Variational description of a quasihole excitation in a quantum antiferromagnet

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
(Received 6 September 1991)

An accurate variational ansatz is proposed for a single quasihole excitation in a two-dimensional quantum antiferromagnet. The trial state includes spin-hole and spin-hole-spin correlations, in addition to background antiferromagnetic spin-spin correlations. Background spin-spin correlations are induced by the Heisenberg antiferromagnetic exchange interaction and describe the zero-point motion of spin waves around the Néel state. Spin-hole and spin-hole-spin correlations describe "strings" of spins displaced by one lattice site along the hole path. This is a generalization of the Brinkman-Rice approach to include quantum spin fluctuations. We have used the Monte Carlo method to compute the variational energy and the spectral weight of the quasihole state in the t-J model on the square lattice, with the proposed ansatz. Comparison with exact results for the 4×4 lattice shows very good agreement for both energy and spectral weight, at $\mathbf{k} = (\pi/2, \pi/2)$ in the range $0 \leq t/J \leq 5$. We report results for lattices of several sizes up to 16×16 in the above range of t/J and for the two values of $\mathbf{k}$ where the hole energy band attains its minimum [$\mathbf{k} = (\pi/2, \pi/2)$] and maximum [$\mathbf{k} = (0, 0)$].

I. INTRODUCTION

The two-dimensional (2D) t-J model[1,2] in the presence of one or more holes has elicited significant interest as a simple attempt to capture the essential physics of the superconducting copper oxides. The t-J model, in the no-hole case, reduces to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model (AFHM), which has proven quite successful in explaining certain magnetic properties of the copper oxide undoped materials.[3] The effect of doping is to create mobile holes in the copper oxide planes; the t-J Hamiltonian attempts to describe the motion of holes in a quantum antiferromagnet by a simple nearest-neighbor hole-hopping term in addition to the spin-$\frac{1}{2}$ AFHM:

$$\hat{H}_{t\text{-}J} = -t \sum_{<ij>s} (\hat{a}^{\dagger}_{i,s} \hat{a}_{j,s} + \text{H.c.}) + J \sum_{<ij>} (\mathbf{s}_i \cdot \mathbf{s}_j - \tfrac{1}{4} \hat{n}_i \hat{n}_j). \tag{1}$$

$\hat{a}^{\dagger}_{i,s} = \hat{c}^{\dagger}_{i,s}(1 - \hat{n}_{i,-s})$, where $\hat{c}^{\dagger}_{i,s}$ creates an electron at lattice site i, with spin projection s in a given direction of the spin space, and $\hat{n}_{i,s} = \hat{c}^{\dagger}_{i,s} \hat{c}_{i,s}$ is the number operator; therefore, $\hat{a}^{\dagger}_{i,s}$ creates an electron only at an empty site, thus avoiding double occupancy. $\mathbf{s}_i$ is the spin operator at lattice site i, which is related to $\hat{c}^{\dagger}_{i,\alpha}, \hat{c}_{i,\alpha}$ via $\mathbf{s}_i = \frac{1}{2} \sum_{\alpha,\beta} \hat{c}^{\dagger}_{i,\alpha} \boldsymbol{\sigma}_{\alpha\beta} \hat{c}_{i,\beta}$; t is the hole-hopping matrix element and $\hat{n}_i = \hat{n}_{i,s} + \hat{n}_{i,-s}$.

Several attempts have been made to study the 2D t-J model in the presence of one or two holes; different analytical approaches[4–9] have predicted certain features of the physics of one hole, such as the existence of a quasiparticle peak in the hole spectral function for $J \neq 0$ and the location of the minimum of the hole band at $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$. Numerical studies have also been performed, both to check the theoretical results obtained with the various approximations and to gain information about those aspects of the problem which are not fully understood, such as the effect of the hole motion on the antiferromagnetic spin background. Important results have been produced by exact diagonalization[10–12] which seem to confirm, to some extent, the above predictions. However, exact diagonalization is limited to lattices of small size (4×4 or $\sqrt{20} \times \sqrt{20}$) because of computer memory constraints; extrapolation to the infinite lattice is also problematic due to the unavailability of calculations on lattices of significantly different sizes. Alternative techniques must then be used in order to extend the numerical investigation to larger lattices and extrapolate the values of the physically relevant quantities in the bulk limit. We perform a variational study, based upon a trial state which includes analytical insight on the correlations introduced by the hole, and we gauge the accuracy of the trial state by comparing the variational estimates for small lattices with the exact diagonalization results. Though intrinsically approximate, variational results can offer an indication of the finite-size scaling behavior of the quantities of interest. Additionally, an accurate trial state can be used to compute the mixed estimates in a quantum Monte Carlo simulation, which affords a more precise estimate of the various expectation values than the one obtained variationally.

In a recent paper[13] we derived a variational state (in the following referred to as Ψ^{I}) for a single hole in the 2D t-J model on the square lattice by using a formal analogy 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. The trial state Ψ^{I} includes two-body correlations and a backflow term analogous to the one introduced by Feynman and Cohen[14] to study the problem of a ^{3}He impurity in liquid ^{4}He. Translated in the spin language, the trial state Ψ^{I} takes the form of a state obtained by acting on an antiferromagnetically correlated

 ©1992 The American Physical Society

hole state with a complex spin-hole correlation operator. This operator generates 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 well localized in the immediate neighborhood of the hole, both depending on the momentum of the excitation. The variational estimate of the hole energy given by the state Ψ^{I} is accurate for $t/J \leq 0.5$. The reason why the state Ψ^{I} is adequate for low values of t/J is that it describes a global response of the spin background, which can rearrange itself coherently with the motion of the hole by means of quantum spin fluctuations associated with the Heisenberg term of the Hamiltonian (1), in order to minimize the energy.

