Quasiparticle structure and coherent propagation in the $t - J_z - J_\perp$ model

Junwu Gan and Per Hedegård

Department of Physics, University of California, Berkeley, CA 94720.

Numerical studies, from variational calculation to exact diagonalization, all indicate that the quasiparticle generated by introducing one hole into a two-dimensional quantum antiferromagnet has the same nature as a string state in the $t - J_z$ model. Based on this observation, we attempt to visualize the quasiparticle formation and subsequent coherent propagation at low energy by studying the generalized $t - J_z - J_\perp$ model in which we first diagonalize the $t - J_z$ model and then perform a degenerate perturbation in $J_\perp$. We construct the quasiparticle state and derive an effective Hamiltonian describing the coherent propagation of the quasiparticle and its interaction with the spin wave excitations in the presence of the Néel order. We expect that qualitative properties of the quasiparticle remain intact when analytically continuing $J_\perp$ from the anisotropic $J_\perp < J_z$ to the isotropic $J_\perp = J_z$ limit, despite the fact that the spin wave excitations change from gapful to gapless. Extrapolating to $J_\perp = J_z$, our quasiparticle dispersion and spectral weight compare well with the exact numerical results for small clusters.

PACS Numbers: 74.20-z, 74.20.Mn, 71.27.+a

I. INTRODUCTION

Since the beginning of the era of high temperature superconductivity, it has been suggested that the one-band Hubbard model or the closely related $t - J$ model describing the CuO$_2$ plane may be the basic model for cuprate superconductors. While the early suggestion was based on the high energy properties of the cuprates, such as electronic structure and spectroscopy, it is remarkable that many peculiar low energy properties of the cuprates have been reproduced in exact numerical studies of the Hubbard or $t - J$ model. Thus, understanding the two-dimensional Hubbard or $t - J$ model stands out as a central problem in the field of high temperature superconductivity.

While the Hubbard and $t - J$ models at half-filling describing the insulating parent compounds are well understood by now, present understanding of the effect of doping mostly derives from numerical studies. Essentially, the numerical results can be summarized as follows: (i) Doping the two-dimensional (2D) antiferromagnet with one hole generates a quasiparticle with finite spectral weight which implies that the quasiparticle carries charge $e$ and spin $1/2$. (ii) The quasiparticle dispersion has a bandwidth of order $J$, is almost flat near $(\pi, 0)$ and $(0, \pi)$, and the general structure agrees with the recent photoemission results. (iii) The remaining spectral weight is mostly distributed in the energy range corresponding to the mid-infrared absorption universally observed in the optical experiments of the high $T_c$ cuprates. (iv) There is tentative evidence indicating that the quasiparticle band found in the one-hole case remains fairly robust under the finite doping. The latter may have already received experimental support.

In this paper, we attempt to provide an intuitive way to understand all numerical results, and derive a low-energy effective Hamiltonian for the one-hole problem. We shall also point out the extension to finite doping when the Néel order is destroyed.

The exact numerical results on the one-hole problem in small clusters suggest an adiabatic picture for the doped antiferromagnet. For the $t - J$ model with $t \gg J$, the hole hopping takes place at a typical time scale of $1/t$ while the time scale of spin fluctuations is at least $1/J (\gg 1/t)$. When considering the hole hopping, it is reasonable to take a snapshot of the spin configuration and freeze it. When the system possesses either long range or short range antiferromagnetic correlation, a typical spin configuration also possesses the same kind of correlation. As the hole hops in two dimensions, it leaves behind a string of overturned spins along its trace. These overturned spins are energetically frustrated with their neighboring spins surrounding the trace. The energy increase due to the frustration is roughly proportional to the length of the string. Therefore, the hole is linearly confined to its original site. Due to this confinement, the hole is dressed by a cloud of local distortion of the spin configuration. The quasiparticle is just such a composite object. The formation of the quasiparticle does not require the existence of long range antiferromagnetic order. The quasiparticle should be stable as long as its size is smaller than the magnetic correlation length. It is also important to realize that the formation of the quasiparticle is a high-energy process at the scale of the hopping amplitude $t$. Exact diagonalization study of small clusters provides accurate description of the quasiparticle...
structure. At the lower-energy scale of order $J$, the physical properties of the doped antiferromagnet are described by the coherent propagation of the quasiparticle and its interaction with the spin wave excitations. It is at this lower-energy scale that an effective Hamiltonian is needed.

