMC method Gros, Yokoyama, and Shiba studied the t-J model. Two types of ground states were mainly studied: a commensurate antiferromagnetic wave function[12,8] with a wave vector $K = (\pi, \pi)$, and a d-wave superconducting BCS-type wave function.[13,14] The former describes a state with a staggered magnetization and no superconductivity, whereas the latter describes a superconducting state with no long-range magnetic order, although it exhibits some short-range antiferromagnetic correlations. Using VMC, Gros[13] and Yokoyama and Shiba[14] have shown that, for the t-J model, close to half filling the antiferromagnetic phase is higher in energy than a d-wave superconducting phase. These results are consistent with small repulsion renormalization calculations (which have nevertheless recently been questioned[15]), which find a d-type pairing away from half filling.[16–18] But such results seem contradictory with the VMC results on the Hubbard model in a related range of parameters (on this model at half filling the energy per particle of an antiferromagnetic wave function is $E = -0.401t$, whereas it is $E{=}-0.244t$ for a d-wave wave function and away from half filling at $\delta{=}0.11$ one has $E = -0.643t$ for antiferromagnetism and $E = -0.634t$ for superconductivity[11]).

This contradiction can be solved only in two ways: either the Hubbard and t-J models describe, in this range of parameters, very different physical systems, or the variational subspaces that have been explored are too small to describe the real ground state.

It was guessed for the t-J model by mean-field theory, that close to half filling the d-wave wave function was unstable towards antiferromagnetism,[19] which was checked numerically by projecting a variational superconducting resonating valence bond (RVB) function to simulate the presence of a staggered magnetic field.[10] This suggested the possibility of a restricted region of coexistence of antiferromagnetism and superconductivity close to half filling and that a pure superconducting or antiferromagnetic wave function was too restricted a variational space. In order to check if a similar behavior could also occur in the Hubbard model, we have introduced[11] a variational wave function that includes superconductivity and antiferromagnetism in a unique variational space. It was found that close to half filling there was indeed the coexistence of antiferromagnetism and superconductivity in the Hubbard model. Later this wave function was studied at half filling for the t-J model and was shown to provide a rather good description of the ground state of the system.[20]

Here we will use this variational wave function, which provides a sufficiently large variational space and gives good energetic results for both the Hubbard and t-J model, to try to make a more quantitative comparison between the two models at intermediate U for a wide range of dopings. In this framework we compute an estimate of the magnetic and superconducting order parameters. Finally we compare this optimized wave function with other proposals (incommensurate antiferromagnetism and flux phases).

II. MODELS AND TRIAL WAVE FUNCTION

We use the two-dimensional Hubbard model on a square lattice, with hopping restricted to nearest neighbors,

$$H_{\text{hub}} = -t \sum_{i,\tau,\sigma} c^\dagger_{i+\tau,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}, \tag{1}$$

where τ connects two nearest neighbors on the lattice, and $c_{i,\sigma}, c^\dagger_{i,\sigma}$ respectively destroys (creates) an electron with spin σ at site i and $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$. U is the on-site Hubbard repulsion ($U > 0$), and t the hopping parameter. In the following we will take $t = 1$, which gives for $U = 0$ a bandwidth of 8, and express all energies in units of t.

As is well known, in the large-U limit a canonical transformation[3] of the Hubbard model gives the t-J model,

$$H_{tJ} = -t \sum_{i,\tau,\sigma} c^\dagger_{i+\tau,\sigma} c_{i,\sigma} + J \sum_{\langle i,j \rangle} (S_i S_j - n_i n_j/4). \tag{2}$$

S_i denotes the spin at site i: $S_{i,\alpha} = \frac{1}{2} c^\dagger_{i,\sigma} \sigma^\alpha_{\sigma,\sigma'} c_{i,\sigma'}$ are $\alpha = x, y, z$, and σ are the Pauli matrices. $\langle i,j \rangle$ stands for a pair of nearest neighbors. H_{tJ} operates only in the subspace where there are no doubly occupied sites. In the large-U limit one has $J = 4t^2/U$.

We compute, by the usual Monte Carlo integration technique,[6-9] the average value of H with a trial wave function $|\psi\rangle$,

$$E = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle . \tag{3}$$

For strongly correlated fermions, $|\psi\rangle$ is usually taken to be of the Jastrow-Gutzwiller type,[21-23]

$$|\psi\rangle = P |\psi_0\rangle , \tag{4}$$

where P is a projector that modifies the weight of configurations with doubly occupied sites, and $|\psi_0\rangle$ is a model wave function that ensures the fermionic antisymmetry.

For the Hubbard model, we will take a prefactor of the form $P = g^{N_d}$,[22,23] where g is a variational parameter and N_d is the number of doubly occupied sites. More refined prefactors have been studied by Yokoyama[9] for the Hubbard model but will not be considered here for simplicity (such an improvement can change slightly the variational energy but not qualitatively the physical content of the wave function).

For the t-J model the constraint of no double occupancy has to be enforced exactly. This can be achieved with the same kind of variational wave function but with a projector P such that $P = 0$ if $N_d \neq 0$ (formally this corresponds to the limit $g \to 0$). In the following we will therefore use *the same* $|\psi_0\rangle$ for the Hubbard and t-J models, with a Gutzwiller projector (g^{N_d} for the Hubbard model) or a complete projector (enforcing $N_d = 0$) for the t-J model.