In order for this picture to be valid, the time scale associated with quantum spin fluctuations ($\sim 1/J$) should be small compared to the one associated to hole hopping ($\sim 1/t$). In other words, the hole should not move too fast, in order to give enough time to the spin background to respond. As t/J grows, the relative "inertia" of the spin background increases, and in the $t/J >> 1$ limit one can neglect quantum spin fluctuations and consider the motion of the hole in a "rigid" spin lattice. It is known[15] that the spin background is ferromagnetic at $J = 0$ and it was shown by Brinkman and Rice[16] that the system approaches this limit by becoming ferromagnetic inside an increasingly larger circular region around the hole, as $t/J \to \infty$. The value of t/J at which ferromagnetism begins to develop can be estimated[4] to be of order 10^2. Therefore, there is a wide range of t/J where the spin background should remain essentially antiferromagnetic, and if spin fluctuations are neglected (at $t/J >> 1$) the hole motion generates "strings" of overturned spins.

In this paper, we propose a trial state (henceforth referred to as Ψ^{II}) to describe an intermediate t/J regime, where t is of the same order of J and where spin fluctuations restore the damage that the hole leaves behind it. In this picture, the effect of the hole motion on the background remains confined within a few lattice sites away from the hole, namely to those lattice sites that can be reached, from the position of the hole, by at least one of the "strings" allowed in the state. Further away, the environment is the same as in the absence of the hole.

The state Ψ^{II} is obtained by acting on an antiferromagnetically correlated hole state, including effects of quantum spin fluctuations, with an operator that generates strings of spins displaced by one site along the hole path; we allow for strings of length up to two sites. Such an operator can be more generally interpreted as a spin-hole correlation operator, including up to three-body correlations.

We used the Monte Carlo method to compute the variational estimate of the hole energy and the spectral weight of the quasihole state, with the trial state Ψ^{II}. Our results for the hole energy are in very good agreement with exact diagonalization results for the 4×4 lattice, at $\mathbf{k} = (\pi/2, \pi/2)$, over the range $0 \leq t/J \leq 5$. At $\mathbf{k} = (0,0)$ we find the same kind of agreement for $0 \leq t/J \leq 1$, whereas for higher values of t/J the agreement is not as good as at $\mathbf{k} = (\pi/2, \pi/2)$, even though there is still a definite improvement with respect to the state Ψ^{I}. We believe this to be due to the need of including strings longer than two sites at $\mathbf{k} = (0,0)$, for $t/J > 1$. However, it should also be noted that at $\mathbf{k} = (0,0)$ the lowest eigenstate has very small spectral weight and the main peak in the spectral function occurs at higher energy.[7,11] The energy estimate given by the state Ψ^{II} compares favorably to the one of the state Ψ^{I} even for small values of t/J, where we would expect the state Ψ^{I} to be more accurate. The reason is that although the two states have different physical motivations, their leading contributions are very similar at small values of t/J, as we show below. In the next section we introduce the variational ansatz Ψ^{II}; our results are discussed in Sec. III.

II. THE VARIATIONAL ANSATZ

It is easier to introduce the state Ψ^{II} by considering the Brinkman-Rice approach to the $t/J \gg 1$ limit. In this limit, as explained above, one can neglect quantum spin fluctuations associated with the Heisenberg term of (1) and consider the motion of the hole in a rigid spin lattice, which we assume to be antiferromagnetically aligned, with alignment in an arbitrary direction of the spin space. Consider the following translationally invariant hole state:

$$|\mathbf{k},0> = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}} \, |\mathcal{N},\mathbf{R}> , \tag{2}$$

where N is the number of sites in the square lattice, $\mathbf{k}$ is the hole Bloch wave vector and $|\mathcal{N},\mathbf{R}>$ is the antiferromagnetically aligned (Néel) state in a given direction, with a hole at $\mathbf{R}$. By acting on (2) with the hole-hopping term of the Hamiltonian (1) we generate four new states:

$$|\mathbf{k},\mathbf{a}> = \hat{\mathcal{P}}_{\mathbf{a}} \, |\mathbf{k},0> , \tag{3}$$

where $\hat{\mathcal{P}}_{\mathbf{a}} = \sum_s \hat{c}^{\dagger}_{\mathbf{R},s} \hat{c}_{\mathbf{R}+\mathbf{a},s}$ is simply the hole-hopping operator in the Hamiltonian (1), which interchanges the positions of the hole and of the spin located at $\mathbf{a}$ with respect to the hole; $\mathbf{a} = \pm\hat{\mathbf{x}}, \pm\hat{\mathbf{y}}$ is a unit vector connecting two nearest-neighboring sites; obviously, $\hat{\mathcal{P}}_{\mathbf{a}}\hat{\mathcal{P}}_{-\mathbf{a}} = 1$. By acting once again with the hole-hopping term on the states $|\mathbf{k},\mathbf{a}>$ we obtain twelve new states:

$$|\mathbf{k},\mathbf{a},\mathbf{a}'> = \hat{\mathcal{P}}_{\mathbf{a}} \, \hat{\mathcal{P}}_{\mathbf{a}'} \, |\mathbf{k},0> , \tag{4}$$

with $\mathbf{a}' \neq -\mathbf{a}$. This procedure can be iterated to generate new states; the ground state of (1) with wave vector $\mathbf{k}$ is written, in this approach, as

$$|\phi,\mathbf{k}> = \sum_{n=0}^{\infty} \sum_{\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(n)}} f_{\mathbf{a}^{(1)},\ldots,\mathbf{a}^{(n)}}(\mathbf{k}) \times \hat{\mathcal{P}}_{\mathbf{a}^{(1)}} \cdots \hat{\mathcal{P}}_{\mathbf{a}^{(n)}} |\mathbf{k},0> . \tag{5}$$

The operator $\hat{\mathcal{P}}_{\mathbf{a}^{(1)}}\hat{\mathcal{P}}_{\mathbf{a}^{(2)}} \cdots \hat{\mathcal{P}}_{\mathbf{a}^{(n)}}$, when acting on the state $|\mathcal{N},\mathbf{R}>$, creates a "string" of length n, i.e., displaces the hole from $\mathbf{R}$ to $\mathbf{R} + \mathbf{a}^{(1)} + \mathbf{a}^{(2)} + \cdots + \mathbf{a}^{(n)}$ and displaces all spins along the hole path by one site. The sum in the state (5) is over all possible string configura-

tions; in the large t/J limit, strings of arbitrary length must be considered.

