Variational Monte Carlo study of incommensurate antiferromagnetic phases in the two-dimensional Hubbard model

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We use a variational Monte Carlo technique to study the ground state of the two-dimensional Hubbard model on a square lattice. We study the stability of the usual commensurate antiferromagnetic phase against the formation of domain walls for various system sizes, band filling, and Hubbard repulsion. An instability towards diagonal domain walls is found for the values of the Hubbard repulsion studied ($U=4-10t$). We compute the condensation energy of the holes in walls. Such an incommensurate antiferromagnetic phase is much stabler than any other solution. Whether paramagnetic or purely superconducting, but superconductivity is found still to coexist with incommensurate antiferromagnetism. We carefully compare our results with those of the Hartree-Fock model and shed some light on the limitations of the Hartree-Fock solutions.

I. INTRODUCTION

Soon after the discovery of high-T_c superconductivity,[1] it was pointed out by Anderson that the two-dimensional Hubbard model could be of some relevance to these compounds.[2] Another model also proposed was the so-called t-J model, which was first introduced as the strong-coupling limit of the Hubbard model[3] and later proved to be an efficient model to describe the two-band structure of the high-T_c compounds.[4,5] This has lead to a renewal of interest for understanding the nature of the ground state of these models. One question of crucial interest is the existence of superconductivity and the competition with the usual antiferromagnetic phase that one can expect for repulsive interactions.

By using a variational Monte Carlo method[6-9] on the t-J model, Gross, Yokoyama, and Shiba[10,11] were the first to prove that close to half-filling the antiferromagnetic phase was superset by a d-wave superconducting phase. These results are consistent with small-repulsion renormalization calculations which also find a d-type pairing away from half-filling.[12-14] These variational results are based on the assumption that under doping the antiferromagnetic phase remains commensurate, i.e., that the wave vector of the magnetization remains at (π,π) (for a unity lattice spacing).

It was soon proposed that this commensurate phase was unstable, and various types of incommensurate phases have been investigated[15-19] leading to a further stabilization of the antiferromagnetic phase. At small U it was shown[15] that the most stable incommensurate phase corresponds to a phase in which the holes are localized in domain walls, and therefore to a linear polarization of the incommensurate modulation. Subsequently the relative stability of vertical and diagonal domain walls was studied, using the Hartree-Fock approximation.[16,17]

However, the wave function obtained with Hartree-Fock (HF) is a poor variational wave function, since it is much too high in energy, as was already the case for a commensurate antiferromagnetic Hartree-Fock wave function.[20,9] The HF wave function has to overestimate the antiferromagnetic order to reduce the Hubbard repulsion, i.e., avoid having a spin-up and spin-down particle on a same site. As is well known, it is best to ensure a part of the correlations between electrons of opposite spins through a Gutzwiller projector.[21,22] It is thus natural to wonder if the results concerning the incommensurate phases subsist when these more complete and energetically more reasonable wave functions are taken into account. Moreover, a more efficient wave function is also needed if one wants to compare with the energies of other types of instabilities (e.g., superconductivity).

Our purpose is to check, by a Monte Carlo variational calculation, the stability of the commensurate antiferromagnetic phase when a full Gutzwiller-type wave function is taken into account. We will also compare the energy of an incommensurate antiferromagnetic phase and a superconducting one. Since, as will be shown, the incommensurate antiferromagnetic phase is stabler than any proposed superconducting wave function[10,11,23] we will examine in a crude approximation if it is still possible to get superconductivity even with a strongly stabilized antiferromagnetic phase.

II. MODEL AND METHOD

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

$$H=-t\sum_{\langle i,j\rangle,\sigma}c^{\dagger}_{i,\sigma}c_{j,\sigma}+U\sum_{i}n_{i,\uparrow}n_{i,\downarrow}\ , \tag{2.1}$$

where $\langle\ \rangle$ stands for nearest neighbors, $c_{i,\sigma}$ ($c^{\dagger}_{i,\sigma}$) 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 ex-

press all energies in units of t.