The nature of $|\psi_0\rangle$ depends on the expected long-range behavior. We will here use the wave function of Ref. 11, which includes paramagnetism, antiferromagnetism, and superconductivity in a unique variational space. Instead of pairing two free electrons of opposite spin, we pair together two quasiparticles describing the excitations of the antiferromagnetic phase. We therefore have

$$|\psi_0\rangle = \prod_k (u_k + v_k d^\dagger_{k,\uparrow} d^\dagger_{-k,\downarrow}) |0\rangle , \tag{5}$$

where the u_k, v_k, are the usual BCS coefficients. Up to a nonimportant normalization factor we get

$$v_k/u_k = \Delta_k / [\epsilon_k - \mu + \sqrt{(\epsilon_k - \mu)^2 + |\Delta_k|^2}]. \tag{6}$$

Δ_k is the BCS variational parameter and is taken to be $\Delta_k = \Delta[\cos(k_x) - \cos(k_y)]$ for d-wave superconductivity. μ is the chemical potential. Note that such a form for Δ_k is not mandatory, and any function can, in principle, be taken into account.

The $d^\dagger$ are the operators diagonalizing the antiferromagnetic Hartree-Fock Hamiltonian

$$\begin{aligned} d^\dagger_{k,\sigma} &= \alpha_k c^\dagger_{k,\sigma} + \sigma \beta_k c^\dagger_{k+K,\sigma} , \\ d^\dagger_{k+K,\sigma} &= -\sigma \beta_k c^\dagger_{k,\sigma} + \alpha c^\dagger_{k+K,\sigma} , \end{aligned} \tag{7}$$

where $K = (\pi, \pi)$ is the commensurate perfect nesting vector, and k is limited to half of the Brillouin zone by $\epsilon_k < 0$. α_k and β_k are the usual Hartree-Fock antiferromagnetic coefficients

$$\alpha_k = [(1 - \epsilon_k/\sqrt{\epsilon_k^2 + D^2})/2]^{1/2},$$
$$\beta_k = [(1 + \epsilon_k/\sqrt{\epsilon_k^2 + D^2})/2]^{1/2}. \quad (8)$$

The gap D is related to the antiferromagnetic staggered magnetization, whereas the gap Δ is related to the superconducting order parameter. It should be noted that a nonzero D or Δ is not the signature of a magnetic or superconducting order. The true order parameters will have to be computed to allow for an answer (see below). If $D = 0$ our function gives the d-wave-type wave function, whereas if $\Delta \to 0$ the usual antiferromagnetic phase is recovered.

To be treated numerically, the function $|\psi\rangle$ is projected on a subspace with a fixed number of particles,[24,13] and Δ, D, μ (and g for the Hubbard model), are taken as variational parameters and fixed by minimizing the energy E. Since in (4) the projectors for the Hubbard and t-J models differ, the optimal variational parameters have no reason to be the same in the nonprojected wave functions. Therefore we will have to perform different minimizations for the Hubbard and t-J models.

III. SIMULATION AND RESULTS

A. Simulation

All the calculations were made on a square lattice, with periodic-antiperiodic conditions on the wave function $[\psi(x + L_x, y) = \psi(x, y),\ \psi(x, y + L_y) = -\psi(x, y)]$, in order to avoid degeneracy of the Fermi surface at half filling.[9,25] We have mainly studied 8×8 lattices for $U = 10.0$. We have taken an intermediate U because the intermediate coupling region is the region of physical interest in application to high-T_c superconductivity.[2,26] For such a value of the coupling, the t-J model is expected to give a correct approximation of the Hubbard one, if one chooses $J = 4t^2/U = 0.4$.

In order to check the size dependence we have also performed some simulations on 6×6 and 10×10 systems, for selected values of the band filling, to be sure that the following qualitative conclusions will not be invalidated by size effects. But we have not systematically performed an extrapolation to infinite size, which would have been extremely time consuming.

The variational parameters were determined by generating a fixed set of configurations and then using them to minimize the energy.[7,27] This offers both the advantage of good computing time performances and of using *correlated* measurements, which allows us to compare energies that differ by much less than the statistical error bars on uncorrelated samples. Note that one could choose instead to minimize the energy variance[27] for which more powerful minimization techniques can be used. This method is efficient for atomic systems where there are well-separated excited states, which is not the case for our many-body problem. We in fact found that, in general, the minimum of the variance does not coincide with the minimum of the energy. For sufficiently badly behaved wave functions the minimum in energy can even be a maximum of the variance as one can convince oneself by looking at the function $|\psi\rangle = |\psi_0\rangle + (\nu^2 + \lambda^2)|\psi_1\rangle$, where $|\psi_0\rangle$ and $|\psi_1\rangle$ are two eigenstates such that $E_0 < E_1$, ν is fixed, and λ a variational parameter. It is easy to see that the minimum of the energy is at $\lambda = 0$, whereas it corresponds, for $\nu > 1$ to a maximum of the variance.

