Quasihole excitation in a quantum antiferromagnet: variational Monte Carlo calculation

Massimo Boninsegni and Efstratios Manousakis
Department of Physics, Center for Materials Research and Technology and Supercomputer Computations Research Institute, Florida State University, Tallahassee, Florida 32306
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We study a single quasihole excitation in a quantum antiferromagnet using a variational wave function that includes spin-spin as well as spin-hole correlations. The wave function can be cast in the form of a complex correlation operator acting on a Marshall-type wave function for the spin background. Such a correlation operator, featuring momentum-dependent spin-hole correlations, is shown to correspond to a coherent local rotation of the spins, which can be also interpreted as a "spin-backflow" current, analogous to the Feynman-Cohen backflow current in helium liquids. The variational Monte Carlo method is used to calculate the hole excitation spectrum on a square lattice for the t-J model with this wave function. Comparing our results with available exact results on a 4×4 square lattice, we find qualitative and semiquantitative agreement. We provide results obtained on much larger lattices. We find that the quasihole energy band attains its minimum at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ while the hole mass is strongly anisotropic in different directions of k space. The quasihole excitation creates both a planar long-range distortion of the antiferromagnetic (AF) moment of the background $\delta m^{\dagger}(r \to \infty) \sim (\mathbf{k}\cdot\mathbf{r})/r^2$ and a ferromagnetic moment localized in the immediate neighborhood of the hole, pointing in the perpendicular direction. The magnitude of the ferromagnetic moment depends on the momentum of the excitation, and at the minimum of the hole band only the long-range AF planar distortion is present.

I. INTRODUCTION

The nearly half-filled, two-dimensional (2D) Hubbard model has been suggested[1] as an appropriate starting point for the study of superconducting copper oxides. In the strong-coupling limit and at half-filling this model reduces to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM). The effect of doping is the creation of mobile holes in the CuO_2 planes, and one considers the strong-coupling limit of the Hubbard model in the nearly half-filled case. In this limit one finds that the spin-$\frac{1}{2}$ AFHM is one piece of the Hamiltonian and the hole motion can be described by including hole-hopping terms such as the first term in the following model:

$$\hat{H}_{t\text{-}J} = -t \sum_{\langle ij\rangle\sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}) + J_z \sum_{\langle ij\rangle} (s^z_i s^z_j - \tfrac{1}{4}\hat{n}_i \hat{n}_j) + \tfrac{1}{2} J_{xy} \sum_{\langle ij\rangle} (s^+_i s^-_j + s^-_i s^+_j), \quad (1)$$

where $J_z = J_{xy} = J$ and $c_{i,\sigma}$ is a hole creation operator and t the electron hopping matrix element. The strong on-site Coulomb repulsion is taken into account by restricting the action of the Hamiltonian operator in a subspace of the Hilbert space having states with singly occupied sites. The Hamiltonian (1), now known as the "t-J model," has received significant attention by various authors because it can be derived from more realistic models which account for the detailed chemical structure of the copper oxide planes.[2] It is worth mentioning that in the derivation of (1) from the Hubbard model one also encounters a three-site interaction term which permits the hole to hop to a next-nearest-neighbor site: such a term is neglected in the present paper; here, we only study the t-J model and we postpone studies of its extensions until the future. The t-J model, in the undoped case, reduces to the spin-$\frac{1}{2}$ AFHM which has proven quite successful in explaining certain magnetic properties of the copper-oxide planes of the undoped materials.[3] Recent analysis of the NMR measurements suggests[4] that the copper oxide materials can be described by a one-component antiferromagnetically correlated Fermi liquid, which is consistent with starting with Hamiltonians such as (1).

Several attempts have been made to study the 2D t-J model in the presence of one or two holes, by using both analytical and numerical techniques. The problem of pairing of two holes has been studied on a small-size cluster,[5] by exact diagonalization; it was found that a range of t/J exists for which pairing, induced by antiferromagnetic (AF) spin correlations, might be possible. Much effort has been devoted in order to achieve a thorough understanding of the single-hole and related problems.[5-10] Some information has been produced[5-9] about certain features of the single-hole dispersion relation and the spectral function, where a quasiparticle peak has been found.

The variational approach, which overcomes the limitations of dealing with small-size lattices, may provide both an analytical understanding of the nature of the correlations introduced by the hole and a deeper insight on the possibility of hole pairing; in addition, a good variational wave function can be used further as a guiding function in a Green's-function Monte Carlo simulation, to obtain a more accurate estimate of the various expectation values. In this work we carry out a variational Monte Carlo (VMC) calculation for the single-hole energy band. A formal analogy is used between this problem and the one of the motion of an impurity in a Bose fluid, with two-body interactions among the bosons and between the impurity and the bosons. In such a context, a variational wave function can be written down with all possible two-body correlations, including a backflow term analogous to the one introduced by Feynman and Cohen[11] to study the problem of a ^{3}He impurity in liquid ^{4}He. Translated into spin language, the trial wave function can be obtained by acting on a Marshall-type antiferromagnetically correlated state with a complex spin-hole correlation operator. The part of this operator deriving from the backflow term generates a "distortion field,"[8] which originates at the position of the hole and decays as $(\mathbf{k}\cdot\mathbf{r})/r^2$ far away from it. Upon comparing our variational results with exact ones for the 4×4 lattice, we find that certain broad features of the hole excitation spectrum are reproduced, and the variational estimate of the hole binding energy is accurate for $t/J \leq 0.5$.

Several of our conclusions agree with those of other works obtained with different methods.[6,8,9] We find that the quasihole excitation creates a planar long-range distortion of the antiferromagnetic (AF) moment of the background $\delta m^{\dagger}(r\rightarrow\infty)\sim(\mathbf{k}\cdot\mathbf{r})/r^2$ and a ferromagnetic moment well localized in the immediate neighborhood of the hole, both depending on the momentum of the excitation. The plane of the distortion in the spin space is parallel to the direction of the staggered magnetization of the square lattice, while the ferromagnetic moment is perpendicular. At the minimum of the hole band, which occurs at $\mathbf{k}=(\pi/2,\pi/2)$, there is only the long-range planar AF distortion. The hole band is strongly anisotropic in different directions of $\mathbf{k}$ space; we find that the effective mass of the hole is much smaller in the direction $(0,0)$ to (π,π) compared with the hole mass in the direction $(0,\pi)$ to $(\pi,0)$.

In Sec. II, we formulate the problem in our convenient language and we discuss the formal analogy of this problem with the problem of an impurity moving in a Bose fluid. In Sec. III, we study certain analytical results obtained by including only hole-spin correlations. In Sec. IV, we provide results obtained with the full wave function and the VMC technique. Finally, we summarize our results and discuss how to improve the variational calculation for large values of t/J.

II. FORMULATION

First, we shall outline a representation where one finds an interesting analogy with the physics of Bose fluids. The analogy of hard-core Bose fluids with spin systems was pointed out by Matsubara and Matsuda,[12] who have shown that liquid ^{4}He, when approximated as a quantum lattice-gas model is equivalent to the ferromagnetic spin-$\frac{1}{2}$ Heisenberg model. Here, using a unitary transformation of the basis, we make use of this analogy for quantum antiferromagnets.