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

$$E=\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle \ . \tag{2.2}$$

In order to take into account the fact that doubly occupied sites are disfavored by the Hubbard repulsion U and to have a tractable function, $|\psi\rangle$ is usually taken of the Jastrow-Gutzwiller type[24,21,22]

$$|\psi\rangle=P|\psi_0\rangle \ , \tag{2.3}$$

where P is a projector which reduces the weight of doubly occupied sites and $|\psi_0\rangle$ is a model wave function which insures the fermionic antisymmetry.

We will take here the simplest form for the prefactor $P=g^{N_d}$,[21,22] where g is a variational parameter and N_d the number of doubly occupied sites. More refined prefactors have been studied by Yokoyama[9] but will not be considered here for simplicity.

$|\psi_0\rangle$ depends on the expected long-range behavior. Since we are interested by an antiferromagnetically ordered phase, we will take $n_i=\langle n_{i,\uparrow}+n_{i,\downarrow}\rangle$ and $m_i=(-1)^{x_i+y_i}\langle n_{i,\uparrow}-n_{i,\downarrow}\rangle$ as order parameters. n_i and m_i are, respectively, the average number of particles and the average staggered magnetization on site i. $|\psi_0\rangle$ is the N particle determinant made from one-particle states, solutions of the Hartree-Fock Hamiltonian

$$H=-\sum_{\langle i,j\rangle,\sigma} c^{\dagger}_{i,\sigma}c_{j,\sigma}+\frac{U}{2}\sum_{i,\sigma}[n_i-\sigma(-1)^{x_i+y_i}m_i]c^{\dagger}_{i,\sigma}c_{i,\sigma} \ . \tag{2.4}$$

Such a wave function describes the usual antiferromagnetic phase if n_i,m_i are constants in space. On the other hand if n_i and m_i are allowed to vary in space and are parameters to be determined self-consistently[16,17] such a wave function can describe incommensurate antiferromagnetism with a linear polarization of the spin modulation. For small U, such a solution has been shown to be stabler than spiral like polarizations.[15] Although in an HF calculation it is possible to keep all the n_i and m_i as variational parameters, here this would mean too much computer time. Instead we will assume a functional form for n_i and m_i which appears to fit very closely the Hartree-Fock results. Since we want to describe an antiferromagnetic phase with domain walls, we choose the n_i and m_i to have the form

$$\begin{aligned} n_i&=1-\alpha/\cosh[(y_i-y_1)/\xi_\rho]-\alpha/\cosh[(y_i-y_2)/\xi_\rho] \ , \\ m_i&=m\tanh[(y_i-y_1)/\xi_\sigma]\tanh[(y_i-y_2)/\xi_\sigma] \ . \end{aligned} \tag{2.5}$$

This corresponds to two vertical domain walls at y_1 and y_2. α is fixed by $\sum_i n_i=N$ where N is the total number of particles. The variational parameters g,ξ_ρ,ξ_σ,m are fixed by minimizing the energy. Note that a pure Hartree-Fock solution means in our case keeping $g=1$. Diagonal domain walls can be treated in the same way by changing $y_i\rightarrow x_i-y_i$. For the commensurate phase n_i and m_i are taken constant in space; thus, $n_i=N/L$ where L is the number of lattice sites, and g and m_i are to be determined variationally.

III. SIMULATION AND RESULTS

A. Simulation

All the calculations were made on a rectangular lattice with walls parallel to the smaller side. We have taken periodic-antiperiodic conditions for vertical domain walls and antiperiodic-antiperiodic conditions for diagonal domain walls in order to avoid degeneracy of the Fermi surface at half-filling.[9,25] The calculations are made on systems between 4×20 and 8×28 depending on U and the doping in holes δ. To avoid important finite-size corrections when comparing the energy of a commensurate system with one with walls, we have to keep exactly the same boundary conditions. It is thus necessary to introduce two domain walls. Since the walls interact, the locations y_1 and y_2 of the walls have been chosen to have the largest separation between the walls on the torus. If this separation is high enough the interaction energy is expected to become negligible compared to the intrinsic energy of a single wall. This has been checked numerically for the systems studied.