For the optimal wave functions, we have then measured the superconducting order parameter:[13,8]

$$\Delta_{\text{mes}} = \left\langle \frac{1}{16L^2} \left(\sum_{i,\tau} c_{i,\uparrow}^\dagger c_{i+\tau,\downarrow}^\dagger (-1)^{\tau_y} \right) \left(\sum_{j,\tau'} c_{j,\downarrow} c_{j+\tau',\uparrow} (-1)^{\tau'_y} \right) \right\rangle^{1/2}, \quad (9)$$

where L is the number of sites, τ denotes the four nearest-neighbor vectors, and the antiferromagnetic order parameter is

$$m = \frac{1}{L} \sum_i \langle (-1)^{x_i + y_i} (n_{i,\uparrow} - n_{i,\downarrow}) \rangle. \quad (10)$$

We have used at least five independent simulations, each of 4×10^5 Monte Carlo steps (MCS's) to determine the minimum energy and parameters and the error bars. Other quantities such as the superconducting order parameter, the staggered magnetization, the kinetic energy,

TABLE I. Optimal parameters for an $L = 8 \times 8$ system at $U = 10$. N is the number of particles, δ the deviation from half filling $(L - N)/L$, D the antiferromagnetic parameter, Δ the superconducting one, μ the chemical potential, g the Gutzwiller prefactor, and N_d is the number of doubly occupied sites.

N	δ	D	Δ	μ	g	N_d
64	0.0	1.55(4)	0.04(2)	−0.00(2)	0.45(1)	2.33(2)
60	0.06	0.80(5)	0.11(2)	−0.19(3)	0.34(1)	2.39(4)
52	0.19	0.05(3)	0.05(2)	−0.55(6)	0.25(3)	1.93(2)
44	0.31	0.00(3)	0.02(1)	−0.69(5)	0.29(2)	1.30(5)
36	0.44	0.00(3)	0.00(3)	−0.87(9)	0.34(2)	1.00(5)

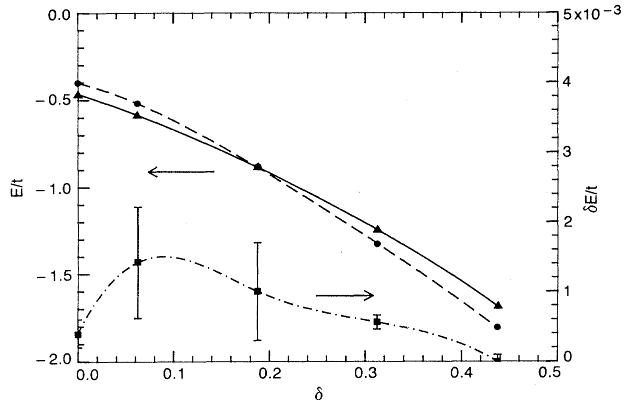

FIG. 1. Energies in units of t for the optimal parameters given in Tables I and II for a Hubbard model at $U = 10$ (circles) and a t-J model for $J = 0.4$ (triangles). The difference in energy δE between a superconducting and a nonsuperconducting phase for the Hubbard model is also indicated (squares).

and the potential energy, were measured over independent samples of 8×10^5 MCS's. The order of magnitude of the time needed to get one minimum is between 1 and 2 h on a Cray-2 computer. The different physical quantities are much easier to compute, and a set of measures takes around 1 h of Cray-2 computer time.

B. Results

The optimal parameters for an 8×8 system at $U = 10$ as a function of the band filling are indicated in Table I for the Hubbard model and Table II for the t-J model, and the results for the optimal variational energies are reported in Fig. 1. By looking at Tables I and II one can see that, in both models, close to half filling, the superconducting variational parameter *and* the antiferromagnetic one are both nonzero suggesting a coexistence of superconductivity and antiferromagnetism. Such a phase diagram, which would be in good qualitative agreement with a mean-field analytical result on the t-J model,[19] will be criticallly discussed in the following, but first we would like to make some comments on the significance of the variational results.

TABLE III. Comparison of the average energy $\langle 2\mathbf{S}_i \cdot \mathbf{S}_j \rangle$ and the average alternate magnetization $\langle M \rangle$ for the Heisenberg model in different recent works.

	$\langle 2\mathbf{S}_i \cdot \mathbf{S}_j \rangle$	$\langle M \rangle$
8×8 lattices		
Gross, Sánchez-Velasco, and Siggia[a]	−0.6715	
Trivedi and Ceperley[b]	−0.6734	0.7
Our variational work	−0.6642	0.7
$\infty \times \infty$		
Gross, Sánchez-Velasco, and Siggia[a]	−0.6672	
Trivedi and Ceperley[b]	−0.6692(2)	0.62
Carlson[c]	−06692(1)	

[a] Reference 28.
[b] Reference 29.
[c] Reference 30.

1. Variational energy

At half filling a detailed comparison with a large body of existing results is possible. Energies and alternate magnetization for the Heisenberg model (which is the limit of the t-J model at half filling) are given in Table III. Inspection of these results shows that our wave function is within $10^{-2}t$, from the best results [obtained by diagonalization on small samples or by quantum Monte Carlo (QMC) calculations]. For the Hubbard model, our result of $0.401t$ is the same as the antiferromagnetic one of Yokoyama and Shiba[12] (see Sec. III B 3). Comparisons done in Ref. 12 show that such an antiferromagnetic wave function is extremely close in energy to QMC (at $U = 8$ $E_{\rm VMC} = 0.493$ and $E_{\rm QMC} = 0.48$). At $U = 10$ our result compares favorably with the QMC value of Sorella *et al.*[31] ($E = -0.42$). For comparison we recall that for $U = 10t$ the Gutzwiller approximation for the paramagnetic state has an energy of $-0.09t$, and the Gutzwiller paramagnetic state has an energy of $-0.13t$.