We construct our variational state by introducing quantum spin fluctuations in the above scheme. Spin fluctuations can be accounted for by replacing the "rigid" state $|\mathbf{k},0>$ with a more general, antiferromagnetically correlated hole state.

In order to obtain such state we start from the no-hole case, i.e., spin-$\frac{1}{2}$ AFHM, and consider the following state:

$$|\Phi>=\sum_c (-1)^{L(c)} \exp\left(-\frac{1}{2}\sum_{i<j} u_{ij} s_i^z s_j^z\right)|c> . \quad (6)$$

This state is widely used as a variational ansatz for the no-hole case;[17–19] $|c>$ is a lattice spin configuration, specified by assigning the value of the projection of the spin in a given direction (which we call z) of the spin space for each lattice site; the function u_{ij} is a spin-spin correlation function which depends on the distance $|\mathbf{r}_i-\mathbf{r}_j|$ between two sites i and j; it has been investigated both analytically and numerically.[18,19] If the sum in (6) is taken over all possible lattice spin configurations and $L(c)$ is chosen to be the number of down spins in one of the two sublattices, then the state (6) can be shown to feature long-range antiferromagnetic order in the x direction of the spin space. The sum can also be restricted to spin configurations with a fixed value of the z component of the total spin, S^z: in this case, although the state (6) retains long-range antiferromagnetic order in the xy plane of the spin space, there is no well-defined direction of the staggered magnetization.[13] In our variational calculation, we have set $S^z=0$ and used the same function u numerically optimized by Liu and Manousakis[18]: with such a choice, the state (6) gives a variational estimate of the energy per site equal to $-1.1638J$ (as opposed to $-J$ given by the simple Néel state), in good agreement with the value $-1.1692J$ found by Trivedi and Ceperley, who used a Green's function Monte Carlo method.[20]

A "bare" hole state with momentum $\mathbf{k}$ and $S^z=-s$ can be created by acting on $|\Phi>$ with the operator $\hat{c}_{\mathbf{k},s}=(1/\sqrt{N})\sum_{\mathbf{R}} e^{-i\mathbf{k}\cdot\mathbf{R}}\,\hat{c}_{\mathbf{R},s}$, where the sum runs over all lattice sites; $\hat{c}_{\mathbf{k},s}$ simply removes a particle with spin projection s in the z direction from the no-hole state $|\Phi>$. The state $\hat{c}_{\mathbf{k},s}|\Phi>$ retains spin-spin correlations associated with the spin of the particle that has been eliminated: such correlations are to be removed and replaced by spin-hole correlations, in our variational ansatz. Therefore, we introduce the following hole state:

$$|\mathbf{k}>=\hat{U}\hat{c}_{\mathbf{k},s}|\Phi> , \quad (7)$$

where

$$\hat{U}=\exp\left(\frac{s}{2}\sum_i u(|\mathbf{r}_i-\mathbf{R}|)\hat{s}_i^z\right) . \quad (8)$$

The operator $\hat{U}$ cancels out the spin-spin correlations associated with the spin of the particle that has been eliminated, in the "bare" hole state $\hat{c}_{\mathbf{k},s}|\Phi>$. The state (7) provides a good variational ansatz for the $t/J=0$ (static hole) case: the extrapolation to the infinite lattice gives a variational energy estimate of $(2.210\pm0.014)J$, in good agreement with the value $(2.193\pm0.007)J$ recently obtained by Barnes and Kovarik by a Monte Carlo algorithm.[21] At $t/J\neq 0$, spin-hole correlations must be introduced to account for the effect of hole hopping: we express such correlations in the same "string"-based form that we found by neglecting background fluctuations [Eq. (5)]; because we are interested in an intermediate regime, where strings just begin to emerge, we only consider strings of up to two sites. The variational state Ψ^{II} is therefore expressed as

$$|\Psi^{\mathrm{II}}_{\mathbf{k}}>=\hat{F}(\mathbf{k})\,|\mathbf{k}> , \quad (9)$$

with

$$\hat{F}(\mathbf{k})=\left(1+\sum_{\mathbf{a}} f_{\mathbf{a}}(\mathbf{k})\hat{\mathcal{P}}_{\mathbf{a}}+\sum_{\mathbf{a},\mathbf{a}'} f_{\mathbf{a}\mathbf{a}'}(\mathbf{k})\hat{\mathcal{P}}_{\mathbf{a}'}\hat{\mathcal{P}}_{\mathbf{a}}\right) . \quad (10)$$

The operator $\hat{F}(\mathbf{k})$ is a spin-hole correlation operator, which contains up to three-body correlations. The spin-hole correlation operator (10) modifies the spin environment only within two sites from the hole. This is consistent with the physical idea that, in an intermediate range of t/J, the time scales associated with hole motion and with spin fluctuations are comparable. Therefore, the damage on the antiferromagnetic order that the hole leaves behind in its motion is restored by quantum spin fluctuations, and remains confined within few sites away from the hole.