The variational parameters were determined by using a method proposed by Umrigar *et al.* for the study of atomic systems.[26] A set of configurations is generated and then used to minimize the energy. This offers both the advantage of good computing time performances and that of using *correlated* measurements, which allows us to compare energies that differ by less than the statistical error bars on uncorrelated samples. We have used at least five independent simulations each of 4×10^5 Monte Carlo steps (MCS) to determine the minimum energy and parameters and the error bars. The order of magnitude of the time needed to get one minimum is half an hour on a Cray-2.

B. Results

The optimal parameters for $U=4,7,10$, for various system sizes, are indicated in Table I. Since the best energy is obtained when there is one hole per site in the wall,[16] we have only considered systems where the number of holes is $2L_y$, where L_y is the width of the system, in order to get exactly two walls of holes. As can be seen in Table II, the commensurate antiferromagnetic phase is unstable, close to half-filling, towards the formation of domain walls in qualitative agreement with the Hartree-Fock results.[16,17] Even for quite large doping ($\delta=0.1$) there is a significant energy gain due to the incommensurate instability.

The formation of domain walls also leads to a strong increase of the antiferromagnetic order parameter as can be seen in Fig. 1. We have shown the density and staggered magnetization for $U=4$ and a 4×20 system, with and without domain walls. At this doping ($\delta=0.1$), antiferromagnetism is nearly destroyed in the commensurate phase as can be seen on the staggered magnetization $m\simeq0.2$ ($m=0.58$ at half-filling). Between walls, con-

TABLE I. Optimal variational parameters and energies for various values of U and either commensurate system (C) or two vertical (V) or diagonal (D) domain walls [see Eqs. (2.4) and (2.5)]. Note that due to the Gutzwiller projection, the parameter m which would correspond to the staggered magnetization for a pure HF wave function is quite different from the measured magnetization (see Table II).

U	Size	N	δ	Type	m	ξ_ρ	ξ_σ	g
4	8×20	72	0.1	C	0.07(3)			0.57(2)
4	8×20	72	0.1	V	0.23(5)	5.6(6)	3.7(3)	0.59(2)
4	8×28	104	0.07	C	0.15(3)			0.58(2)
4	8×28	104	0.07	V	0.27(3)	5.9(3)	3.7(2)	0.60(2)
4	8×28	104	0.07	D	0.27(3)	5.9(3)	3.7(3)	0.60(2)
7	4×20	36	0.1	C	0.13(3)			0.41(2)
7	4×20	36	0.1	V	0.27(3)	3.1(2)	3.3(2)	0.43(2)
7	4×28	52	0.07	C	0.19(4)			0.42(4)
7	4×28	52	0.07	V	0.28(4)	3.2(4)	3.5(4)	0.45(2)
7	4×28	52	0.07	D	0.28(4)	3.4(4)	3.2(4)	0.45(2)
10	4×20	36	0.1	C	0.10(2)			0.29(1)
10	4×20	36	0.1	V	0.23(3)	2.9(2)	2.5(2)	0.35(2)
10	4×28	52	0.07	C	0.14(2)			0.32(2)
10	4×28	52	0.07	V	0.27(3)	3.2(2)	3.3(3)	0.37(2)
10	4×28	52	0.07	D	0.26(3)	3.4(3)	2.8(4)	0.35(2)

versely, the staggered magnetization in the incommensurate phase nearly keeps its half-filling value $m \simeq 0.5$. For $U=4$ the walls are quite wide, and for the system shown in Fig. 1 the modulation of the measured magnetization is nearly sinusoidal due to a strong interaction between the two walls. The properties of a single wall will have to be measured on a much larger system in order to avoid such an interaction between walls. Note that the incommensurate modulation of the spin density is matched with a significant charge density modulation at a double period.