Let us first consider the case of no hole, i.e., the spin-$\frac{1}{2}$ AFHM. The eigenstates of this model can be expressed as

$$|\Psi\rangle=\sum_{\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u}}\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u})\times(-1)^{L(c)}|\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u}\rangle, \tag{2}$$

where the configuration $|c\rangle$ is labeled by the location of the up spins,

$$|\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u}\rangle=s^+_{\mathbf{r}_1}s^+_{\mathbf{r}_2}\cdots s^+_{\mathbf{r}_{N_u}}|F\rangle; \tag{3}$$

$|F\rangle$ is the ferromagnetic state with all spins "facing" down and N_u is the number of up spins. The amplitude $\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u})$ is symmetric under exchange of any two coordinates $\mathbf{r}_i,\mathbf{r}_j$, as it can be easily inferred from the commutation rule $[s^+_{\mathbf{r}_i},s^+_{\mathbf{r}_j}]=0$. Moreover, $\Psi(\ldots,\mathbf{r}_i,\ldots,\mathbf{r}_j,\ldots)=0$, if $\mathbf{r}_i=\mathbf{r}_j$ for any pair i,j as a result of $(s^+_{\mathbf{r}})^2|F\rangle=0$. Spins pointing up can therefore be regarded as particles, namely "hard-core" bosons. The phase $(-1)^{L(c)}$ is separated from the amplitude ψ in order to have a non-negative ψ for any ground-state configuration.[13] $L(c)$ is the number of up spins in one sublattice. In this representation, it is straightforward to show that the eigenvalue problem, $H|\Psi\rangle=E|\Psi\rangle$, reduces to a difference equation, for the amplitude $\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u})$, identical to the many-particle Schrödinger equation on a square lattice:

$$-\tfrac{1}{4}J\sum_{i=1}^{N_u}\tilde{\nabla}_i^2\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u})+\sum_{1\leq i<j\leq N_u}V_{ij}\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u})=\epsilon\psi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_{N_u}), \tag{4}$$

where

$$\tilde{\nabla}_i^2\psi(\mathbf{r}_1,\ldots,\mathbf{r}_i,\ldots,\mathbf{r}_{N_u})\equiv\sum_{\delta}[\psi(\mathbf{r}_1,\ldots,\mathbf{r}_i+\delta,\ldots,\mathbf{r}_{N_u})-\psi(\mathbf{r}_1,\ldots,\mathbf{r}_i,\ldots,\mathbf{r}_{N_u})]$$

is the Laplacian operator on the discrete square lattice and δ is a vector of unit length that connects the site located at $\mathbf{r}_i$ with each of the four NN. Here, $\epsilon = E - \frac{1}{2}NJ + 3N_uJ$ with E being the ground-state energy eigenvalue of the Heisenberg model. The "particles" correspond to up spins and the wave function ψ is symmetric with respect to "particle" permutations; hence, this is a quantum lattice gas of bosons with "mass" $m = 2/J$ (we use units in which a=1 and $\hbar$=1) that interact via a pair potential V_{ij} having an infinite on-site repulsion, $V_{ij} = J$ if i, j are NN, otherwise V_{ij}=0.

It is known that the ground state of a Bose liquid has a broken symmetry (condensate) which in the magnetic language corresponds to AF long-range order (LRO). A simple and nontrivial ground-state wave function which takes into account short-range correlations due to the existence of the hard-core [$V(\mathbf{r} = 0) = \infty$] is the Jastrow wave function

$$\psi_0(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}) = \prod_{1 \le i < j \le N_u} f_{ij}, \tag{5}$$

where f_{ij}=0 for $i = j$ and $f_{ij} > 0$ for $i \neq j$. It is customary to write

$$f_{ij} = e^{-u_{ij}/2}, \tag{6}$$

where $u_{ij} = u(\mathbf{r}_i - \mathbf{r}_j)$. Substituting the number operator counting the "particles" (up spins) by $s_i^z + \frac{1}{2}$ we can go back to the spin variables. We obtain the Marshall[13] state

$$|\psi_0\rangle = \sum_c (-1)^{L(c)} \exp\left(-\frac{1}{2}\sum_{i<j} u_{ij} s_i^z s_j^z\right) |c\rangle, \tag{7}$$

where the sum now runs over all lattice sites. If we extend the sum not only over those configurations with N_u up spins but over all possible configurations, then the state (7) takes the following form

$$|\psi_0\rangle = \exp\left(-\frac{1}{2}\sum_{i<j} u_{ij} \hat{s}_i^z \hat{s}_j^z\right) |x\rangle . \tag{8}$$

$|x\rangle$ is the Néel state with antiferromagnetic order in the x direction

$$|x\rangle = \prod_{i\epsilon+} |+\hat{x}\rangle_i \prod_{i\epsilon-} |-\hat{x}\rangle_i, \tag{9}$$

where

$$|\pm\hat{x}\rangle_i \equiv \frac{1}{\sqrt{2}}(|+\rangle_i \pm |-\rangle_i), \tag{10}$$

i.e., they are eigenstates of $\hat{s}_i^x$. The variational state (8) features a reduced antiferromagnetic order. A straightforward calculation yields $\langle \hat{s}_i^y \rangle = \langle \hat{s}_i^z \rangle = 0$ and $\langle \hat{s}_i^x \rangle = \pm m^\dagger$, where $m^\dagger$ is $\le \frac{1}{2}$ and depends on the function u. If we restrict the sum in (7) over configurations with zero z component of the net spin (i.e., $N_u = N/2$), we find that $\langle \hat{s}_i^x \rangle = \langle \hat{s}_i^y \rangle = \langle \hat{s}_i^z \rangle = 0$; however, each of the two correlation functions $\langle \hat{s}_i^x \hat{s}_j^x \rangle$ and $\langle \hat{s}_i^y \hat{s}_j^y \rangle$ at large distances approaches the value $\frac{1}{2}(-1)^{i+j} m^{\dagger 2}$ while $< \hat{s}_i^z \hat{s}_j^z >$ approaches zero. Therefore, even though there is no well-defined direction for the staggered magnetization, there is still long-range antiferromagnetic order in the x-y plane.

The elementary excitations in the Bose system are density fluctuations (phonons in the long-wavelength limit) which in the magnetic system correspond to spin waves and the Bose condensate to antiferromagnetic long-range order. Chester and Reatto[14] have shown that the zero-point motion of the long-wavelength modes of the Bose system (zero sound) gives rise to a long-range tail in the Jastrow wave function. For a square lattice spin-$\frac{1}{2}$ quantum antiferromagnet we obtain $u(r \to \infty) = c/J\pi r$, c being the spin-wave velocity. The optimization of the Jastrow wave function has been numerically carried out by Liu and Manousakis,[15] who used the values of u_{ij} for the first few neighbors as variational parameters and determined the long-range part by satisfying sum rules.

Let us next consider the Hilbert space of all possible states of the system, with N_u up spins and one hole. A basis vector can be written as $|\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}\rangle$, with $\mathbf{R} \neq \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}$, where $\mathbf{R}$ is the position of the hole and $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}$ are the positions of the N_u up spins. More precisely,

$$|\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}\rangle = s^+_{\mathbf{r}_1} s^+_{\mathbf{r}_2} \cdots s^+_{\mathbf{r}_{N_u}} |\mathbf{R}, F\rangle, \tag{11}$$

where the reference state $|\mathbf{R}, F\rangle$ is the "down" ferromagnetic state with the hole at $\mathbf{R}$. The most general eigenstate of (1) having N_u up spins can be written as

$$|\Psi\rangle = \sum_{\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}} (-1)^{L(c)} \Psi(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}) \times |\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}\rangle. \tag{12}$$