The coefficients $f_{\mathbf{a}}(\mathbf{k})$, $f_{\mathbf{a}\mathbf{a}'}(\mathbf{k})$ are variational parameters; there are sixteen altogether, corresponding to all nonretracing hole paths which can be constructed with one- and two-hole hops. Upon neglecting background spin fluctuations, such parameters can be evaluated analytically by diagonalizing the Hamiltonian (1) in the subspace spanned by the seventeen states $|\mathbf{k},0>$, $|\mathbf{k},\mathbf{a}>$, $|\mathbf{k},\mathbf{a},\mathbf{a}'>$; such diagonalization can be done exactly (see also Ref. 9). The eigenvector corresponding to the lowest eigenvalue is a linear combination of the above states with coefficients $f_{\mathbf{a}}$, $f_{\mathbf{a}\mathbf{a}'}$. In our variational approach with the state (9) (which includes spin fluctuations) we perform a minimization in the sixteen-parameter space, using the Monte Carlo method to compute the energy expectation value. We start from the values of the parameters found analytically by neglecting spin fluctuations and vary them to find the energy minimum. The optimal values of these parameters are found to be very close to those computed analytically for $t/J>1$.

Next we investigate the low t/J limit, and make contact with the variational state Ψ^{I} proposed in Ref. 13. Let us consider such variational state:

$$|\Psi^{\mathrm{I}}_{\mathbf{k}}>=\hat{G}(\mathbf{k})\,|\mathbf{k}>, \quad (11)$$

with

$$\hat{G}(\mathbf{k})=\exp\left(-\sum_i[\lambda_{\mathbf{k}}(\mathbf{r_i}-\mathbf{R})+i\phi_{\mathbf{k}}(\mathbf{r}_i-\mathbf{R})]\hat{s}^z_{\mathbf{r}_i}\right) . \quad (12)$$

The spin-hole correlation operator $\hat{G}(\mathbf{k})$ contains two variational functions, $\lambda_{\mathbf{k}}(\mathbf{r})$ and $\phi_{\mathbf{k}}(\mathbf{r})$; $\lambda_{\mathbf{k}}$ describes a

ferromagnetic moment in the neighborhood of the hole, perpendicular to the staggered magnetization vector, whereas the spin-backflow function $\phi_{\mathbf{k}}$ is associated with a planar rotation of the spins, in the plane of the staggered magnetization. Both $\lambda_{\mathbf{k}}(\mathbf{r})$ and $\phi_{\mathbf{k}}(\mathbf{r})$ are decreasing functions of the distance between the spin and the hole, and $\lambda_{\mathbf{k}}, \phi_{\mathbf{k}} \rightarrow 0$ when $t/J \rightarrow 0$. In this limit, we can take $\lambda_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ to be simple nearest-neighbor functions, and approximate the operator (12) by

$$\hat{G}(\mathbf{k}) \approx 1 - \sum_{\mathbf{a}} [\lambda_{\mathbf{k}}(\mathbf{a}) + i\phi_{\mathbf{k}}(\mathbf{a})] \hat{s}^z_{\mathbf{R}+\mathbf{a}} \, . \tag{13}$$

A straightforward calculation shows that, upon setting $\lambda_{\mathbf{k}}(\mathbf{a}) + i\phi_{\mathbf{k}}(\mathbf{a}) = 2f_{\mathbf{a}}(\mathbf{k})$ and $f_{\mathbf{a}\mathbf{a}'}(\mathbf{k}) = 0$, (13) and (10) are equivalent if they act on $|\mathbf{k}, 0>$ (the antiferromagnetic order is assumed to be in the x direction). In this limit, therefore, the operators (12) and (10) are very close. To make this more quantitative, consider the two states $|G> = \hat{G}(\mathbf{k})|\mathbf{k}, 0>$, with $\lambda_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ equal to zero for distances beyond nearest neighbors, and $|F> = \hat{F}(\mathbf{k})|\mathbf{k}, 0>$ with $f_{\mathbf{a}\mathbf{a}'}(\mathbf{k}) = 0$; the variational minimization for the Hamiltonian (1) with these two states can be done analytically (see Ref. 13 for the state $|G>$). The expectation values are independent of $\mathbf{k}$; in the first two columns of Table I, we report the expectation values of the Hamiltonian (1) on the states $|G>$ and $|F>$, with the expectation value of the spin-$\frac{1}{2}$ AFHM on the Néel state taken as reference energy. As we can see, the energy estimates for the two states are very close at small values of t/J (< 0.5); as t/J grows, the one given by the state $|F>$ is increasingly lower. Spin fluctuations, which can be included by replacing the state $|\mathbf{k}, 0>$ with the correlated state $|\mathbf{k}>$, do not fundamentally alter the argument given above, because the state $|\mathbf{k}>$ still features substantial antiferromagnetic order; thus, we can expect the variational state Ψ^{II} to have a significant overlap with the state Ψ^{I} in the low t/J limit, for which the state Ψ^{I} is an accurate variational ansatz. We also note that the state Ψ^{II} can be obtained from the perturbative treatment of the Hamiltonian (1) in the low t/J limit: the state $|\mathbf{k}>$, as mentioned above, is a good variational ansatz at $t/J = 0$, and therefore can be taken as unperturbed ground state. In conclusion, although the state Ψ^{II} was introduced to describe an intermediate t/J range, it can be expected to give good variational energy estimates in the low t/J limit as well.

TABLE I. Comparison between the variational energy δE obtained with the states $|G>$ and $|F>$ (first two columns). The third and fourth columns report the hole energy from the diagonalization in the seventeen-state basis, neglecting spin fluctuations, at $\mathbf{k} = (0,0)$ and $(\pi/2, \pi/2)$. The expectation value of the spin-$\frac{1}{2}$ AFH Hamiltonian on the Néel state is taken as reference energy. The results are in units of J.

t/J	$\|G>$	$\|F>$	$\mathbf{k} = (\pi/2, \pi/2)$	$\mathbf{k} = (0,0)$
0.05	1.994	1.994	1.108	1.113
0.1	1.974	1.974	1.098	1.112
0.2	1.904	1.900	1.045	1.098
0.3	1.802	1.790	0.960	1.075
0.5	1.546	1.500	0.711	1.002
1.0	0.778	0.614	−0.221	0.542
2.5	−1.777	−2.306	−3.856	−2.733
5.0	−6.164	−7.278	−10.349	−9.201