If U increases, the walls become narrower as shown in Fig. 2. We have also shown on this figure the important *quantitative* differences with the HF solution. The Hartree-Fock results were obtained with the same method and keeping $g=1$. The walls are considerably enlarged compared to what is predicted by Hartree-Fock. The physical reason is that the condensation of holes in walls results from a competition between the loss of kinetic energy if the holes are localized in walls, and the gain in potential energy if the holes do not destroy the antiferromagnetic order. But there is an artefact of the Hartree-Fock wave function: In the HF wave function the antiferromagnetic order is essential in order to minimize the on-site repulsion. It is thus very difficult to destroy this order due to the increase of available double oc-

TABLE II. Physical parameters measured with the optimal wave functions given in Table I. For the incommensurate systems the staggered magnetization [for a commensurate system the staggered magnetization is defined as $\langle S \rangle = 2L^{-1} \sum_i \langle (-1)^i S_i \rangle$ and normalized to be 1 for a full antiferromagnetic order] is defined as the staggered magnetization at mid distance between the wall (well defined if the walls are sufficiently apart). $E_{\rm inc}$ is always smaller than $E_{\rm com}$; thus, the holes will always condense in walls. One can also notice that diagonal walls are stabler than vertical ones.

U	Size	δ	Type	$\langle S \rangle$	$-E$	$-E/(2N)$
4	8×20	0.1	C	0.19(3)	153.8(1)	1.068
4	8×20	0.1	V	0.53(3)	154.9(2)	1.075
4	8×28	0.07	C	0.38(3)	207.1(3)	0.996
4	8×28	0.07	V	0.59(3)	208.7(3)	1.004
4	8×28	0.07	D	0.56(3)	209.5(2)	1.006
7	4×20	0.1	C	0.54(3)	55.8(3)	0.775
7	4×20	0.1	V	0.77(3)	57.3(3)	0.795
7	4×28	0.07	C	0.61(4)	72.9(2)	0.701
7	4×28	0.07	V	0.81(4)	74.7(3)	0.718
7	4×28	0.07	D	0.79(4)	75.8(3)	0.728
10	4×20	0.1	C	0.60(2)	44.2(2)	0.613
10	4×20	0.1	V	0.88(3)	46.1(3)	0.640
10	4×28	0.07	C	0.72(2)	56.2(3)	0.540
10	4×28	0.07	V	0.90(3)	58.8(2)	0.565
10	4×28	0.07	D	0.88(3)	59.6(3)	0.573

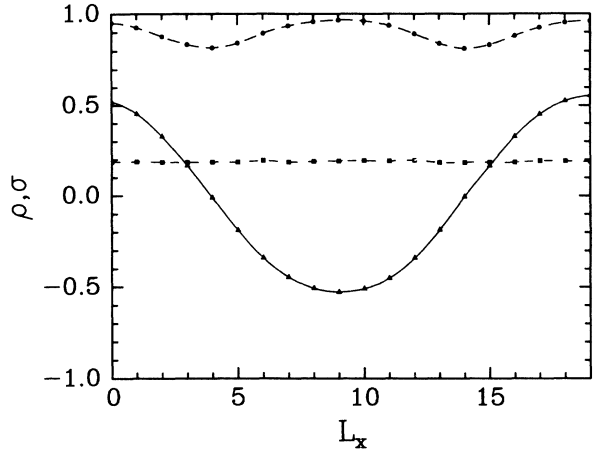

FIG. 1. Profiles of density (solid dots and dashed line) and staggered magnetization (triangles and solid line) for a 4×20 system at $U=4$. The staggered magnetization for a commensurate system is also indicated (squares). Whereas the commensurate system is nearly paramagnetic, the order parameter for the incommensurate one is nearly the same as at half-filling ($m=0.58$) due to the localization of holes. The creation of domain walls strongly stabilizes the antiferromagnetism. Note that, even for small values of U ($U=4$), the density fluctuation is not a small effect.

cupancy. The thinner the walls are, the better. In the Gutzwiller wave function the prefactor already takes care of the double occupancy, so that in order to minimize the kinetic energy, it becomes energetically favorable to enlarge the walls. The idea that due to the Gutzwiller projection the kinetic energy term plays a more important role seems to favor the idea at large U of a homogeneous incommensurate phase (e.g., spiral like) or of a spin liquid.