The phase factor $(-1)^{L(c)}$ is defined as in the no-hole case. In this representation we can write down the eigenvalue equation $\hat{H}\Psi = \epsilon\Psi$ for the function $\Psi(\mathbf{R}, \mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u})$, with

$$\hat{H} = -t\tilde{\nabla}^2_{\mathbf{R}} - \tfrac{1}{4}J\sum_{i=1}^{N_u} \tilde{\nabla}^2_{\mathbf{r}_i} + \sum_{1 \le i < j \le N_u} V(\mathbf{r}_i - \mathbf{r}_j) + \sum_{i=1}^{N_u} U(\mathbf{r}_i - \mathbf{R}) - t\sum_{\{\mathbf{r}_i\}} \hat{P}(\mathbf{r}_i, \mathbf{R})\delta_{\langle \mathbf{r}_i \mathbf{R}\rangle}, \tag{13}$$

where $\epsilon = E + 3JN_u - 4t$, E being the ground-state energy eigenvalue of (1) and $\hat{P}(\mathbf{r}, \mathbf{r}')$ being a two-"particle" exchange operator, whereas $\delta_{\langle \mathbf{r}_i \mathbf{R}\rangle}$ is equal to one for nearest neighbors and zero otherwise. The first two terms of the Hamiltonian are kinetic-energy terms, one for the hole, whose "mass" is $m_h = 1/2t$, the other for the bosons introduced above, whose "mass" is $m_b = 2/J$. V_{ij} has been defined before and U_i is the interaction potential between a hole and a boson, featuring an infinite on-site repulsion and it is equal to $J/2$ for nearest-neighbor sites and zero otherwise. Apart from the fifth term, that we shall examine below, (13) is the lattice version of the Hamiltonian

for an interacting boson gas with an impurity, in this case the hole. This is analogous, for instance, to the problem of a ^{3}He atom in liquid ^{4}He. The fifth term of the Hamiltonian (13) represents the exchange taking place between the impurity and a nearest-neighboring boson. This exchange term expresses the possibility for the impurity and a nearest-neighboring boson to interchange without involvement of a third or more particles. Because of that, unlike the case of ^{3}He atom inside a liquid ^{4}He background, hole motion inside the boson "fluid" may not necessarily cause a rearrangement of the fluid itself in the vicinity of the moving hole (backflow). A variational ansatz for the wave function describing the motion of an impurity inside a Bose fluid can be obtained as a generalization of the state (5), allowing for two-body boson-impurity correlations:

$$\Psi_T(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{R}} \exp\left(-\sum_j [i\phi_{\mathbf{k}}(\mathbf{r}_j - \mathbf{R}) + \lambda_{\mathbf{k}}(\mathbf{r}_j - \mathbf{R})]\right) \times \exp\left(-\frac{1}{2}\sum_{i<j} u(\mathbf{r}_i - \mathbf{r}_j)\right), \tag{14}$$

where u accounts for the hard-core repulsion between pairs of bosons, as in the no-impurity case, and the term $\lambda_{\mathbf{k}} + i\phi_{\mathbf{k}}$ describes two-body boson-impurity correlations. The imaginary part can describe "backflow" effects, as in the Feynman-Cohen treatment of the problem of a ^{3}He impurity in liquid ^{4}He;[11] in that context, $\phi_{\mathbf{k}}$ refers to the collective motion of ^{4}He atoms which move out of the way, in order to make room for a ^{3}He impurity to pass through, filling the empty space it leaves behind. Due to this effect, the ^{3}He particle embedded in liquid ^{4}He has an effective mass which is larger than its true mass. Mathematically, the form of the function $\phi_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R})$ can be determined by imposing on the wave function (14) the condition that it give a divergence-free current when plugged into Eq. (13). Upon paralleling the calculation outlined in Ref. 10, we obtain the large-distance behavior of $\phi_{\mathbf{k}}(\mathbf{r})$, as $\propto (\mathbf{k}\cdot\mathbf{r})/r^2$, in the low-density limit, that is, when the number of bosons (spins pointing up) is small compared to the number of empty sites (spins pointing down), or, in other words, when the system has a large negative z component of the total spin (see the Appendix). We can now go back to spin variables, by using the identity $\hat{n}(\mathbf{r}) = \hat{s}^z_{\mathbf{r}} + \frac{1}{2}$, where $\hat{n}(\mathbf{r})$ is the boson number operator at lattice site $\mathbf{r}$ (1 if there is an up spin, zero otherwise); $\Psi_T(\mathbf{k})$, within a multiplicative constant, is given by

$$|\Psi_T(\mathbf{k})\rangle = \sum_{\mathbf{R},c}(-1)^{L(c)} e^{-i\mathbf{k}\cdot\mathbf{R}} \exp\left(-\sum_i [\lambda_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R}) + i\phi_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R})] s^z_{\mathbf{r}_i}\right) \exp\left(-\frac{1}{2}\sum_{\mathbf{r}_i,\mathbf{r}_j} u(\mathbf{r}_i - \mathbf{r}_j) s^z_{\mathbf{r}_i} s^z_{\mathbf{r}_j}\right) |\mathbf{R}, c\rangle, \tag{15}$$

where the sum over i and j now runs over all lattice sites. As in the no-hole case, if we allow the sum in the state (15) to run over all possible configurations rather than just those with a fixed number of bosons (i.e., with a fixed value of the net z component of the spin), then we can express the state as

$$|\Psi_T(\mathbf{k})\rangle = \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} \exp\left(-\sum_i [\lambda_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R}) + i\phi_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R})] \hat{s}^z_{\mathbf{r}_i}\right) \exp\left(-\frac{1}{2}\sum_{\mathbf{r}_i,\mathbf{r}_j} u(\mathbf{r}_i - \mathbf{r}_j) \hat{s}^z_{\mathbf{r}_i} \hat{s}^z_{\mathbf{r}_j}\right) |\mathbf{R}, x\rangle, \tag{16}$$

where

$$|\mathbf{R}, x\rangle = \prod_{i\epsilon+} |+\hat{x}\rangle_i \prod_{i\epsilon-} |-\hat{x}\rangle_i |\mathbf{R}\rangle. \tag{17}$$

The states $|\pm x\rangle_i$ have been defined before, and $|\mathbf{R}\rangle$ refers to the vacuum at the site $\mathbf{R}$; the two products run over all lattice sites except $\mathbf{R}$. As in the no-hole case, the basic difference between the states (15) and (16) is that the latter features a well-defined direction of the staggered magnetization.

The wave function (15) ignores physical processes arising from multiple hole hops. In our formalism, such processes appear as hole-spin exchanges and can be included by appropriate modification of the correlation operator acting on the Marshall state with the mobile hole. Such processes are known as "strings" of overturned spins which follow the path of the hole in the Brinkman-Rice approach; such an approach, however, neglects the role of quantum spin fluctuations. Thus, we expect our wave function to give unsatisfactory results for the hole energy at large t/J, where hole-spin exchange becomes important. The wave function can be improved by modifying the correlation operator; this is discussed to some degree also in Sec. IV.

III. IGNORING BACKGROUND CORRELATIONS

If one sets u=0 in the state (16), the variational problem can be solved almost analytically, and this provides further insight. We shall see that the $\lambda_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ correlations, which can also be interpreted as local spin rotations, are necessary in order to relieve the local spin environment from the incoherence created by the hole motion. Let us consider the state (16) and set u=0:

$$|\Psi_0(\mathbf{k})\rangle = \frac{1}{\sqrt{M}} \sum_{\mathbf{R}\in\pm} e^{-i\mathbf{k}\cdot\mathbf{R}} \prod_{\mathbf{r}_i\ (\neq\mathbf{R})} |\chi(\mathbf{r}_i)\rangle_\pm, \tag{18}$$

where

$$|\chi(\mathbf{r}_i)\rangle_\pm = |\lambda_i, \phi_i\rangle_\pm \equiv \exp[-(\lambda_i + i\phi_i)\hat{s}^z_{\mathbf{r}_i}]|\pm\hat{x}\rangle_i, \tag{19}$$

and $|\pm\hat{x}\rangle_i$ are eigenstates of $\hat{s}^x_i$ given by Eqs. (9) and (10) and the functions λ_i and ϕ_i are abbreviations for $\lambda_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R})$ and $\phi_{\mathbf{k}}(\mathbf{r}_i - \mathbf{R})$, respectively. We have suppressed the index $\mathbf{k}$ for simplicity. The state $\chi(\mathbf{r}_i)$ after normalization can be expressed as

$$|\chi(\mathbf{r}_i)\rangle_\pm = |\theta^\pm_i, \phi_i\rangle \equiv \exp(-\tfrac{1}{2}i\theta^\pm_i \hat{n}_i\cdot\boldsymbol{\sigma}) \times \exp(-i\phi_i\hat{s}^z_{\mathbf{r}_i})|\pm\hat{x}\rangle_i, \tag{20}$$

where $\boldsymbol{\sigma}$ are the Pauli matrices and $\hat{n}_i = (-\sin\phi_i, \cos\phi_i, 0)$. This state can be interpreted as a local rotation of the spin vector which points in the $\pm\hat{x}$ direction by an angle ϕ_i around the positive z axis and subsequently by an angle θ_i around the vector $\hat{n}_i$ out of the x-y plane towards the positive direction. The angle $\theta^\pm_i$ is related to the parameter λ_i as follows:

$$\theta^+_i = 2\tan^{-1}\left(\tanh\left(\frac{\lambda_i}{2}\right)\right) \tag{21}$$

$$\theta^-_i = -2\tan^{-1}\left(\coth\left(\frac{\lambda_i}{2}\right)\right). \tag{22}$$