Away from half filling the results are scarce. There are no "exact" (QMC or diagonalization) results for the energy of these models with such a large on-site repulsion but only variational ones. To give some idea of the differences in energy we are encountering, let us consider as an example the case of the Hubbard model for a 6×6 lattice with four holes ($\delta = 0.11$). The energy per particle obtained for the different wave functions are the following:

TABLE II. Same as Table I but for the t-J model. Here $g = 0$ (no doubly occupied sites).

N	δ	D	Δ	μ
64	0.0	0.276(5)	0.55(2)	−0.00(1)
60	0.06	0.18(1)	0.56(6)	−0.38(4)
52	0.19	0.00(1)	0.34(3)	−0.54(4)
44	0.31	0.00(1)	0.20(3)	−0.69(5)
36	0.44	0.00(1)	0.00(2)	−0.87(9)

$-0.6341t$ for a pure d-wave superconducting wave function, $-0.6428t$ for a pure commensurate antiferromagnetic wave function, $-0.6447t$ for a mixed wave function containing both superconducting and antiferromagnetic correlations.

These results as well as those of Table III are a good illustration of how near in energy, states with really different long-range order could be. We nevertheless think that our comparison is meaningful: due to the correlated measurements described in the preceding section, the statistical uncertainties are under control and our simulations on 6×6 and 10×10 samples indicate that size effects do not seem to affect the hierarchy of variational states. This does not predetermine what kind of order will be preferred in the thermodynamical limit in the *true* ground state. This important question is still certainly open both in analytical and numerical work, and the answer to this question is beyond the reach of any variational method. With these points and restrictions in mind, we will now proceed to the study of the order parameters measured in our wave function with optimal values of the variational parameters.

2. Magnetism

The alternate magnetization measured in each model is shown in Fig. 2. These results, combined with the information on the energy, show that the antiferromagnetic instability is at $T = 0$—a very strong feature of the Hubbard model.

For the t-J model the antiferromagnetism is also quite strong close to half filling, and the two models are in that sense in good qualitative agreement. The more rapid disappearance of antiferromagnetism (for $\delta \sim 0.1$) is perhaps to be related to the absence in the t-J model of the three-site term, which allows the jumping of holes onto second-neighbor sites.

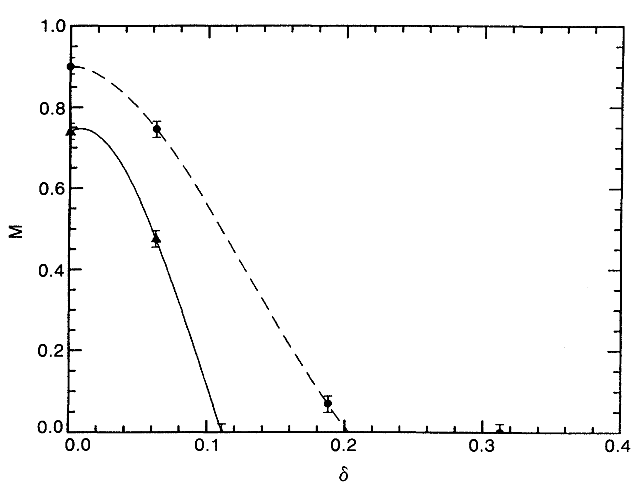

FIG. 2. Measured staggered magnetization for the Hubbard (circles) and t-J (triangles) models as a function of the band filling for a 8×8 system at $U = 10$. The lines are simply a guide to the eye.

The critical doping for the disappearance of antiferromagnetism in the Hubbard model ($\delta_c = 0.2$) is nearly identical to the values found for the disappearance of a pure antiferromagnetic phase.[32,33] This indicates that, at least for this kind of wave function, antiferromagnetism is not drastically affected by the possibility of superconducting pairing in the Hubbard model.

A comparison of these results to those of the mean-field calculation of Inui *et al.*[19] shows that the mean-field calculation overestimates the magnetization and the range of existence of antiferromagnetism. It has been pointed out[12,9] that a pure antiferromagnetic Gutzwiller wave function still overestimates the alternate magnetization. But the inclusion of the superconducting pairing in (5) also has the effect of introducing more fluctuations.

The study of the t-J model at half filling is an interesting benchmark (see also Ref. 20). The inclusion of a "superconducting" gap decreases the energy from $E = -0.4568$ per particle[32] to $E = -0.4656$ (which would correspond to $\langle S_i S_j \rangle = -0.3321$) and decreases the staggered magnetization from $m \sim 0.9$ (Ref. 32) to $m \sim 0.7$. This is extremely close to the best QMC estimates for the same system size,[29] $E = -0.4694$ and $m \sim 0.7$, and to the variational results of Liang, Douçot, and Anderson[34] $E = -0.4675$ ($m \sim 0.6$). So this wave function appears to be variationally interesting to restore spin fluctuations that were frozen in the pure classical antiferromagnetic wave function.