Our approach amounts to a degenerate perturbative treatment of the transverse spin fluctuation term $J_\perp$ of the $t-J_z-J_\perp$ model. We first construct a basis of states by diagonalizing the $t-J_z$ model. Then we project the transverse $J_\perp$ term onto the constructed basis of states and use the resulting matrix elements as an effective representation of the transverse spin fluctuation term. Previous analytical studies have concentrated on solving Bogoliubov-deGennes-type equations (summing up the noncrossing diagrams) in which the spin wave excitations are represented by Holstein-Primakoff bosons and the hole hopping term is treated as the interaction. Although the plausible argument for the “dominant-pole approximation” put forward by Kane, Lee, and Read indicated the existence of a low-energy quasiparticle, it has been found that a self-consistent solution is needed to obtain the correct features of the quasiparticle dispersion and spectral weight. The self-consistent solution can be obtained only numerically.

The advantage of our approach is the clear separation between the quasiparticle formation at high energy from the low-energy coherent propagation of the quasiparticle. The parameters in the effective Hamiltonian describing the quasiparticle propagation are evaluated directly, though approximately. Most importantly, the form of the effective Hamiltonian does not depend on the detailed calculations and is completely determined by the spin and charge quantum numbers of the quasiparticle.

The specific nature of the quasiparticle, that it is essentially same as a string state as explicitly shown by Eder and Ohta, implies that the qualitative properties of the quasiparticle remain intact when analytically continuing $J_\perp$ from the anisotropic $J_\perp < J_z$ to the isotropic limit $J_\perp = J_z$, despite the fact that the spin wave excitations change from gapful to gapless. We have evaluated the parameters of the effective Hamiltonian to first order in $J_\perp$ which is appropriate when $J_\perp \ll J_z$. Nevertheless, by taking $J_\perp = J_z$ our quasiparticle dispersion and spectral weight compare qualitatively and quantitatively well with the exact diagonalization results for the isotropic $t-J$ model. The quantitative agreement is expected to improve should our results be compared with the exact numerical results for the anisotropic $t-J_z-J_\perp$ model if available. These expectations can be critically tested.

Although the hole hopping amplitude $t$ is much larger than $J$, the bare hole hopping is localized inside the quasiparticle and the associated excitations are gapful. The true low-energy charge excitations are those corresponding to the coherent propagation of the quasiparticle. The velocity of the quasiparticle near the bottom of the quasiparticle band is much smaller than the spin wave velocity. Therefore, the spin wave excitation is not dissolved into the quasiparticle-hole continuum excitations. As a result, the low-energy spin wave excitations cannot decay by exciting the quasiparticle into a higher-energy state of the quasiparticle band. The linear dispersion of the spin excitations is preserved contrary to naive expectation based on the fact $t \gg J$.

The layout of the paper is as follows. In Sec. II, we derive the effective Hamiltonian for one hole in the antiferromagnet. In Sec. III we compare our quasiparticle dispersion and spectral weight with the exact diagonalization results in small clusters. We conclude the paper in Sec. IV.

## II. ADIABATIC DESCRIPTION OF A DOPED ANTIFERROMAGNET

In this section, we shall derive an effective Hamiltonian describing the quasiparticle motion in a doped antiferromagnet and the interaction of the quasiparticle with long wavelength spin wave excitations in the presence of Néel order. We shall first construct all low-energy eigenstates of the $t-J_z$ Hamiltonian. Then we represent the transverse Heisenberg interaction $J_\perp$ term by its matrix elements within the basis of these eigenstates of the $t-J_z$ Hamiltonian.