When λ_i and ϕ_i are nearest-neighbor functions the problem can be solved analytically. The wave function (19) can be parametrized as follows:

$$|\chi(\mathbf{r}_i)\rangle_\pm = |\rho_i, \phi_i\rangle \equiv \rho_i|\pm\hat{x}\rangle_i + \sqrt{1-\rho_i^2}e^{i\omega_i}|\mp\hat{x}\rangle_i, \tag{23}$$

The states (23) and (19) apart from a multiplicative constant can be made identical provided that the functions λ_i, ϕ_i ρ_i, ω_i are related in the following way:

$$\phi_i = -\tan^{-1}\left(\frac{2\rho_i\sqrt{1-\rho_i^2}}{2\rho_i^2 - 1}\sin\omega_i\right), \tag{24}$$

$$\lambda_i = -\frac{1}{2}\ln\left(\frac{1 + 2\rho_i\sqrt{1-\rho_i^2}\cos\omega_i}{1 - 2\rho_i\sqrt{1-\rho_i^2}\cos\omega_i}\right). \tag{25}$$

In this form, the expectation value of the potential energy (J term) is given by

$$\langle V\rangle = -\tfrac{3}{2}J\sum_i \rho_i^2 + \text{const}\ , \tag{26}$$

which is independent of ω_i. Therefore the relative phase ω_i can be found by minimizing the hopping energy only. Now, when a hole, in an antiferromagnetically aligned spin lattice, moves to a nearest-neighboring site, it creates a state which is orthogonal to the original state. In order to minimize the hopping energy, one has to allow for maximum overlap between the initial and the final state, and this can be achieved if the spins around the hole are in a nonpure spin state. It is straighforward to see that the overlap between the state obtained by acting with $H_{t\text{-}J}$ on (18) and the state (18) itself attains its maximum magnitude by choosing

$$\omega_\delta = -\mathbf{k}\cdot\boldsymbol{\delta}\ , \tag{27}$$

where phase coherence is achieved. Choosing $\rho_\delta = \rho$ the expectation value of the Hamiltonian (1) is obtained as

$$\langle H_{t\text{-}J}\rangle = E(\rho) = -8t\rho^7\sqrt{1-\rho^2} - 6J\rho^2 + \text{const} \tag{28}$$

and the optimal value of the parameter ρ lies in the interval $\rho_c \le \rho \le 1$ and depends monotonically on t/J with $\rho(t/J = 0) = 1$ and $\rho(t/J \to \infty) \equiv \rho_c = \sqrt{7/8}$. We further obtain $E(t/J \to \infty) = -1.772t$ and $\tan\phi_\delta = \sqrt{7}/3\sin(\mathbf{k}\cdot\boldsymbol{\delta})$, i.e., the maximum value of ϕ is somewhat less that 45°. Since ρ is close to 1 for small t/J the parameters (24), (25) can be approximated by $\phi_\delta = A_0\sin(\mathbf{k}\cdot\boldsymbol{\delta})$ and $\lambda_\delta = A_0\cos(\mathbf{k}\cdot\boldsymbol{\delta})$ where $A_0 = 2\rho\sqrt{1-\rho^2}$.

One can also calculate the expectation values of the NN spin operators

$$\langle s^x_\delta\rangle_\pm = \pm\tfrac{1}{2}(2\rho^2 - 1), \tag{29}$$

$$\langle s^y_\delta\rangle_\pm = \pm\rho\sqrt{1-\rho^2}\sin(\mathbf{k}\cdot\boldsymbol{\delta}), \tag{30}$$

$$\langle s^z_\delta\rangle_\pm = \rho\sqrt{1-\rho^2}\cos(\mathbf{k}\cdot\boldsymbol{\delta}). \tag{31}$$

For large distances, the problem can be solved by assuming that $\lambda(\mathbf{r}\to\infty)\to 0$ and $\phi(\mathbf{r}\to\infty)\to 0$ and expanding the energy expectation value and keeping up to terms quadratic in λ, ϕ and $\nabla\lambda$ and $\nabla\phi$. Minimizing the resulting expression we find that the function λ should decay within a few lattice spacings from the hole, whereas the function ϕ may have significant large-distance behavior. Namely, the planar distortion survives at long distances from the hole, while the magnetization along the direction orthogonal to the plane is confined within the neighborhood of the hole. The minimization with respect to ϕ gives $\nabla^2\phi = 0$ as $r\to\infty$. ϕ can be therefore written as a multipole expansion in which the lth multipole coefficient is proportional to $1/r^l$. If we impose the condition that the large-distance symmetry of the wave function be the same as at short distances then only odd multipoles contribute. Upon retaining the dominant $l = 1$ (dipole) contribution, we can write $\phi(\mathbf{r}) = A(k)(\hat{\mathbf{k}}\cdot\hat{\mathbf{r}})/r$.

Summarizing the results of this section, the operator $\exp[-i\phi_{\mathbf{k}}(\mathbf{r})\hat{s}^z_{\mathbf{r}}]$ rotates the spin, which lies on the x-y plane in the uncorrelated state, by an angle $\phi_{\mathbf{k}}$ which behaves, at large distances, as $(\mathbf{k}\cdot\hat{\mathbf{r}})/r$, whereas $\exp[-\lambda_{\mathbf{k}}(\mathbf{r})\hat{s}^z_{\mathbf{r}}]$ generates the magnetization along the z direction. This operation maximizes the overlap between states where the hole is displaced by one lattice site by the hopping term of (1).

IV. VARIATIONAL MONTE CARLO CALCULATION

The state (15) with $u \neq 0$ is the variational state that has been used in our variational Monte Carlo (MC) calculation. We have obtained results with and *without*

TABLE I. Comparison between VMC and exact diagonalization results for the 4×4 lattice case, at $\mathbf{k} = (\pi/2, \pi/2)$. The wave function has the restriction on the total $S^z = \pm\frac{1}{2}$. The results are given in units of J. The T column reports the VMC expectation values of the hopping energy.