Finally we want to compare our VMC results to the QMC ones[35–37] for the Hubbard model. At half filling the QMC calculation predicts an antiferromagnetically ordered ground state in agreement with the variational calculation but with a smaller staggered magnetization (for $U = 10$, QMC results give $m \sim 0.5$ instead of $m \sim 0.9$ for VMC).[12] Such a quantitative discrepancy is clearly due to the lack of fluctuations in the variational wave function. This can be cured, at least partially, by improving the wave function in order to take into account such fluctuations. Nevertheless the variational method gives the correct long-range order. Away from half filling there is a large difference that remains to be explained: the QMC results seem to predict the absence of antiferromagnetic order[35–37] in the thermodynamical limit, although antiferromagnetic fluctuations are found in the finite-size samples. A possible explanation of the discrepancy with the QMC results could still be a lack of fluctuations in the variational wave function (5). But some facts appear to be at variance with that conclusion: firstly the good agreement of the VMC with the exact diagonalisation studies,[33] secondly the correct qualitative agreement with the t-J model, where antiferromagnetism is much less favored and where the wave function—at half filling at least—is expected to be rather good (see above), and finally the unphysical nature of the phase diagram that QMC calculations would predict (antiferromagnetism at half filling and nothing away from half filling). So we are inclined to believe that the discrepancy between VMC and QMC results originates from the fact that VMC results mainly give information on the ground state of the system, whereas QMC results are intrinsically a $T \neq 0$ method: the problem of the criticality of the phase transition being still largely open, as well as the problem of size effects, the results obtained by QMC calculation could be in too high a temperature region to exhibit full long-range order on the finite systems studied here. Note that the study of the antiferromagnetic order is made more complicated by the fact that away from half filling the wave vector of the staggered magnetization becomes incommensurate.[37,38]

3. Superconductivity

The values of the variational parameters (see Tables I and II) indicate that, for a wide range of dopings, the inclusion of a superconducting variational parameter does improve, in both models, the energy of the state.

The results obtained for the superconducting variational parameter Δ at half filling call for some comments. Due to a local SU(2) symmetry the t-J model at half filling is not superconducting even with a nonzero Δ.[39,13,14] This is not the case for the Hubbard model, where a nonzero Δ could imply superconductivity, since $g \neq 0$ allows double occupancy and charge fluctuations. The results obtained for the 8×8 system at half filling should thus be analyzed in more detail. To do so we have looked at the finite-size effects by considering the size dependence of the superconducting variational parameter at half filling and around $\delta \sim 0.1$ where Δ seems to be at its maximum. The results are reported in Fig. 3. One clearly sees in this figure the different behavior of the $\delta = 0$ and 0.1 systems and the strong decrease of the Δ parameter at half filling with its probable extrapolation towards a zero value. We can therefore expect, in the thermodynamical limit, a pure antiferromagnetic phase at half filling, which is in agreement with previous results[12,10,8,35] and with the t-J model result. Since the number of doubly occupied sites is quite small on the smallest systems ($N_d = 2.3$ for an 8×8 system), the local number of fluctuations at half filling is severely restricted, and both solutions ($\Delta \neq 0$ and $\Delta = 0$) are certainly very close in energy, which explains the important size effect for $\delta = 0$. However, the results for a doped sample do not exhibit the same size effect. True extrapolation is difficult as the different samples do not have exactly the same doping, but examination of Fig. 3 gives us a firm indication, at $T = 0$, of the existence of d-wave superconductivity for $\delta \sim 0.1$. Figure 3 also indicates that, except at half filling, the size effects are not drastic and our 8×8 system is probably adequate.

The measured superconducting order parameter is shown in Fig. 4 for both models. The above discussion on magnetism accurately shows how subtle the problem of superconductivity in these models is. In the t-J model the superconducting d-wave component helps introduce short-range spin fluctuations, and the present calculation alone cannot decide definitively whether the superconducting long-range order is a necessary ingredient.

In that sense, the fact that the Hubbard model, where the superconducting gap is zero at half filling and where a pure superconducting wave function being unfavored also

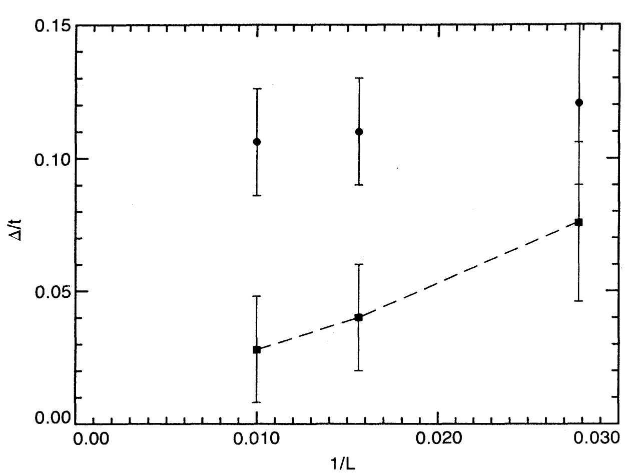

FIG. 3. Size dependency of the variational parameter Δ. Squares correspond to half filling, whereas solid circles stand for systems with 32 (6×6), 60 (8×8), or 44 (10×10) particles. These three points correspond to slightly different δ ($\delta = 0.11$, $\delta = 0.0625$, and $\delta = 0.12$, respectively), and therefore no extrapolation to infinite size can be made directly.