In order to measure the stability of the incommensurate phase we introduce the condensation energy of holes into walls at half-filling by[16]

$$E_c=\lim_{\delta\to 0}[E_{\rm inc}(\delta)-E_{\rm com}(\delta)]/\delta\ , \tag{3.1}$$

where $E_{\rm com,inc}(\delta)$ is the total energy of a commensurate (incommensurate) system. If $E_c<0$ the holes will always condense into walls. We have measured the condensation energy on the largest system (smallest δ) which was obtained in the simulation. Since quite large systems were already necessary to avoid the interactions between walls, especially at small U, no systematic extrapolation has been tried, due to computer time limitations. Note that especially for small U, where the walls are quite large, very large systems (typically 4×28) were necessary to avoid the finite-size effects due to the walls' repulsion. Such a repulsion leads to a reduction (in absolute value) of the condensation energy and thus destabilizes the incommensurate phase. Since the commensurate antiferromagnetic phase is little affected by the finite-size effects,[9] this will lead to an underestimate of the incommensurate instability energy.

The results for vertical and diagonal domain walls are shown in Fig. 3, together with the Hartree-Fock results of Ref. 16. The condensation energy is lowered in the presence of a Gutzwiller prefactor, as expected. Another *qualitative* important different between the HF and the full solution is that here, for all studied values of U, the diagonal walls are stabler as shown in Fig. 3, whereas for the HF solution a transition from vertical to diagonal

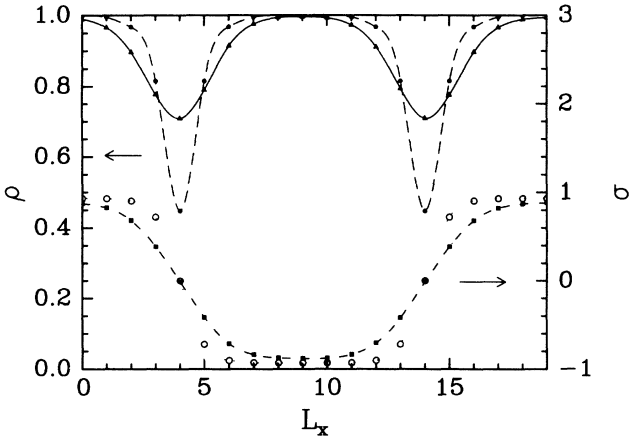

FIG. 2. Profiles of density (ρ) and staggered magnetization (σ) for two vertical domain walls (solid and dash-dotted lines), for a 4×20 system at $U=10$. In dashed and dotted lines is the pure Hartree-Fock solution (obtained with the same method by fixing $g=1$). The effect of the Gutzwiller prefactor is to considerably enlarge the walls. Since it weakens the Hubbard repulsion, the gain is kinetic energy associated with a larger wall supersedes the loss in magnetic energy.

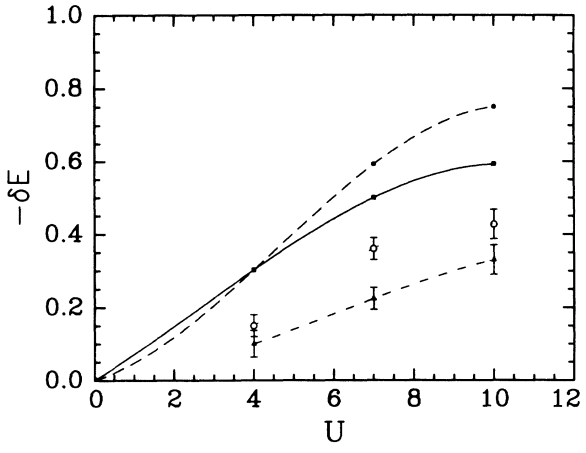

FIG. 3. Condensation energy of holes in walls as given by (3.1). A negative δE indicates that the homogeneous phase is unstable. Hartree-Fock results for vertical walls (squares) and diagonal walls (bullets), from Ref. 16. Monte Carlo results for vertical walls (triangles) and diagonal walls (circles). δE is still important but much lower than predicted by the HF calculations. As expected when $U\to0$ the effect of the Gutzwiller prefactor becomes less important. For the values of U considered here, diagonal domain walls are stabler. The lines are simply a guide to the eye.