We conclude this section by noticing that the diagonalization of (1) on the seventeen-state basis $|\mathbf{k}, 0>$, $|\mathbf{k}, \mathbf{a}>$, $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$, which ignores background spin fluctuations, can be used to gain insight about the structure of the hole band,[9] but cannot provide quantitative estimates of the hole energy δE, defined as the difference between the ground-state energies of the single-hole and the no-hole case. To illustrate this point, consider the third [$\mathbf{k} = (\pi/2, \pi/2)$] and fourth [$\mathbf{k} = (0,0)$] columns of Table I, where we report the energy differences between the lowest eigenvalue found from the above simple diagonalization and the energy of the Néel state for the no-hole case. If we compare these numbers with those in the first two columns and also with the exact results for the 4×4 lattice[11] we conclude that the hole energy is largely underestimated, particularly at $t/J \leq 1$. The reason is that by extending the Hilbert space of minimization to include the states $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$, we also allow for processes of "flipping" of a pair of nearest-neighboring spins adjacent to the hole; such processes are allowed by the Heisenberg part of (1) in both the hole and the no-hole cases (of course, not just in the vicinity of the hole but everywhere in the lattice): therefore, they must be consistently accounted for in both cases.

To further clarify this issue, consider the static hole (i.e., $t = 0$) case, within the approximation of neglecting spin fluctuations. Again, we start from the state $|\mathbf{k}, 0>$; if we take $|\mathbf{k}, 0>$ as the static hole ground state and the Néel state as the no-hole ground state, we obtain a static hole energy $\delta E = 2J$. The introduction of string states [Eq. (5)], in the absence of a hole-hopping term, is no longer justified; however, if we replace $|\mathbf{k}, 0>$ by a linear combination of $|\mathbf{k}, 0>$ and the twelve states $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$ and minimize the variational energy, we find a value of $\delta E = 1.115J$, with the Néel state taken as the no-hole ground state. This is because, even at $t = 0$, the Hamiltonian (1) can "flip" pairs of nearest-neighboring antiparallel spins, therefore the inclusion of the states $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$ can lower the variational energy of the static hole. The inconsistency of such a way to estimate δE lies in the fact that we are allowing for the flipping of a spin pair in the neighborhood of a particular site (the hole) in the hole case only, whereas it should be allowed in both the hole and the no-hole case, everywhere in the lattice. To show how this can affect the estimate of δE, we can perform a simple calculation, that is, we can diagonalize the Heisenberg Hamiltonian in the subspace spanned by the Néel state $|\mathcal{N}>$ and the twelve states $|\mathcal{N}>$, $|\mathcal{N}, \mathbf{a}, \mathbf{a}'>$, where $|\mathcal{N}, \mathbf{a}, \mathbf{a}'>$ is the Néel state with two overturned spins at $\mathbf{a}$ and $\mathbf{a} + \mathbf{a}'$ with respect to a given site, chosen as the origin: these states correspond to the states $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$ of the static hole case. If the eigenstate corresponding to the lowest eigenvalue is taken as the no-hole ground state, as opposed to the Néel state, the static hole energy δE becomes $1.904J$, i.e., close to the value of $2J$ we found when we did not introduce the states $|\mathbf{k}, \mathbf{a}, \mathbf{a}'>$ and $|\mathcal{N}, \mathbf{a}, \mathbf{a}'>$ at all. Note that the ground-state energy

is an extensive quantity, i.e., of order N, and the energy of the new ground state for the no-hole case only differs from that of the Néel state by a correction of order 1; however, this correction is significant in estimating the hole energy δE, which is also of order 1.

In conclusion, quantum spin fluctuations must be systematically allowed everywhere in the lattice, not just around the hole, in both the hole and no-hole state. In our approach, spin fluctuations are automatically included in the hole state (7) and in the state (6) for the no-hole case; the hole energy is computed by subtracting, from the total variational energy of the system in the single-hole case, the same quantity for the no-hole case . This way, the role of spin fluctuations is consistently taken into account in both the hole and no-hole state.

III. VARIATIONAL CALCULATION

We performed variational calculations for the hole energy and the spectral weight of the quasihole state (9) on lattices of several sizes up to 16×16, using the Monte Carlo technique. We found that the optimal values of the variational parameters depend very weakly on the lattice size. As previously mentioned, for $t/J > 1$ the optimal values of the variational parameters are very close to the values determined analytically within the approximation of neglecting background spin fluctuations; this was expected, as in this range of t/J such approximation is a valid one. For $t/J \leq 1$ we determined numerically the values of the optimal parameters $f_{\mathbf{a}}(\mathbf{k})$ and $f_{\mathbf{aa'}}(\mathbf{k})$. At low values of t/J ($t/J \sim 0.2$) the variational energy estimate given by the ansatz Ψ^{II} is the same as the one obtained with the state Ψ^{I}; moreover, the optimal values of the parameters $f_{\mathbf{a}}(\mathbf{k})$ can be related to the optimal values of the parameters for the state Ψ^{I} via $\lambda_{\mathbf{k}}(\mathbf{a}) + i\phi_{\mathbf{k}}(\mathbf{a}) = 2f_{\mathbf{a}}(\mathbf{k})$, which is what we found analytically in the previous section, neglecting spin fluctuations; this confirms the analogy outlined above between the states Ψ^{I} and Ψ^{II}, in the low t/J limit.

The hole band attains its minimum at $\mathbf{k} = (\pi/2, \pi/2)$ and the maximum at $\mathbf{k} = (0,0)$. In Fig. 1 we compare variational results for the hole energy δE at $\mathbf{k} = (\pi/2, \pi/2)$ on a 4×4 lattice, obtained with the state Ψ^{I} (squares) and Ψ^{II} (open circles), with exact diagonalization results (solid line) from Ref. 11, for different values of t/J. In the range $t/J > 1$ the variational estimate for the hole energy given by the state Ψ^{II} is significantly lower than the one given by the state Ψ^{I}: in particular, at $\mathbf{k} = (\pi/2, \pi/2)$ the agreement with the exact results on the 4×4 lattice is very good, which indicates the validity of the string picture. At $\mathbf{k} = (0,0)$, the agreement with exact results is not as good as at $\mathbf{k} = (\pi/2, \pi/2)$ (see Table II). We believe this to be due to the need of including longer strings at $\mathbf{k} = (0,0)$ than at $\mathbf{k} = (\pi/2, \pi/2)$. This argument is supported by the results of our ground-state spectral weight calculation, which are given below.