### A. Construction of the basis states

The $t-J$ model Hamiltonian has the form

$$H = H_0 + H_1,$$

$$H_0 = -t \sum_{<i,j>} [(1 - n_{i,-\sigma})c_{i\sigma}^\dagger c_{j\sigma}(1 - n_{j,-\sigma}) + h.c.] + J_z \sum_{<i,j>} S_i^z S_j^z, \tag{2}$$

$$H_1 = J_\perp \sum_{<i,j>} (S_i^x S_j^x + S_i^y S_j^y), \tag{3}$$

where $c_{i\sigma}^\dagger$ creates an electron at lattice site $i$ with spin $\sigma$, $n_{i,\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the electron density operator, and $S_i^\mu = \sum_{\nu\nu'} c_{i\mu}^\dagger \sigma_{\mu\nu} c_{i\nu}/2$ is the spin operator. The summation $<i,j>$ is limited to the nearest neighbor links. Unlike the Néel
state in the undoped case, the ground state of the $t - J_z$ Hamiltonian $H_0$ in the presence of one hole has macroscopic near degeneracy. These ground states can be generated by removing a spin at an arbitrary site in the Néel state and allowing the hole to hop. As the hole hops, it leaves behind a string of overturned spins. Therefore, the hole suffers a linear binding potential to its original site. The eigenstates of the hole consist of discrete bound states with energy spacing uniquely characterized by an energy scale $(J_z/t)^{2/3}$. For the purpose of deriving a low-energy effective theory, we only need to retain the ground state.

There is an excellent approximation to obtain the ground states of the $t - J_z$ Hamiltonian \[ H_0 \] The approximation amounts to neglecting winding paths (Bethe lattice approximation). We briefly describe this approximation here with some minor improvement. We shall also use slightly more concrete notations to meet our needs. The perfect classical Néel state with only one hole can be labeled by the position of the hole, $\mathbf{r}$. There are no frustrated spins in this state. Applying the hole hopping operator in $H_0$ to this state generates four new configurations, each with a string of a length of one lattice spacing, $|\mathbf{r}, \{a_i\}\rangle$, where $a$ can be one of the four unit lattice vectors $\pm \mathbf{x}$ or $\pm \mathbf{y}$, representing the hopping of the hole from $\mathbf{r}$ to $\mathbf{r} + \mathbf{a}$. From the four configurations we construct an “$s$-wave” state with string length 1,

$$|\mathbf{r}, 1\rangle = \frac{1}{2} \sum_{\mathbf{a} = \pm \mathbf{x}, \pm \mathbf{y}} |\mathbf{r}, \{\mathbf{a}\}\rangle. \quad (4)$$

Other states with longer strings are constructed similarly,

$$|\mathbf{r}, l\rangle = \frac{1}{2 \times 3^{(l-1)/2}} \sum_{\mathbf{a}_1 \cdots \mathbf{a}_l} |\mathbf{r}, \{\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_l\}\rangle, \quad (5)$$

where the summation is implicitly subject to the constraint $\mathbf{a}_i \neq -\mathbf{a}_{i-1}$ to prevent hole retracing, here and throughout the paper. The Bethe lattice approximation is to use the matrix elements within the set of states $|\mathbf{r}, l\rangle$ to represent the $t - J_z$ Hamiltonian for the corresponding subspace,

$$H_0|\mathbf{r}, 0\rangle = J_z|\mathbf{r}, 0\rangle - 2t|\mathbf{r}, 1\rangle,$$

$$H_0|\mathbf{r}, 1\rangle = \frac{5}{2} J_z|\mathbf{r}, 1\rangle - 2t|\mathbf{r}, 0\rangle - \sqrt{3} t|\mathbf{r}, 2\rangle,$$

$$H_0|\mathbf{r}, l\rangle \approx \epsilon_l|\mathbf{r}, l\rangle - \sqrt{3} t (|\mathbf{r}, l-1\rangle + |\mathbf{r}, l+1\rangle), \quad l \geq 2,$$

where

$$\epsilon_l = J_z(l, \mathbf{r}) \sum_{i,j \neq l} \left( S_i^z S_j^z + \frac{1}{4} \right) |\mathbf{r}, l\rangle. \quad (7)$$