t/J	E	E (exact)	T	ΔE	ΔE (exact)
0.0	−16.661(02)	−16.880	0	2.380(04)	2.349
0.20	−16.768(02)	−16.981	−0.177	2.273(04)	2.248
0.50	−17.162(02)	−17.465	−0.731(01)	1.879(04)	1.764
1.00	−18.019(03)	−18.573	−1.837(02)	1.022(05)	0.656
2.50	−20.869(06)	−22.534	−4.852(06)	-1.828(08)	-3.305
5.00	−25.770(11)	−29.719	−9.848(11)	-6.729(13)	-10.49

restricting the sum in (15) over configurations with fixed total S^z. We found the same optimal values of the variational parameters in the two cases. Restricting the sum over configurations with $S^z = +m$ (or $-m$) produces a finite-size correction to the hole binding energies at different $\mathbf{k}$, that has the same sign as S^z and scales as $1/N$. One can eliminate such a correction by allowing for configurations with $S^z = \pm\, m$ in the simulation. If this is done, the optimal variational parameters are insensitive to the lattice size. We performed VMC calculations on several lattices with periodic boundary conditions. The Metropolis algorithm with single-spin updates was used. The function u was chosen to be the same as that determined by Liu and Manousakis[15]. We have found that taking u to be a function of the distance between i and j, i.e., $u(\mathbf{r}_i - \mathbf{r}_j) = u(r)$, $r = |\mathbf{r}_i - \mathbf{r}_j|$, and

$$u(1) = \alpha, \tag{32}$$

$$u(\sqrt{2}) = \beta, \tag{33}$$

$$u(r > \sqrt{2}) = \frac{\gamma}{r}, \tag{34}$$

gives energies for the no-hole and one-hole state very close to those obtained with the u determined in Ref. 15. This is a simpler trial function and it has the important features, namely the long-range $1/r$ tail (consistent with spin-wave theory). We have numerically found the following simple parametrization of the functions $\phi_{\mathbf{k}}(\mathbf{r})$ and $\lambda_{\mathbf{k}}(\mathbf{r})$:

$$\phi_{\mathbf{k}}(\delta) = A_o \sin(\mathbf{k}\cdot\delta)\ , \tag{35}$$

$$\lambda_{\mathbf{k}}(\delta) = B_o \cos(\mathbf{k}\cdot\delta), \tag{36}$$

for the short-range part, which is consistent with the solution for $u = 0$ and small t/J. In fact the symmetries of ϕ and λ, namely $\phi_{\mathbf{k}}(-\delta) = -\phi_{\mathbf{k}}(\delta)$ and $\lambda_{\mathbf{k}}(-\delta) = \lambda_{\mathbf{k}}(\delta)$, require only four parameters for each value of $\mathbf{k}$. We have found that allowing for all four parameters to vary independently for each value of $\mathbf{k}$, the best energies, within our MC error bars, cannot be better than those obtained with the parametrization (35) and (36). We further found that the optimal values for A_o are such that $A_o \simeq -B_o$, and by allowing for their values to be different we can only gain small amounts of energy, lying within the error bars of the values summarized in the Tables I–VI. In order to resolve the difference one needs higher precision which requires computational resources much beyond the ones available for this project, and for simplicity we took $A_o = -B_o$, therefore keeping only one variational parameter. For distances larger than one lattice spacing away from the hole we took

$$\phi_{\mathbf{k}}(\mathbf{r}) = A_k \frac{\mathbf{k}\cdot\mathbf{r}}{r^2}, \tag{37}$$

i.e., the expression for the dipolar backflow discussed in Secs. II and III and derived in the Appendix. We found λ not to be significantly different from zero beyond nearest neighbors.

In Fig. 1 we compare our results to those obtained by numerical exact diagonalization for the hole binding energy on a 4×4 lattice, from Ref. 6, for several values of t/J and at $\mathbf{k} = (\pi/2, \pi/2)$. In the figure we give ΔE in units of t, which is the dominant scale at large t/J, while in the inset we give ΔE in units of J, which is the dominant energy scale at small t/J. For $t = 0$, i.e., the static hole case, we find $\phi = \lambda = 0$. The difference between the

TABLE II. VMC results for the 8×8 lattice , with the restriction on $S^z = \pm\frac{1}{2}$.

t/J	E	T	ΔE
0.0	−72.375(06)	0	2.237(09)
0.20	−72.492(06)	−0.180(01)	2.120(09)
0.50	−72.911(07)	−0.738(02)	1.701(10)
1.00	−73.815(08)	−1.852(05)	0.797(11)
2.50	−76.753(14)	−4.920(13)	-2.141(17)
5.00	−81.837(25)	−10.072(25)	-7.225(28)

TABLE III. VMC results for the 16×16 lattice, with the restriction on $S^z = \pm\frac{1}{2}$.

t/J	E	T	ΔE
0.0	−295.807(21)	0	2.187(31)
0.20	−295.923(21)	−0.179(01)	2.071(31)
0.50	−296.332(15)	−0.741(07)	1.662(25)
1.00	−297.252(22)	−1.848(09)	0.742(32)
2.50	−300.203(30)	−4.920(23)	−2.240(40)
5.00	−305.320(49)	−10.097(45)	−7.326(59)

TABLE IV. Comparison between VMC and exact diagonalization results for the 4×4 lattice case, at $\mathbf{k} = (\pi/2, \pi/2)$, obtained without restriction on S^z.

t/J	E	E (exact)	T	ΔE
0.0	−16.547(02)	−16.880	0.000	2.247(03)
0.20	−16.652(02)	−16.980	−0.175	2.142(03)
0.50	−17.044(02)	−17.465	−0.725(01)	1.750(03)
1.00	−17.892(03)	−18.573	−1.822(02)	0.902(04)
2.50	−20.732(06)	−22.533	−4.811(05)	−1.938(07)
5.00	−25.572(11)	−29.718	−9.760(11)	−6.778(12)

exact ground-state energy and the variational energy at small values of t/J can be attributed to an incomplete description of spin background fluctuations given by the factor $\exp(-\frac{1}{2}\sum_{i<j} u_{ij} s_i^z s_j^z)$, whereas hole motion effects are, in this regime, correctly described by the variational wave function. For $t/J \geq 0.5$ the difference between variational and exact results begins to increase.

For $\mathbf{k} = (\pi/2, \pi/2)$, $\phi_x = \phi_y = A_0$. In Fig. 2, we compare the value of the variational parameter ϕ_δ found for this value of $\mathbf{k}$ with that found analytically in Sec. III by minimizing $E(\rho)$ given by (28). Notice that there is only a small difference. The difference is mostly due to the fact that (24) and (25) are found by minimizing the energy without allowing for the tail (37). The difference in the optimal values of the variational parameter due to the fact that $u \neq 0$, is smaller. In Fig. 3, the solid line gives the results for λ obtained from (24) and (25) and $\mathbf{k} = 0$ and the open circles the optimal values for the parameter λ found by the VMC procedure where we have set $A_0 = -B_0$. We notice that they are very close. In fact, calculating the energy with MC and $u \neq 0$ and the value for λ given by (24) and (25) gives the same energy within error bars.

The hole band $E(\mathbf{k})$ was also computed for several values of t/J. A typical result is shown in Figs. 4 and 5 for $t/J = 0.5$ obtained by restricting to configurations with total $S^z = \pm\frac{1}{2}$. The structure of the hole band agrees reasonably well with the one of Fig. 14 of Ref. 6. The fact that the energy of the hole at $(\pi/2, \pi/2)$ is degenerate with $(0, \pi)$ and $(\pi, 0)$ in the exact diagonalization[6] is believed to be due to additional symmetries of the 4×4 lattice[6] which are not present in other lattices. We numerically searched for the optimal value of A_k at a few

TABLE V. VMC results for the 8×8 lattice, without restriction on S^z.

t/J	E	T	ΔE
0.0	−72.296(05)	0	2.193(07)
0.20	−72.412(05)	−0.179(01)	2.077(07)
0.50	−72.831(05)	−0.737(02)	1.658(07)
1.00	−73.735(06)	−1.850(04)	0.754(08)
2.50	−76.669(11)	−4.914(10)	−2.180(13)
5.00	−81.747(21)	−10.059(21)	−7.258(23)

TABLE VI. VMC results for the 16×16 lattice, without restriction on S^z.