We found that we could obtain a further slight lowering of the variational estimate, at large values of t/J (> 2.5), by allowing for a small rotation of the spins in the neighborhood of the hole, in the state $\mathbf{k}$. Such rotation can be

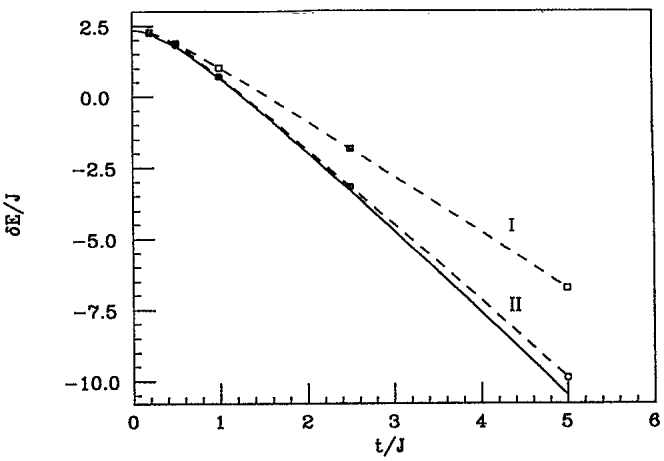

FIG. 1. Comparison between exact diagonalization (solid line) and variational results for the hole energy at $\mathbf{k} = (\pi/2, \pi/2)$, for the 4×4 lattice. Squares joined by a dashed line labeled I refer to the values obtained with the trial state Ψ^{I}, whereas open circles joined by a dashed line labeled II refer to the values obtained with the state Ψ^{II}. The improvement obtained with the state Ψ^{II} is especially evident at large values of t/J, where strings play a significant role.

obtained by acting on the state $|\mathbf{k}>$ with the operator $\hat{G}$, that is the operator that creates the trial state Ψ^{I}, with $\lambda_{\mathbf{k}}$ and $\phi_{\mathbf{k}}$ nearest-neighbor functions.[13] We interpret this further improvement in the variational energy, which is more significant at $\mathbf{k} = (0,0)$, as due to contributions coming from strings longer than two sites, which are absent in the operator $\hat{F}(\mathbf{k})$ and which are partly accounted for by the additional rotation. Explicit inclusion of longer strings in the trial state Ψ^{II} would eliminate the need for this degree of freedom.

Our variational results are summarized in Tables II and III, where we report the expectation values of the hole energy and of the hopping energy, computed with the trial state Ψ^{II}, for the two wave vectors $\mathbf{k} = (0,0)$ and $\mathbf{k} = (\pi/2, \pi/2)$, on the various lattices. We obtained the extrapolated values for the hole energy in an infinite lattice by performing finite-size-scaling analysis of the results in Table II. We assumed the hole energy for an $L \times L$ lattice to scale as $\delta E_L = \delta E_\infty + \alpha_{\mathbf{k}}/L^2$. The $1/L^2$ dependence of the hole-hopping energy in our calculation is mainly due to the fact that S^z is fixed, in the state (7). If we compute the expectation value of the hole-hopping term with the state (7) and $u = 0$, we find it to be equal to $(2t/N)[\cos(k_x) + \cos(k_y)]$. This k-dependent finite-size effect, which is also present when $u \neq 0$, can explain the lattice size dependence of the expectation value of the hole-hopping term of (1) with the trial state Ψ^{II} at $\mathbf{k} = (0,0)$ and for small values of t/J. At $\mathbf{k} = (\pi/2, \pi/2)$, on the other hand, the hole-hopping energy is insensitive to the lattice size for $L > 4$. Note that, at $\mathbf{k} = (\pi/2, \pi/2)$, the extrapolated estimates for the hole energy on an infinite lattice fall within the statistical error bars of the results for the 16×16 lattice: therefore, we believe that such results can be considered as a good estimate of those for the infinite lattice with the trial state (9). Also, at $\mathbf{k} = (\pi/2, \pi/2)$ the difference

TABLE II. Variational results for the hole energy at $\mathbf{k} = (\pi/2, \pi/2)$ and $\mathbf{k} = (0,0)$, at different values of t/J and for lattices of different sizes. The first column reports the exact values for the 4×4 lattice. The results are in units of J. Statistical errors (in parentheses) are on the last two digits.

t/J	Exact	4×4	8×8	12×12	16×16	Extrapolated
			$\mathbf{k} = (\pi/2, \pi/2)$			
0.20	2.248	2.268(02)	2.111(08)	2.093(11)	2.081(15)	2.075(15)
0.50	1.764	1.796(02)	1.594(08)	1.575(12)	1.564(16)	1.557(16)
1.00	0.656	0.698(02)	0.447(09)	0.427(13)	0.415(16)	0.407(16)
2.50	−3.305	−3.156(02)	−3.552(09)	−3.568(13)	−3.579(18)	−3.584(17)
5.00	−10.49	−9.880(05)	−10.448(11)	−10.454(15)	−10.479(19)	−10.476(19)
			$\mathbf{k} = (0,0)$			
0.0	2.349	2.374(03)	2.232(05)	2.221(09)	2.212(18)	2.210(14)
0.20	2.500	2.451(04)	2.253(08)	2.221(11)	2.207(15)	2.193(15)
0.50	2.579	2.500(04)	2.114(09)	2.062(12)	2.039(16)	2.017(16)
1.00	1.849	2.000(05)	1.644(11)	1.561(15)	1.538(19)	1.499(19)
2.50	−1.638	−0.875(08)	−1.374(12)	−1.447(17)	−1.467(21)	−1.501(22)
5.00	−9.14	−6.667(14)	−7.546(15)	−7.613(23)	−7.618(25)	−7.651(27)