The usage of the average energy $\epsilon_l$ slightly improves the approximation \[ (6) \] for the $t - J_z$ Hamiltonian used by Shraiman and Sigija.\[ \] In this paper, we shall directly evaluate the first few values of $\epsilon_l$ up to $l = 7$. For larger $l$ values, we shall use the extrapolation of $\epsilon_l$ from small $l$. The values of $\epsilon_l$ used in this paper are listed in Table \[ \] The extrapolation is $\epsilon_l = 2.574 - 0.0156(-1)^l - 0.7857/l + 0.6857l$. Numerically diagonalizing \[ (6) \] determines the coefficients $u_l$ in the approximate ground state of the $t - J_z$ Hamiltonian,

$$H_0|\mathbf{r}\rangle = -E_0|\mathbf{r}\rangle, \quad |\mathbf{r}\rangle = \sum_{l=0}^{\infty} u_l |\mathbf{r}, l\rangle. \quad (8)$$

There is a macroscopic number of such ground states since we can choose $\mathbf{r}$ to be any lattice site. The size of $|\mathbf{r}\rangle$ depends on $J_z/t$ ratio: The smaller the ratio, the bigger the size.

In the two-dimensional square lattice, the macroscopic degeneracy of $|\mathbf{r}\rangle$ is removed by the winding paths (so-called Trugman process)\[ ] This is reflected in the fact that the approximate ground states $|\mathbf{r}\rangle$ labeled by $\mathbf{r}$ and given by Eq. \[ (8) \] are not strictly orthogonal to each other. In the presence of Néel order, we can divide the two-dimensional square lattice into $\mathcal{A}$ and $\mathcal{B}$ sublattices. For $\mathbf{r}$ belonging to the same sublattice, there is a small overlap. An example is shown in Fig. \[ \] This configuration belongs to both $|\mathbf{r} = \mathbf{r}_0, l = 5\rangle$ and $|\mathbf{r} = \mathbf{r}_2, l = 1\rangle$ according to the prescription \[ (8) \], causing an overlap between $|\mathbf{r}_0\rangle$ and $|\mathbf{r}_2\rangle$ states. For $J_z/t = 0.3$, the overlap between $|\mathbf{r}\rangle$ and $|\mathbf{r} + \mathbf{x} + \mathbf{y}\rangle$ is 0.0049. The overlap between $|\mathbf{r}\rangle$ and $|\mathbf{r} + 2\mathbf{x}\rangle$ is 0.0019, negligible even compared to $\langle \mathbf{r}|\mathbf{r} + \mathbf{x} + \mathbf{y}\rangle$. For $\mathbf{r}$ belonging to different sublattices, any two states are orthogonal since they have different $S_{tot}^z = \sum_i S_i^z$. The small corrections due to the nonorthogonality of $|\mathbf{r}\rangle$ will be taken into account later by using tight-binding approximation to study the propagation of $|\mathbf{r}\rangle$ as a whole.
The set of states $|r\rangle$ is far from complete. One way to complement the set of states $|r\rangle$ is to include “non-s-wave” string states. Instead (6), for instance, we can form the $d$ state,

$$|r, 1\rangle_d = \frac{1}{2} (|r, \{x\}⟩ - |r, \{y\}⟩ + |r, \{-x\}⟩ - |r, \{-y\}⟩).$$

Applying the hole hopping operator in $H_0$ to (6) will generate a new set of states. Diagonalizing the $t - J_z$ Hamiltonian within the corresponding new subspace will give us new eigenstates of the $t - J_z$ Hamiltonian whose energies are about $1.5J_z$ higher than the states $|r\rangle$ given by Eq. (6). Obviously, the new eigenstates are also localized around $r$. For the same reason — the existence of the winding paths — the new eigenstates centered at $r$ are not strictly orthogonal to the “s-wave” states $|r'\rangle$ centered at a different site $r'$ in the same sublattice and not too far away from $r$. We note that if $r = r'$ there is no overlap due to the different rotational symmetries. The spin fluctuation term (6) also has nonvanishing matrix elements between the “s-wave” states $|r'\rangle$ and the new eigenstates. However, both overlaps and matrix elements are very small. Thus, these new eigenstates of the $t - J_z$ Hamiltonian generated from “non-s-wave” string configurations are almost disconnected from the subspace where the states $|r\rangle$ “live”. The “non-s-wave” states will be omitted in our low-energy effective theory.