t/J	E	T	ΔE
0.0	−295.756(15)	0	2.192(20)
0.20	−295.873(14)	−0.179(01)	2.075(19)
0.50	−296.293(15)	−0.737(03)	1.655(20)
1.00	−297.199(16)	−1.850(07)	0.749(21)
2.50	−300.151(22)	−4.923(16)	−2.203(27)
5.00	−305.270(35)	−10.101(32)	−7.322(40)

different values of $\mathbf{k}$ and obtained A_k for the remaining wave vectors by linear interpolation. We found $A_k = 0$ at $\mathbf{k} = (0,0)$, $(\pi,0)$, (π,π), $(\pi,\pi/2)$, and $A_k \sim 0.085$ at $\mathbf{k} = (\pi/2,0)$, $(\pi/2,\pi/2)$. The curve features a minimum at $\mathbf{k} = (\pi/2,\pi/2)$, and attains its maximum value at $\mathbf{k} = (0,0)$ and (π,π). We found the effective mass of the hole to be smaller in the direction $(0,0)$ to (π,π) than in the direction $(0,\pi)$ to $(\pi,0)$ (compare Fig. 4 with Fig. 5). This feature of the quasiparticle band agrees with other theories and calculations.[5,7–9,17,18] Results for the bandwidth W, obtained as the difference between $E(\pi/2,\pi/2)$ and $E(\pi,\pi)$, are shown in Fig. 6. They show a linear behavior for W/t versus t/J for small values of t/J. In Fig. 15 of Ref. 6, it can observed that the bandwidth increases moving from $t/J = \frac{1}{10}$ to $t/J = \frac{1}{2}$, but then it starts decreasing. The increase of the bandwidth for $t/J < 0.5$ is also a result of the variational calculation; however, for larger values of t/J the behavior of W disagrees with the exact results of Ref. 6. This was expected because of the inadequacy of the wave function to describe the physical processes (such as multiple hole

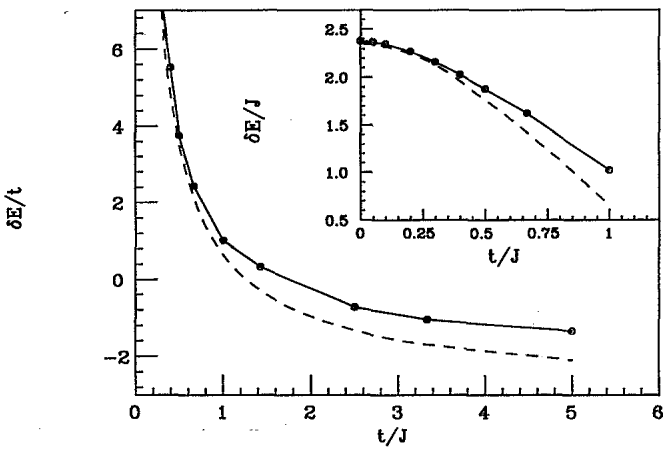

FIG. 1. Comparison between VMC (open circles) and exact diagonalization (dashed lines) results for the 4×4 lattice, at $\mathbf{k} = (\pi/2, \pi/2)$. In the figure we give ΔE in units of t, which is the dominant scale at large t/J, while in the inset we give ΔE in units of J, which is the dominant energy scale at small t/J.

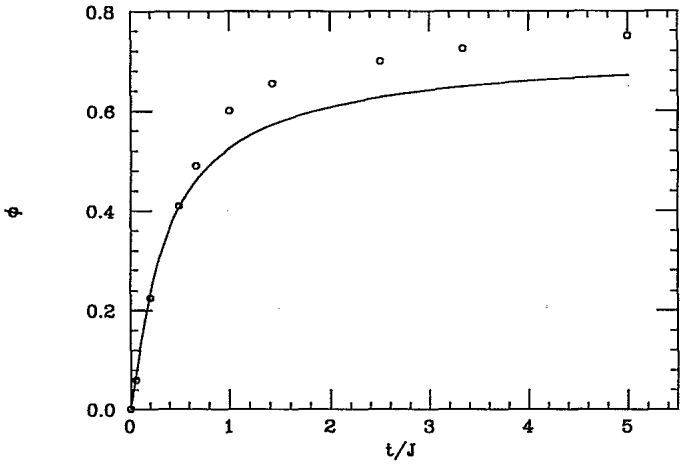

FIG. 2. Comparison between the values of the variational parameter ϕ_δ found at $\mathbf{k} = (\pi/2, \pi/2)$ (open circles) and the values obtained by minimizing $E(\rho)$ given by (28) (solid line), for different values of t/J.

hops) which have been neglected in the present study. We are in the process of improving the wave function by allowing for such processes as also explained below.

In Tables I–VI we give the total energy E, i.e., the expectation value of (1) with the state (15) at $\mathbf{k} = (\pi/2, \pi/2)$, where this quantity is found to attain its minimum, for several lattice sizes, with the restriction on the total $S^z = \pm\frac{1}{2}$ (Tables I–III) and without such restriction (Tables IV–VI). We also give the hole binding energy ΔE, as obtained by subtracting from E the variational ground-state energy for the no-hole case computed with the wave function (7), with and without the restriction on S^z. Assuming the hole binding energy ΔE_L for an

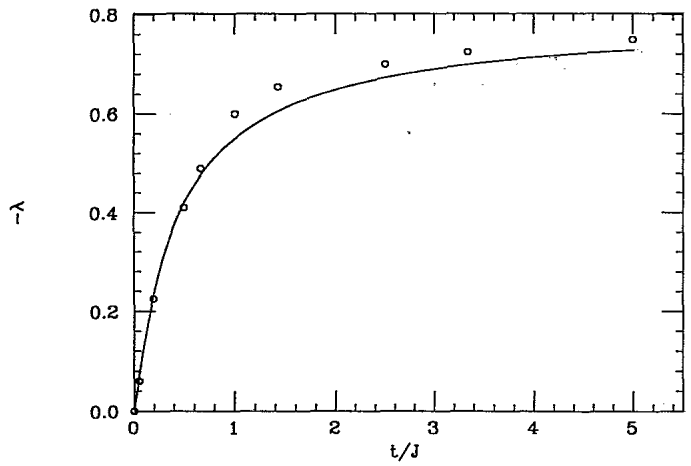

FIG. 3. Comparison between the values of the variational parameter λ_δ found at $\mathbf{k} = (\pi/2, \pi/2)$ (open circles) and the values obtained by minimizing $E(\rho)$ given by (28) (solid line), for different values of t/J.

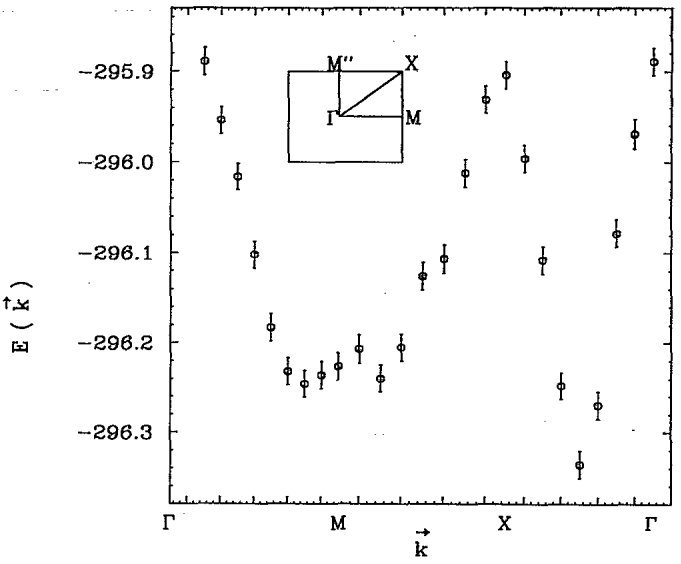

FIG. 4. Hole dispersion curve $E(\mathbf{k})$, plotted along the direction $\Gamma M X \Gamma$ in the Brillouin zone (see inset), for a 16×16 lattice, for $t/J = 0.5$.