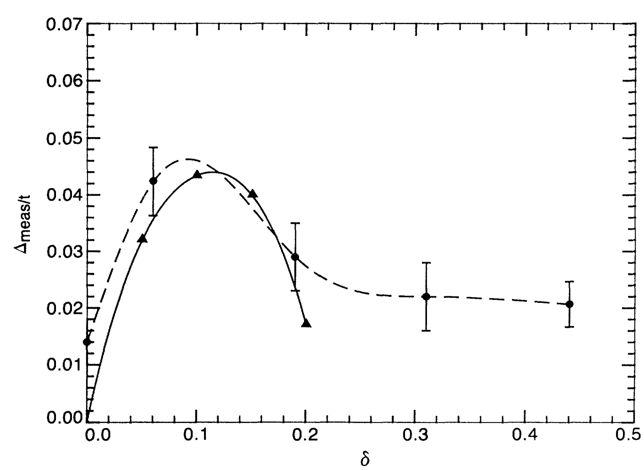

FIG. 4. Our measured superconducting order parameter for the Hubbard model (circles) and the Yokoyama and Shiba measurement (Ref. 14) (triangles) for the t-J model as function of the band filling for a 8×8 system at $U = 10$. The lines are simply a guide to the eye. Note that the measured order parameter $\Delta_{\rm meas}$ always keeps a finite value even in the paramagnetic phase. This is an artefact of formula (9), which gives only the off-diagonal long-range order parameter in the limit $L \to \infty$.

exhibits superconductivity upon doping, seems to provide confirmation that the presence of the d-wave pairing is not an artefact of the variational wave function. The difference in energy between the phase of coexistence and the antiferromagnetic phase with no superconducting gap could then, with more confidence, be attributed to the superconducting pairing. We have indicated in Fig. 1 the total energy per particle for both models and the difference in energy between the phase of coexistence and the same phase but with no superconducting gap ($\Delta = 0$) for the Hubbard model. It is seen to be very weak, a few hundredths of the magnetic energy.

Such a result calls for additional comments. It is numerically significant for the finite-size sample that we have studied. The use of correlated measurements allows one to extract significant results from the numerical noise. The error bars in Tables I and II come from statistics on five different samples. The small size of the pairing energy can explain why superconductivity has not been seen up to now in quantum Monte Carlo calculations.[40] The QMC method is essentially a $T \neq 0$ method and it will be necessary to go to lower temperatures and larger size samples to see so tiny an effect.

The superconducting order parameter has been measured (see Fig. 4) and is at its maximum around $\delta \simeq 0.1$ and of the order of $0.04t$. It does not seem to extrapolate to zero with the size of the sample. After the coexistence phase ($\delta \sim 0.2$ for Hubbard $\delta \sim 0.1$ for t-J) and up to $\delta \sim 0.3$ a pure d-wave superconducting phase is found, as is clearly seen in Table I, Table II, and Fig. 4.

The values for the t-J model are extracted from the work of Yokoyama and Shiba[14] who used a method allowing them to compute the order parameter directly without bias due to finite-size effects. Again both models are in good agreement. The upper limit for the existence of superconductivity is similar in both models and a little bigger than the one predicted by Shiba[41] ($\delta = 0.2$) with a slightly different wave function.

Although clearly the theory is much too crude to be directly related to high-T_c experiments, one can note that the agreement in the ratio between the superconducting gap and the magnetic energy is weak—though not completely unreasonable—in comparison to experimental values for high T_c. To the best of our knowledge no coexistence of long-range order has been observed so far. Nevertheless, if, as in our wave function, the system possesses an antiferromagnetic gap at points where the superconducting gap vanishes (i.e., $k_x = k_y$), all the unusual aspects of d-wave superconductivity linked to the presence of zeros of the gap on the Fermi surface would not be observable, and the experimental distinction between s- and d-wave superconductivity will become more difficult.[42]

4. Comparison of the two models

Finally we would like to stress the following points: the phase diagrams calculated here are qualitatively and, for the superconductivity, quantitatively in agreement. The energies per particle are in qualitative agreement over a wide range of dopings. This seems to confirm that, at the present level of accuracy, and in the range of parameters here studied, the two models (Hubbard and t-J) essentially describe the same physics. But if the "neglected terms" of the t-J model do not seem to change the physics much, they nevertheless have an appreciable importance. At half filling, due to double occupancy, the energy in the Hubbard model is $E = -0.4015$ per particle, whereas it is $E = -0.4656$ for the t-J Hamiltonian. On the other hand, the neglect in the t-J model of the three-site term, which allows the hopping of holes to next neighbor position, probably explains why the energy of the Hubbard Hamiltonian becomes lower upon doping.

IV. COMPARISON WITH OTHER WAVE FUNCTIONS

A. Incommensurate antiferromagnetism

The mixed antiferromagnetic and superconducting wave function seems a reasonably good wave function for strongly correlated systems when the Hubbard repulsion is of the order of the bandwidth. Nevertheless, the increase of the variance of this wave function under doping is a sign that it is not the best one when holes are introduced.