The eigenstates of the $t - J_z$ Hamiltonian that we have discussed so far contain overturned spins only along the trace of the hole. If we neglect the winding paths, the overturned spins form a continuous string in each spin configuration. We need to complement the set of states $|r\rangle$ by including one or more isolated overturned spins outside the string. Inside the eigenstates $|r\rangle$, the hole is localized around the site $r$, and so are all the strings of overturned spins. Thus, if the isolated overturned spins are far from $r$, they will not interfere with the strings. In this case, we have simple superposition of the isolated overturned spins and the string state $|r\rangle$. More delicate situations occur when the isolated overturned spins are located close to the center site $r$ of the string state. Our goal is to find all new eigenstates of the $t - J_z$ Hamiltonian that can be connected to the string states $|r\rangle$ by applying $H_1$.

We start from a configuration with one isolated overturned spin at $r_s$ and a hole at $r$ in an otherwise perfect Néel background. We demand that a new subspace be generated by applying the hole hopping operator to this configuration and new eigenstates of the $t - J_z$ Hamiltonian be generated by diagonalizing the $t - J_z$ Hamiltonian within this new subspace. In order for $H_1$ to have nonvanishing matrix elements between the new states and the old states given by Eq. (6), the site of the hole $r$ and the site of the overturned spin $r_s$ must belong to different sublattices. Otherwise, the generated new state has $S_{\text{tot}}^z = \pm 3/2$ and cannot be connected to the states (6) by $H_1$ since the states (6) have $S_{\text{tot}}^z = \pm 1/2$. Since we require $r_s$ to be close to $r$, the first possibility is for $r_s$ to be a nearest neighbor of $r$. But this is a string of length 1 $|r_s, \{r - r_s\}\rangle$ which we have already considered. Thus, no new subspace will be generated from this configuration. The next possibility is for $r_s$ to be farther away from $r$: $r_s - r = 2x + y$ or $r_s - r = 3x$. Letting the hole hop in these configurations will generate new subspaces. In principle, we have to diagonalize the $t - J_z$ Hamiltonian within these new subspaces and keep the low-energy eigenstates. In practice, we shall do it approximately as in (6). In complete analogy with (6), we construct generalized states

$$|r_s, r, l\rangle = \frac{1}{2 \times 3^{l_1/2}} \sum |r_s, r, \{a_1, a_2, \ldots a_l\}\rangle.$$

Then we use the matrix elements of the $t - J_z$ Hamiltonian within the set of states $|r_s, r, l\rangle$ for $l = 0, 1, \cdots \infty$ as an approximate representation of the $t - J_z$ Hamiltonian. This representation has exactly the same form as (6) except for different diagonal energies $\epsilon'_l$:

$$H_0|r_s, r, 0\rangle = 3J_z|r_s, r, 0\rangle - 2t|r_s, r, 1\rangle,$n
$$H_0|r_s, r, 1\rangle = \frac{9}{2}J_z|r_s, r, 1\rangle - 2t|r_s, r, 0\rangle - \sqrt{3}t|r_s, r, 2\rangle,$$ (11)
$$H_0|r_s, r, l\rangle \simeq \epsilon'_l|r_s, r, l\rangle - \sqrt{3}t (|r_s, r, l - 1\rangle + |r_s, r, l + 1\rangle), \quad l \geq 2,$$}

where

$$\epsilon'_l = J_z \langle l, r, r_s \mid \sum_{<i,j>} (S_i^z S_j^z + \frac{1}{4}) \rangle |r_s, r, l\rangle.$$