TABLE III. Variational results for the hole-hopping energy at $\mathbf{k} = (\pi/2, \pi/2)$ and $\mathbf{k} = (0,0)$, for several values of t/J and for lattices of different sizes. The results are in units of J. Statistical errors (in parentheses) are on the last two digits.

t/J	4×4	8×8	12×12	16×16
		$\mathbf{k} = (\pi/2, \pi/2)$		
0.20	−0.232(01)	−0.234(01)	−0.234(01)	−0.234(01)
0.50	−0.992(01)	−1.010(01)	−1.010(01)	−1.010(01)
1.0	−2.354(02)	−2.404(02)	−2.404(02)	−2.404(02)
2.5	−6.599(05)	−6.785(03)	−6.783(03)	−6.783(03)
5.0	−13.441(06)	−13.801(06)	−13.798(07)	−13.799(06)
		$\mathbf{k} = (0,0)$		
0.20	0.075	0.018	0.008(01)	0.005(01)
0.50	−0.051(02)	−0.229(02)	−0.250(02)	−0.259(02)
1.00	−1.634(04)	−1.710(03)	−1.704(04)	−1.705(03)
2.50	−4.936(09)	−5.223(08)	−5.202(09)	−5.200(08)
5.00	−11.292(17)	−11.930(15)	−11.894(16)	−11.877(16)

TABLE IV. Spectral weight of the quasihole state at $\mathbf{k} = (\pi/2, \pi/2)$ and at $\mathbf{k} = (0,0)$, for several values of t/J and for lattices of different sizes. The first column reports the exact values for the 4×4 lattice. Statistical errors (in parentheses) are on the last two digits.

t/J	Exact	4×4	8×8	12×12	16×16	Extrapolated
			$\mathbf{k} = (\pi/2, \pi/2)$			
0.20	0.91	0.856(03)	0.831(03)	0.815(04)	0.805(04)	0.780(08)
0.50		0.709(02)	0.684(03)	0.670(03)	0.663(03)	0.642(06)
1.00	0.59	0.575(03)	0.553(03)	0.543(03)	0.536(03)	0.520(06)
2.50	0.40	0.421(02)	0.388(02)	0.380(04)	0.375(02)	0.362(04)
5.00	0.28	0.377(02)	0.348(02)	0.341(03)	0.337(02)	0.326(04)
			$\mathbf{k} = (0,0)$			
0.20		0.923(03)	0.894(03)	0.877(03)	0.872(04)	0.848(07)
0.50		0.756(04)	0.703(04)	0.679(04)	0.673(05)	0.639(09)
1.00		0.154(03)	0.207(03)	0.202(03)	0.204(04)	
2.50		0.067(03)	0.118(03)	0.115(02)	0.118(03)	
5.00		0.011(01)	0.045(02)	0.046(02)	0.048(02)	

between the exact results for the 4×4 lattice and the variational results for the same lattice is small, i.e., the variational ansatz is quite accurate, as previously mentioned (Table II); it is noteworthy that in general such a difference is small compared to the difference between the variational results for the 4×4 and the 16×16 lattice. This gives an estimate of the magnitude of the finite-size effects on the 4×4 lattice.

Another observable quantity of interest is the spectral weight, which we also computed using our variational state. Let us define the spectral weight as

$$Z_{n,\mathbf{k}} = | < \Psi_{n,\mathbf{k}} | \hat{c}_{\mathbf{k},s} | \Phi > |^2 , \qquad (14)$$

where $|\Psi_{n,\mathbf{k}}>$ is the exact normalized nth eigenstate of the $(N-1)$-particle system (single hole) with momentum $\mathbf{k}$, and $|\Phi>$ is the exact normalized ground state of the N-particle (no-hole) system. $Z_{n,\mathbf{k}}$ is the residue of pole of the hole Green's function corresponding to the nth eigenstate of the $(N-1)$-particle system for the given value of $\mathbf{k}$. The sum of the residues of all quasiparticle peaks for a specific value of $\mathbf{k}$ is equal to one ($\sum_n Z_{n,\mathbf{k}} = 1$). In our calculation $|\Phi>$ is approximated by the state (6) and we study the spectral weight of the lowest single-hole eigenstate with the state $|\Psi^{\mathrm{II}}_{\mathbf{k}}>$ with the optimal values of the variational parameters.

In Table IV we report our results for the spectral weight Z of the quasihole state, computed by Monte Carlo. In Fig. 2 we compare the spectral weight at $\mathbf{k} = (\pi/2, \pi/2)$, calculated on a 4×4 lattice with the trial states Ψ^{I} (squares) and Ψ^{II} (open circles), with exact diagonalization results, from Ref. 11 (solid line). At small values of t/J (~ 0.2) the spectral weight computed with the state Ψ^{I} is closer to the exact one than the one computed with the state Ψ^{II}; notice that in this range of t/J the energy estimate is the same for the two states, within statistical error bars. For larger values of t/J (> 0.5) the state Ψ^{II} gives a much better estimate of the spectral weight, in good agreement with exact diagonalization results up to $t/J \sim 2.5$; at $t/J = 5$ the spectral weight is overestimated by roughly 30%. Our results at $\mathbf{k} = (0,0)$ clearly indicate that the residue of the quasiparticle peak falls off at large t/J, in agreement with other calculations.[7,11] We obtained the extrapolated values for the infinite lattice by assuming the scaling law $Z_L = Z_\infty + \beta_{\mathbf{k}}/L$; at $\mathbf{k} = (0,0)$ the spectral weight results are, within our statistical error bars, insensitive to the lattice size for $t/J \geq 1$. The results for the spectral weight provide a possible explanation for the better agreement with exact results for the hole energy we find at $\mathbf{k} = (\pi/2, \pi/2)$ than at $\mathbf{k} = (0,0)$. Because we construct our trial state $|\Psi^{\mathrm{II}}_{\mathbf{k}}>$ by acting with the operator $\hat{F}(\mathbf{k})\,\hat{U}$ on the "bare" hole state $\hat{c}_{\mathbf{k},s}|\Phi>$, it is reasonable to assume that the variational state $|\Psi^{\mathrm{II}}_{\mathbf{k}}>$ will be more accurate for those values of $\mathbf{k}$ for which the initial overlap