$L \times L$ lattice to scale as $\Delta E_L = \Delta E_\infty + \alpha/L^2$, we have performed finite-size scaling analysis of the results of Tables I–VI. Our extrapolated estimates for ΔE_∞ fall inside the error bars of the results for the 16×16 lattice (Tables III and VI). Therefore we believe that the results for the 16×16 lattice give a good estimate, within error bars, of the infinite-size lattice, with the wave function (15). As discussed earlier and as can be seen by comparing the data of the last two columns of Table I, the

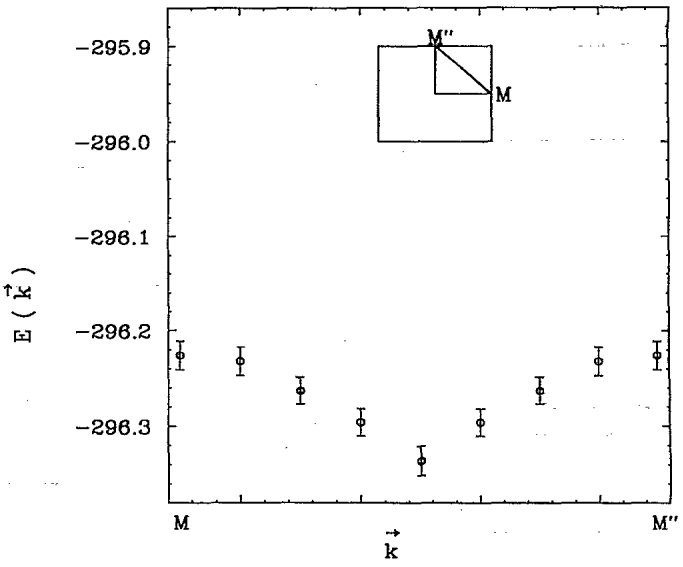

FIG. 5. Hole dispersion curve $E(\mathbf{k})$, plotted along the direction MM'' in the Brillouin zone, for a 16×16 lattice, for $t/J = 0.5$.

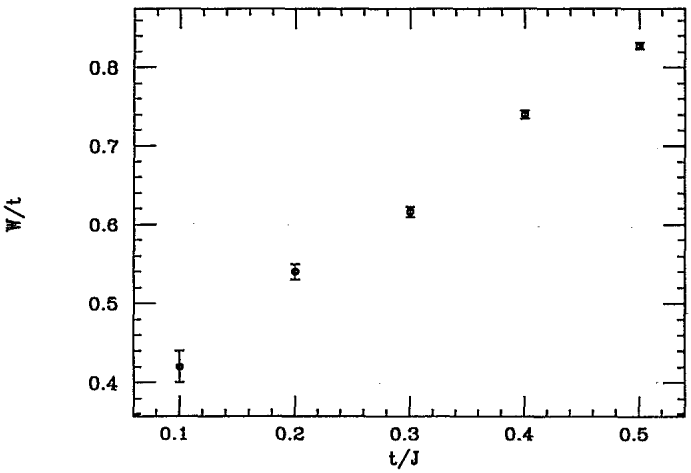

FIG. 6. Hole bandwidth, W/t, plotted vs t/J.

variational estimate of the energy for $t/J < 0.5$ is in good agreement with the results of the exact diagonalization.[6] Assuming that in this range we can trust the variational results, both because they agree with the exact diagonalization results and because of the physical arguments given previously, we can give an estimate of the magnitude of the finite-size effects on the exact diagonalization calculation. For example, for $t/J = 0.2$ we find that ΔE(exact)=2.25 while ΔE(variational)=2.27 in units of J for the 4×4 lattice; this difference, which is due to the approximate nature of the variational calculation, is significantly smaller, in this region, than the difference of about 0.2 between the results on the 4×4 and those obtained on the 16×16 lattice [ΔE(variational)=2.07]; this might give an idea about the finite-size effects affecting the calculation on small-size lattices.

The dipolar distortion of the antiferromagnetic order can be determined by computing the expectation values of the three components of the spin at each lattice site with the state (16), i.e., with no restriction on the total S^z. As explained before, such a state features, in the no-hole case, a nonzero expectation value of the spin at every lattice site, along the x direction. The distortion, induced by the hole, has the effect of rotating the spins. Fig. 7 shows results for a 16×16 lattice, for $t = J$ and $\mathbf{k} = (\pi/2, \pi/2)$, when only the planar distortion is present and $\langle s^z \rangle = 0$ at every site. (a) and (b) refer to the two different sublattices. The vector at each lattice site is proportional to the expectation value of the spin at that lattice site. By computing the expectation value of s^2 at every lattice site we found that quantum fluctuations, that reduce the magnitude of s with respect to its classical value, are less important in the neighborhood of the hole than far away from it, a fact already noticed by Bulut *et al.* for the case of a static hole in a 4×4 lattice.[19] The reduction of the staggered magnetization[17] in the neighborhood of the mobile hole is accomplished by a coherent rotation of the spins, within our wave function.

In conclusion, we have carried out variational Monte Carlo calculations for a single hole in the 2D t-J model. The wave function includes "Jastrow"-type spin-spin and hole-spin correlations. The latter are analogous to Feynman-Cohen backflow correlations introduced to describe elementary excitations in liquid ^{4}He. We find that the hole creates a long-range dipolar distortion of the antiferromagnetic order. The wave function is accurate for small values of t/J ($t/J < 0.5$), while for higher values of t/J we need to generalize our wave function by introducing higher-body static as well as exchange correlations between the hole and the spin background. These effects

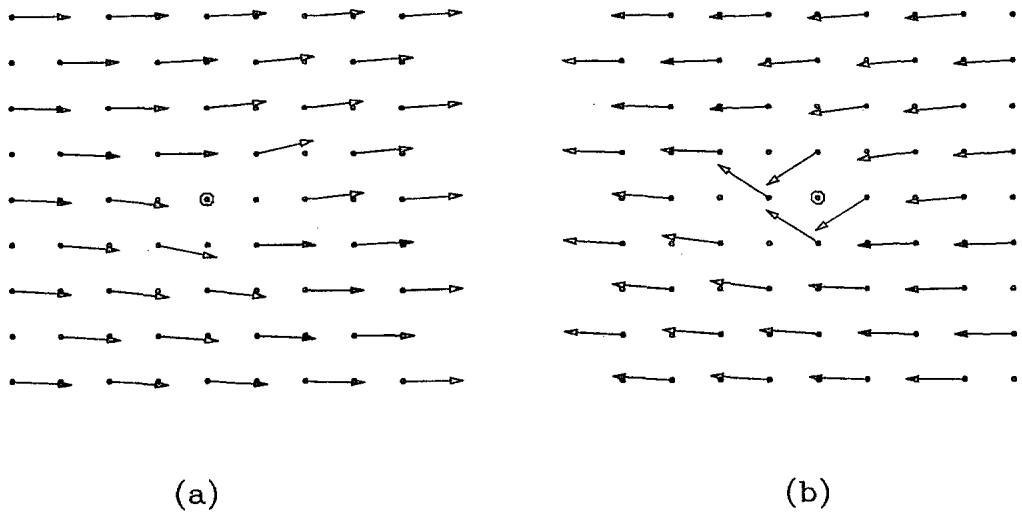

FIG. 7. Distortion of the antiferromagnetic alignment for a 16×16 lattice, at $\mathbf{k} = (\pi/2, \pi/2)$ and $t/J = 1$. (a) refers to the even sublattice, where the hole is residing, (b) to the odd sublattice. The arrows represent the expectation values of the spin at the lattice sites.

modify the correlation operator which acts on the Marshall state in such a way that "string" states, where the spins along the hole path are displaced by one site, are allowed. At large values of t/J, the contributions from such states become increasingly important. Such states have been studied within the Brinkman-Rice[20] approach where the effect of background fluctuations is suppressed. In our approach such fluctuations as well as backflow correlations have been included; thus, it seems attractive to attempt to improve the wave function along these lines. In addition, it would be interesting to study the effects of such "string"-like correlations on the coherent distortion of the AF order. At the present time we are also using the variational wave function as a guidance function for a Green's-function Monte Carlo simulation.