TABLE III. Minimum energy and parameters for a 6×6 system with 4 holes and $U/t=10$. SU and CAF denote, respectively, the numerical results for a pure d-wave superconducting wave function and a commensurate antiferromagnetic one. SU+CAF is a wave function with both superconductivity and commensurate antiferromagnetism (Ref. 23) [obtained by keeping $\nu=0$ in (4.3)]. The results described under the subscript IAF and IAF+SU are those which are built on the crude incommensurate wave function (4.3). The energy of the domain wall phase (incommensurate) is estimated using the condensation energy given in Fig. 3. The fact that the antiferromagnetic phase is stabilized in both cases by the addition of superconductivity seems to suggest that incommensurate antiferromagnetism and superconductivity can coexist. Note that a pure superconducting phase is not a good variational wave function for the Hubbard model.

Type	Δ	μ	D	ν	g	$-E$	$-\delta E$
SU	0.19(2)	−0.35(4)			0.22(1)	20.29(3)	
CAF			0.45(4)		0.28(1)	20.57(3)	
CAF+SU	0.12(2)	−0.49(7)	0.45(4)		0.28(1)	20.63(5)	0.10(7)
IAF			0.25(3)	−0.5(1)	0.29(2)	20.77(8)	
IAF+SU	0.07(3)	−0.4(1)	0.25(3)	−0.5(1)	0.29(2)	20.86(6)	0.09(4)
DW						~ -22.25	

domain walls was found around $U=4$. Since we know, from small U analytical calculations,[15] that when $U\to0$ vertical domain walls are stabler we expect the transition between vertical and diagonal domain walls to happen at much smaller values of U than $U=4$. It is, however, numerically difficult to investigate such small values of U, since the system sizes needed to avoid interactions between walls demand too much computer time.

IV. INCOMMENSURATE ANTIFERROMAGNETISM AND SUPERCONDUCTIVITY

The gain in energy due to incommensurate effects is considerable compared to other instabilities, e.g., superconductivity. At doping 0.1, it has been found that the commensurate antiferromagnetic phase was unstable against superconductivity and that the energy gain was $\delta E\simeq0.0085$ per particle[23] for $U=10$. The incommensurate instability gives an energy gain of $\delta E=0.33$ per hole, thus $\delta E=0.033$ per particle for the same doping. Therefore the incommensurate antiferromagnetic phase has the lowest energy actually exhibited and the superconductive wave function no longer is a good variational candidate. In order to know if superconductivity can occur in the Hubbard model one has to wonder if the incommensurate antiferromagnetic phase presents the same instability as the commensurate one regarding superconductivity.

It is difficult to use the same method straightaway on an incommensurate phase due to the importance of finite-size effects in presence of an incommensurate wave vector. One can, however, get a glimpse of the answer by looking at the incommensurability effects in an oversimplified and naive way.

The nesting vector is kept to (π,π) and the energy is changed in the usual Hartree-Fock expression by $\varepsilon_k=\varepsilon_k-\nu$ where ν is a variational parameter. This allows the antiferromagnetic gap to be opened at the Fermi surface even away from half-filling, but since the nesting vector is kept to (π,π) we do not mix the proper states and such a solution is expected to be worse than a real incommensurate antiferromagnetic wave function. The one-particle antiferromagnetic wave functions ($d^\dagger$) are thus given by

$$\begin{aligned} d^\dagger_{k,\sigma}&=\alpha_k c^\dagger_{k,\sigma}+\sigma\beta_k c^\dagger_{k+K,\sigma}\ ,\\ d^\dagger_{k+K,\sigma}&=-\sigma\beta_k c^\dagger_{k,\sigma}+\alpha c^\dagger_{k+K,\sigma}\ , \end{aligned} \tag{4.1}$$

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

$$\begin{aligned} \alpha_k&=\{[1-(\varepsilon_k-\nu)/\sqrt{(\varepsilon_k-\nu)^2+D^2}]/2\}^{1/2}\ ,\\ \beta_k&=\{[1+(\varepsilon_k-\nu)/\sqrt{(\varepsilon_k-\nu)^2+D^2}]/2\}^{1/2}\ . \end{aligned} \tag{4.2}$$

These quasiparticle states are paired to make a superconducting d-wave wave function

$$\begin{aligned} |\psi_0\rangle&=\prod_k(u_k+v_k d^\dagger_{k,\uparrow}d^\dagger_{-k,\downarrow})|0\rangle\ ,\\ v_k/u_k&=\Delta_k/[\varepsilon_k-\mu+\sqrt{(\varepsilon_k-\mu)^2+|\Delta_k|^2}]\ ,\\ \Delta_k&=\Delta[\cos(k_x)-\cos(k_y)]\ . \end{aligned} \tag{4.3}$$

Such a function exhibits superconductivity and antiferromagnetism. Using this wave function we have computed the different energies for various phases in 6×6 systems at $U=10$ with four holes.