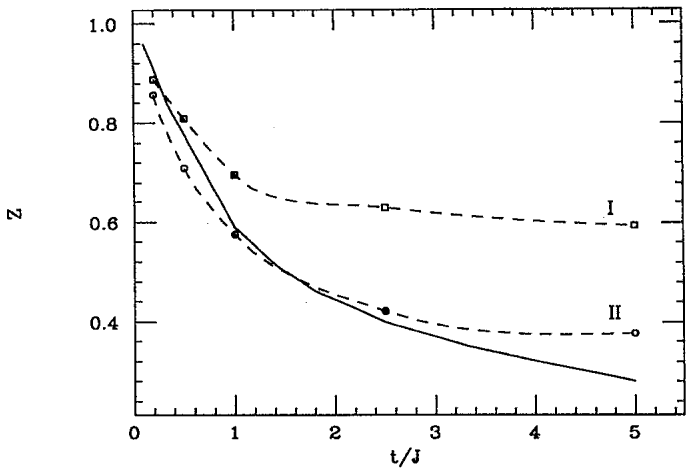

FIG. 2. Comparison between the ground-state spectral weight computed on a 4×4 lattice at $\mathbf{k} = (\pi/2, \pi/2)$ by exact diagonalization (solid line) and with the variational states Ψ^{I} (squares joined by a dashed line labeled I) and Ψ^{II} (open circles joined by a dashed line labeled II).

of the bare state with the exact state is larger. We therefore believe that a more complex form of $\hat{F}(\mathbf{k})$, including strings longer than two sites, is needed in order to obtain the same accuracy at $\mathbf{k} = (0,0)$, since the overlap of the exact state with the bare hole state is much smaller than at $\mathbf{k} = (\pi/2, \pi/2)$. At $\mathbf{k} = (0,0)$ the lowest-energy peak in the spectral function has very small spectral weight and the main peak occurs at higher energy.

In conclusion, we carried out a variational calculation for a single hole in the 2D t-J model. We obtained a variational ansatz which includes spin-spin and up to three-body spin-hole correlations; the latter describe "strings" of spins displaced by one site along the hole path. The trial state is aimed at describing an intermediate range of t/J, where the time scales for hole-hopping and background spin fluctuations are comparable and thus spin fluctuations play the role of removing the damage due to the hole motion and restoring the original background configuration. As we discussed, however, such a state can also give good variational estimates in the low t/J limit. We obtained very accurate results for the hole energy at $\mathbf{k} = (\pi/2, \pi/2)$, where the hole band is found to attain its minimum, over the range $0 < t/J < 5$. This range includes part of the so-called physical regime of the t-J model.

ACKNOWLEDGMENT

This work was supported by the Supercomputer Computations Research Institute, which is partially funded by the U.S. Department of Energy under Contract No. DE-FC05-85ER-250000.

[1] P. W. Anderson, Science **235**, 1196 (1987).
[2] F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).
[3] E. Manousakis, Rev. Mod. Phys. **63**, 1 (1991), and references therein.
[4] B. Shraiman and E. Siggia, Phys. Rev. Lett. **60**, 740 (1988).
[5] B. Shraiman and E. Siggia, Phys. Rev. Lett. **61**, 467 (1988).
[6] C. Kane, P. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989); C. Gros and M. D. Johnson, *ibid.* **40**, 9423 (1989).
[7] Z. Liu and E. Manousakis, Phys. Rev. B **44**, 2414 (1991).
[8] S. A. Trugman, Phys. Rev. B **37**, 1597 (1988); S. Sachdev,

ibid. **39**, 12 232 (1989); R. Shankar, Phys. Rev. Lett. **63**, 203 (1989).
[9] J. M. F. Gunn and B. D. Simons, Phys. Rev. B **42**, 4370 (1990).
[10] E. Kaxiras and E. Manousakis, Phys. Rev. B **38**, 866 (1988); J. A. Riera and A. P. Young, *ibid.* **39**, 9697 (1989); V. Elser, D. A. Huse, B. Shraiman, and E. Siggia, *ibid.* **41**, 6715 (1990); D. Poilblanc and E. Dagotto, *ibid.* **42**, 4861 (1990).
[11] E. Dagotto, R. Joynt, A. Moreo, S. Bacci, and E. Gagliano, Phys. Rev. B **41**, 9049 (1990).
[12] T. Itoh, M. Arai, and T. Fujiwara, Phys. Rev. B **42**, 4834 (1990).
[13] M. Boninsegni and E. Manousakis, Phys. Rev. B **43**, 10 353 (1991).
[14] R. P. Feynman, Phys. Rev. **94**, 262 (1954); R. P. Feynman and M. Cohen, *ibid.* **102**, 1189 (1956).
[15] Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[16] W. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[17] W. Marshall, Proc. R. Soc. London, Ser. A **232**, 48 (1955).
[18] E. Manousakis, Phys. Rev. B **40**, 4904 (1989); Z. Liu and E. Manousakis, *ibid.* **40**, 11 437 (1989).
[19] D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988).
[20] N. Trivedi and D. M. Ceperley, Phys. Rev. B **40**, 2747 (1989).
[21] T. Barnes and M. D. Kovarik, Phys. Rev. B **42**, 6159 (1990).