ACKNOWLEDGMENTS

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APPENDIX:

In this appendix, following Feynman and Cohen,[11] we calculate the large-distance behavior of the spin-backflow function $\phi_{\mathbf{k}}(\mathbf{r})$, $\mathbf{r}$ being the coordinate of a boson relative to the impurity. We first rewrite (14) as

$$\Psi_T^{\mathbf{k}} = C\, e^{-i\mathbf{k}\cdot\mathbf{R}} \exp\left(-i\sum_j \phi_{\mathbf{k}}(\mathbf{r}_j)\right) \Xi_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}), \tag{A1}$$

with

$$\Xi_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u}) = \exp\left(-\sum_j \lambda_{\mathbf{k}}(\mathbf{r}_j)\right) \exp\left(-\frac{1}{2}\sum_{i<j} u(\mathbf{r}_i - \mathbf{r}_j)\right) \tag{A2}$$

where $\mathbf{r}_1, \ldots, \mathbf{r}_{N_u}$ are the coordinates of the bosons relative to the impurity and $L(c)$ is the number of "empty" sites, corresponding to down spins, in the negative sublattice. C is a normalization constant. A differential equation for $\phi_{\mathbf{k}}(\mathbf{r})$ can be obtained by imposing that (A1) satisfy the single-particle continuity equation $\sum_{\mathbf{r}_2}\cdots\sum_{\mathbf{r}_{N_u}}(\Psi_T^*\hat{H}\Psi_T - \Psi_T\hat{H}\Psi_T^*) = 0$. Upon retaining up to terms of the order of $(\nabla\phi_{\mathbf{k}})^2$, $\nabla\Xi_{\mathbf{k}}^2$ and $\nabla\phi_{\mathbf{k}}\cdot\nabla\Xi_{\mathbf{k}}$, one obtains

$$\sum_{\delta}\Bigg[\sin(\mathbf{k}\cdot\delta)\delta\cdot\nabla p(\mathbf{r}) - \cos(\mathbf{k}\cdot\delta)\delta\cdot\nabla p(\mathbf{r})\delta\cdot\nabla\phi_{\mathbf{k}}(\mathbf{r}) - \cos(\mathbf{k}\cdot\delta)\delta\cdot\nabla\left(\sum_{\mathbf{r}'}\delta\cdot\nabla'\phi_{\mathbf{k}}(\mathbf{r}')p(\mathbf{r},\mathbf{r}')\right)$$
$$-\sin[\mathbf{k}\cdot\delta+\phi_{\mathbf{k}}(\delta)-\phi_{\mathbf{k}}(-\delta)]\delta\cdot\nabla A_\delta(\mathbf{r})$$
$$+\cos[\mathbf{k}\cdot\delta+\phi_{\mathbf{k}}(\delta)-\phi_{\mathbf{k}}(-\delta)]\delta\cdot\nabla\left(\sum_{\mathbf{r}'}\delta\cdot\nabla A_\delta(\mathbf{r},\mathbf{r}')\right)\Bigg] + (J/2t)\nabla\phi_{\mathbf{k}}(\mathbf{r})\cdot\nabla p(\mathbf{r}) = 0\ , \tag{A3}$$

where $\delta = \hat{x}, \hat{y}$, and with the definitions

$$p(\mathbf{r}_1) = C^2\ N_u \sum_{\mathbf{r}_2}\sum_{\mathbf{r}_3}\cdots\sum_{\mathbf{r}_{N_u}}\Xi_{\mathbf{k}}^2(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u})\ , \tag{A4}$$

$$p(\mathbf{r}_1, \mathbf{r}_2) = C^2 N_u(N_u-1)\sum_{\mathbf{r}_3}\cdots\sum_{\mathbf{r}_{N_u}}\Xi_{\mathbf{k}}^2(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_{N_u})\ , \tag{A5}$$

$$A_\delta(\mathbf{r}_2) = C^2 N_u(N_u-1)\sum_{\mathbf{r}_3}\cdots\sum_{\mathbf{r}_{N_u}}\Xi_{\mathbf{k}}(\delta, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_{N_u})\Xi_{\mathbf{k}}(-\delta, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_{N_u})\ , \tag{A6}$$

$$A_\delta(\mathbf{r}_2, \mathbf{r}_3) = C^2 N_u(N_u-1)(N_u-2)\sum_{\mathbf{r}_4}\cdots\sum_{\mathbf{r}_{N_u}}\Xi_{\mathbf{k}}(\delta, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_{N_u})\Xi_{\mathbf{k}}(-\delta, \mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_{N_u})\ . \tag{A7}$$

The first two terms in Eq. (A3) refer to the hopping of the hole to a nearest-neighboring site occupied by a down spin, whereas the other two terms refer to the hopping to a site where an up spin is residing. If we confine ourselves to the low-density limit, that is, we consider the situation where the number of spins pointing down is much larger than the number of those pointing up (low density of bosons), then it is reasonable to assume that the hole will be surrounded most of the time by spins pointing down, i.e., it will mostly hop to "empty" sites, in the boson

representation. We can therefore neglect the second two terms of Eq. (A3) because they are small compared to the first two. At $\mathbf{k} = (\pi/2, \pi/2)$, we have

$$\nabla\cdot[\hat{k}p(\mathbf{r}) + (J/2t)\nabla\phi_{\mathbf{k}}(\mathbf{r})\ p(\mathbf{r})] = 0 \tag{A8}$$

$p(\mathbf{r})$ is the probability of finding one particle at the position $\mathbf{r}$ relative to the impurity. At large distances from the impurity, the function $p(\mathbf{r})$ approaches a constant value p_0. On assuming $\nabla\phi_{\mathbf{k}}(\mathbf{r})\to 0$ when $r \to \infty$ we find that the leading contribution to $\phi_{\mathbf{k}}(\mathbf{r})$ is given by $A_{\mathbf{k}}\ (\mathbf{k}\cdot\mathbf{r})/r^2$.

The same long-distance behavior can be obtained for small values of $\mathbf{k}$. In this case, we have

$$\nabla\cdot\left[\mathbf{k}\ p(\mathbf{r}) - \nabla\Phi_{\mathbf{k}}(\mathbf{r})p(\mathbf{r}) + \left(\sum_{\mathbf{r}'}\phi_{\mathbf{k}}(\mathbf{r}')\nabla' p(\mathbf{r},\mathbf{r}')\right) + (J/2t)\nabla\phi_{\mathbf{k}}(\mathbf{r})p(\mathbf{r})\right] = 0\ . \tag{A9}$$

At low density, the distribution function $p(\mathbf{r},\mathbf{r}')$ can be approximated by $\rho(\mathbf{r})p(\mathbf{r}')$, where $\rho(\mathbf{r})$ is the boson density. The $\mathbf{k}$ dependence of ρ is contained in the function $\lambda_{\mathbf{k}}$. With the ansatz that $\phi_{\mathbf{k}}$ and $\lambda_{\mathbf{k}}$ are both functions of $\mathbf{k}\cdot\mathbf{r}$, we can set

$$\sum_{\mathbf{r}}{}'\phi_{\mathbf{k}}(\mathbf{r}')\nabla'\rho(\mathbf{r}') = \beta_{\mathbf{k}}\mathbf{k}. \tag{A10}$$

Therefore, our differential equation is

$$\nabla\cdot[(1+\beta_{\mathbf{k}})\mathbf{k}p(\mathbf{r}) - \nabla\Phi_{\mathbf{k}}(\mathbf{r})p(\mathbf{r}) + (J/2t)\nabla\phi_{\mathbf{k}}(\mathbf{r})p(\mathbf{r})] = 0. \tag{A11}$$

Using the same reasonings as before, we find that the leading term of $\phi_{\mathbf{k}}(\mathbf{r})$ is again $A_{\mathbf{k}}\ (\mathbf{k}\cdot\mathbf{r})/r^2$.

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