The results are shown in Table III. As was the case for commensurate antiferromagnetism, the addition of superconductivity to the "incommensurate" antiferromagnetic phase lowers the energy. One can therefore assume that the incommensurate antiferromagnetic phase will show the same instability towards superconductivity as the commensurate one. However, taking into account the proper incommensurate wave vector could change this result. Note that from a strict variational point of view the domain wall phase still has the lowest variational energy.

V. CONCLUSIONS

In this paper we have presented a variational Monte Carlo study of incommensurate antiferromagnetic phases in the Hubbard model. This incommensurate phase with

diagonal walls is the lowest phase ever exhibited for the Hubbard model at small doping and U between 4 and 10.[8,9,27]

We have found that away from half-filling the commensurate antiferromagnetic phase is unstable toward the formation of domain walls in qualitative agreement with Hartree-Fock calculations. The condensation energy of holes in walls, although considerably lowered by the Gutzwiller prefactor compared to the HF result, is still sufficiently big to ensure that the domain wall phase is the lowest variational phase.

Contrary to what was predicted by HF calculations, diagonal domain walls are found to be stabler for all the values of U studied (4–10). This contradicts also quantum Monte Carlo results[28,29] (see also Refs. 30 and 31). Although an incommensurate antiferromagnetic structure is observed, the wave vector of the modulation seems to be located along the Brillouin zone $(\pi,\pi-\delta)$, corresponding in our case to vertical domain walls, for values of U as high as $U=4$. So far the origin of the discrepancy is not clear. But, as pointed out, finite-size effects are quite important in the presence of an incommensurate wave vector, and this could be sufficient to lock the wave vector of the modulation along one of the directions of the lattice in the quantum Monte Carlo simulations. Note that in our simulations we have notable finite-size effects for systems as large as 8×20 (for $U=4$) and that for the systems considered in quantum Monte Carlo (usually 6×6 or 10×10) the surface is about 40% of the system. Of course, we cannot rule out the possibility of an artefact of the projected Hartree-Fock wave function in our results.

The condensation energy of holes in walls, although considerably lowered by the Gutzwiller prefactor compared to the HF result, is still sufficiently big to ensure that the domain wall phase is the lowest variational phase.

We have used a variational wave function allowing a coexistence between antiferromagnetism and superconductivity to show that the incommensurate antiferromagnetic phase, as well as the commensurate one, seems to be unstable towards superconductivity. Further studies are necessary to understand this effect clearly, in particular for domain walls, where carriers are not free. Nevertheless, the results of these variational calculations definitely point out a hierarchy in the order of magnitude of the different phenomena, the energy related to the magnetism being about 20 times larger than the energy of pairing in the range of U of interest.

Clearly the theory is much too crude to be related to high-T_c experiments. Although some incommensurate structure has been observed in La compounds,[32] in ytrium compounds the structure seems to remains always commensurate, at least when looking along the diagonal of the Brillouin zone.[33] This is in contradiction to what would be seen if diagonal domain walls occurred in the system. Of course, many effects can affect the idealized behavior predicted here for a real system. The domain walls are charged objects and are easily pinned by impurities, which can lead to a very different behavior. The effect of temperature on the walls is not clear. Moreover, if nonlocal interactions were taken into account, such as long-range Coulomb repulsion, it is not clear whether or not walls would remains stable, or would be replaced by a phase where the holes are homogeneously distributed.

The existence of other incommensurate phases[18,19] (e.g., spiral) can be studied by the same method, although such a study would be more delicate due to boundary condition problems. Particularly, the transition between a linear incommensurate phase and a spiral state would be interesting to study.

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