In fact, in qualitative agreement with Hartree-Fock results[43] it appears that an incommensurate antiferromagnetic phase is much more stable than the commensurate one.[38]

The lowest phase presently exhibited in that kind of finite-size study is one where holes align in diagonal walls. The energy gain due to the incommensurate instability is huge[38] even for quite large dopings (of order t per hole). For example, at $\delta = 0.1$ and $U = 10$ the coexistence phase (commensurate antiferromagnetism and superconductivity) has an energy per particle $E = -0.643$, against $E = -0.695$ for a phase with diagonal walls.[38] But such a phase is almost certainly an artefact of the Hubbard model and will disappear if long-range Coulombic repulsion is included. One can then argue that only the homogeneous solutions of the Hubbard model can have a physical meaning. Among these solutions the coexistence phase of antiferromagnetism and superconductivity has, to the best of our knowledge, the lowest energy.

Note that the question of coexistence of incommensurate antiferromagnetism and superconductivity has been addressed. As for the commensurate case, a small energy ($\sim 10^{-3}t$) is gained by a d-wave pairing.[38]

B. Flux phases

For the t-J model another important class of wave functions studied are the so-called flux-phase wave functions.[44–47] At half filling it can be shown that the best flux phase[48] is equivalent under an SU(2) symmetry[39] to various superconducting phases. The most important are the $s+id$ phase of Kotliar and Liu[49] and a special d-wave superconducting wave function with a variational superconducting parameter $\Delta = 1$.[48]

Away from half filling two kinds of flux phase have been considered: the staggered ones[44,50] and the commensurate one.[46,47] In the staggered ones the flux changes sign on alternate plaquettes. These phases have the advantage of giving a good kinetic energy but have been shown by using the Gutzwiller approximation to be higher in energy than a d-wave superconducting wave function,[51] a result confirmed by VMC calculations.[52] Our wave function is therefore better than such a wave function.

The commensurate flux phase frustrates the kinetic energy and for a wide range of values of J is higher in energy than a projected Fermi liquid phase.[53,47,54] For example, if one takes the values of Ref. 53, which are one of the most favorable estimates, the flux phase is more stable than a Fermi-liquid phase only for $J > 0.6$ at $\delta = 0.07$. For the values of J considered here the commensurate flux phase is not stable away from half filling. At half filling, since the most favorable flux phase corresponds by SU(2) symmetry to a d-wave superconducting phase with $\Delta = 1$ (Ref. 48) it is also higher in energy than the best estimate with the coexistence wave function (5).

A function similar to (5) but with a mixing of flux phases and antiferromagnetism has been considered for the half-filled case[55] and gives a slightly higher energy.

V. CONCLUSION

In this paper we have presented a variational Monte Carlo study of the coexistence of superconductivity and antiferromagnetism in the Hubbard model and the t-J model on a square lattice. We have used a variational wave function introduced previously for the Hubbard model[11] that allows a continuous description of the paramagnetic, antiferromagnetic, and superconducting phases, as well as a coexistence between antiferromagnetism and superconductivity.

We have found that at intermediate coupling in *both* models a pure antiferromagnetic phase seems to exist only at half filling. Between zero and a critical doping, whose precise value depends on the model ($\delta \sim 0.2$ for Hubbard $\delta \sim 0.1$ for t-J), the most stable phase exhibits both antiferromagnetism and superconductivity. The energy gained in the pairing compared to those of the pure antiferromagnetic phase is very small for the Hubbard model. For the t-J model it is difficult to define the energy really associated with superconducting pairing because of the lack of a good nonsuperconducting reference state. In our opinion the fact that *both models* give superconductivity, although a pure superconducting phase is unfavorable for the Hubbard model, can be a good indication that the d-wave pairing is a real effect in these models. A definite answer to this question would require a more powerful technique.

Above the threshold for antiferromagnetism the system becomes purely superconducting. Here again the two models have approximately the same order parameter and phase diagrams. Finally above $\delta \sim 0.3$ the most stable phase is the paramagnetic one.

It could be added that, within the present study, the optimized superconducting state appears to be a weak coupling superconductor, which only involves the pairing of a small fraction of the electrons around the Fermi surface. Whether a true RVB state[56,34] describing a disordered spin liquid could be a better approximation for the ground state of the Hubbard model remains to be proved. Our preliminary attempts in this direction have been so far without success.

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[1] J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).
[2] P. W. Anderson, Science **235**, 1196 (1987).
[3] J. E. Hirsch, Phys. Rev. Lett. **54**, 1317 (1985).
[4] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[5] B. S. Shastry, Phys. Rev. Lett. **63**, 1288 (1989).
[6] W. L. McMillan, Phys. Rev. **138**, A442 (1965).
[7] D. Ceperley, G. V. Chester, and K. H. Kalos, Phys. Rev. B **16**, 3081 (1977).
[8] C. Gros, Ann. Phys. **189**, 53 (1989).
[9] H. Yokoyama, Ph.D. thesis, University of Tokyo, 1988.
[10] T.K. Lee and S. Feng, Phys. Rev. B **38**, 11 809 (1988).
[11] T. Giamarchi and C. Lhuillier, in *Condensed Matter Theories,* edited by V. Aguilera-Navarro (Plenum, New York, in press), Vol. 5.
[12] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 3582 (1987).
[13] C. Gros, Phys. Rev. B **38**, 931 (1989).
[14] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **57**, 2482 (1988).
[15] A. Georges and J. S. Yedidia, Phys. Rev. B **43**, 3475 (1991).
[16] I. Dzyaloshinskii, Zh. Eksp. Teor. Fiz. **93**, 1487 (1987) [Sov. Phys. JETP **66**, 848 (1987)].
[17] I. Dzyaloshinskii and V. M. Yakovenko, Zh. Eksp. Teor. Fiz. **94**, 344 (1988) [Sov. Phys. JETP **67**, 844 (1988)].
[18] H. J. Schulz, Europhys. Lett. **4**, 609 (1987).
[19] M. Inui, S. Doniach, P. J. Hirschfeld, and A. E. Ruckenstein, Phys. Rev. B **37**, 2370 (1988); and the erratum Phys. Rev. B **39**, 7300(E) (1989).
[20] C. Gros, Phys. Rev. B **42**, 6835 (1990).
[21] R. Jastrow, Phys. Rev. **98**, 1479 (1955).
[22] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963).
[23] M. C. Gutzwiller, Phys. Rev. **137**, A1726 (1965).
[24] J. P. Bouchaud, A. Georges, and C. Lhuillier, J. Phys. (Paris) **49**, 553 (1988).
[25] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987).

[26]P. W. Anderson, in *Frontiers and Borderlines in Many-Body Physics, Varenna Lectures* (North-Holland, Amsterdam, 1987).
[27]C. J. Umrigar, K. G. Wilson, and J. W. Wilkins, Phys. Rev. Lett. **60**, 1719 (1988).
[28]M. Gross, E. Sánchez-Velasco, and E. Siggia, Phys. Rev. B **39**, 2484 (1989).
[29]N. Trivedi and D.M. Ceperley, Phys. Rev. B **41**, 4552 (1990).
[30]J. Carlson, Phys. Rev. B **40**, 846 (1990).
[31]S. Sorella, E. Tosatti, S. Baroni, R. Car, and M. Parinello, Int. J. Mod. Phys. B **1**, 993 (1988).
[32]H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 3570 (1987).
[33]E. Kaxiras and E. Manousakis, Phys. Rev. B **37**, 656 (1988).
[34]S. Liang, B. Douçot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).
[35]J. E. Hirsch, Phys. Rev. B **31**, 4403 (1985).
[36]J. E. Hirsch and S. Tang, Phys. Rev. Lett. **62**, 591 (1989).
[37]M. Imada and Y. Hatsugai, J. Phys. Soc. Jpn. **58**, 3752 (1989); A. Moreo, D.J. Scalapino, R.L. Sugar, S.R. White and N.E. Bickers, Phys. Rev. B **41**, 2313 (1990).
[38]T. Giamarchi and C. Lhuillier, Phys. Rev. B **42**, 10 641 (1990).
[39]I. Affleck, Z. Zou, T. Hsu, and P. W. Anderson, Phys. Rev. B **38**, 745 (1988).
[40]J. E. Hirsch and H. Q. Lin, Phys. Rev. B **37**, 5070 (1988).
[41]H. Shiba, in *Two Dimensional Strongly Correlated Electronic Systems* (Gordon and Breach, New York, 1988).
[42]We are grateful to H. J. Schulz (private communication) for having pointed out this point.
[43]J. Zaanen and O. Gunnarsson, Phys. Rev. B **40**, 7391 (1989); D. Poilblanc and T. M. Rice, *ibid.* **39**, 9749 (1989); H. J. Schulz, Phys. Rev. Lett. **64**, 1445 (1990); H. J. Schulz, J. Phys. (Paris) **50**, 2833 (1989); M. Kato, K. Machida, H. Nakanishi, and M. Fujita, J. Phys. Soc. Jpn. **59**, 1047 (1990).
[44]I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).
[45]G. Kotliar, Phys. Rev. B **37**, 3664 (1988).
[46]P. W. Anderson, B. S. Shastry, and D. Hristopulos, Phys. Rev. B **40**, 8939 (1989).
[47]P. Lederer, D. Poilblanc, and T. M. Rice, Phys. Rev. Lett. **63**, 1519 (1989).
[48]F. C. Zhang, C. Gros, T. M. Rice, and H. Shiba, Supercond. Sci. Technol. **1**, 36 (1988).
[49]G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988).
[50]J. B. Marston and I. Affleck, Phys. Rev. B **39**, 11 538 (1988).
[51]F. C. Zhang, Phys. Rev. Lett. **64**, 974 (1990).
[52]T. K. Lee and L. N. Chang, Phys. Rev. B **42**, 8720 (1990).
[53]J. P. Rodriguez and B. Douçot, Europhys. Lett. **11**, 451 (1990).
[54]S. Liang and N. Trivedi, Phys. Rev. Lett. **64**, 232 (1990).
[55]T. Hsu (private communication).
[56]J. P. Bouchaud and C. Lhuillier, Europhys. Lett. **3**, 1273 (1987).