The values of $\epsilon'_l$ used in this paper are also listed in Table 1. For large $l$, we use extrapolated values from $\epsilon'_l$ listed in Table 1 in the same way as we did for $\epsilon_l$. Diagonalizing (10) gives us new approximate eigenstates

$$H_0 |r_s, r\rangle = -E_0' (r_s - r) |r_s, r\rangle,$$
$$|r_s, r\rangle = \sum_{l=0}^{\infty} u'_l (r_s - r) |r_s, r, l\rangle.$$ (13)
Following the same line of reasoning, we can construct further approximate eigenstates of the $t - J_z$ Hamiltonian. A straightforward extension is to consider $r_s$ being further away from $r$, for instance, $r_s - r = 5x, 4x + y$, or $3x + 2y$. Since in the realistic situation $J/t = 0.2 \sim 0.4$, the size of the string state $|\langle r \rangle|$ is limited within $l \leq 5$ inside $[4]$. Therefore, we can approximately treat the isolated overturned spin at $r_s$ as independent of $r$ if their separation is five or more lattice spacings. We should also try to generate new eigenstates by applying the hole hopping operator in $H_0$ to configurations with one hole and an isolated pair of neighboring overturned spins in an otherwise perfect Néel background. If the hole is a nearest neighbor of the pair of overturned spins, this is a string of length 2 that we have already considered in $[4]$. As the next possibility, the hole could be separated from the pair of overturned spins by one lattice site. One such example is shown in the upper panel of Fig. [5]. However, this configuration again has already appeared in $[10]$ in the $l = 3$ state as illustrated in the lower panel of Fig. [5]. No new eigenstates of the $t - J_z$ Hamiltonian can be generated from this configuration. Thus, we only need to consider configurations in which the hole is separated from the pair of overturned spins by two or more lattice sites. In this paper we shall neglect the correlation between the hole hopping and the pair of overturned spins in this kind of configurations. Later we shall see that what we have neglected are the interaction vertices with four operators, two quasiparticle and two magnon operators.

B. Derivation of the effective Hamiltonian

To obtain the low-energy effective Hamiltonian, we identify the many-body state $|r\rangle$ with a quasiparticle located at site $r$. It is obvious that the quasiparticle carries charge $e$ and spin $1/2$ as a hole because there is local deficiency of both charge and spin. Furthermore, the quasiparticle spin points in the opposite directions for $r$ belonging to different sublattices. Thus we introduce a fermionic operator $f_{r, \sigma}$ to create the state $|r\rangle$ from the Néel background. In the Néel state, we divide the square lattice into $A$ and $B$ sublattices and assume that the spins in the $A$ sublattice point in the up direction. If $r \in A$, then the quasiparticle spin is down. We shall approximate $|r_s, r\rangle \simeq S^z_{r_s} f_{r, \uparrow}^\dagger |\text{Néel}\rangle$ for $r \in A$ and $r_s \in B$. Using the Holstein-Primakoff representation of the spin operator; $S^z_{r_s} \simeq b_{r_s, 1}^\dagger$ for $i \in A$ and $S^z_{r} \simeq b_{r_s, 2}^\dagger$ for $i \in B$, we can write

$$|r_s, r\rangle \simeq b_{r_s, 2}^\dagger f_{r, \uparrow}^\dagger |\text{Néel}\rangle \quad \text{for } r \in A, \ r_s \in B. \quad (14)$$

The expression for $r \in B$ and $r_s \in A$ is similar. The correlation between the hole hopping and the overturned spin at $r_s$ lowers the energy of the state $|r_s, r\rangle$ with respect to that of two independent $b_{r_s, 2}^\dagger$ and $f_{r, \uparrow}^\dagger$. This energy difference amounts to an interaction vertex of the type $f_{r, \uparrow}^\dagger f_{r, \sigma} b_{r_s, \sigma}^\dagger b_{r_s, \uparrow}$. In this paper, we shall neglect all interaction vertices with four operators and assume that their effects can be properly accounted for by small renormalization of the parameters in the effective Hamiltonian. This is supported by the fact that quantum fluctuations only generate a small density of overturned spins in the ground state of the 2D Heisenberg antiferromagnet.

We have pointed out that the essential difference from the undoped case lies in the macroscopic near degeneracy of the ground states of the $t - J_z$ Hamiltonian. The transverse spin fluctuation $J_\perp$ term in the $t - J_z - J_\perp$ Hamiltonian lifts this degeneracy and generates quasiparticle dispersion. Therefore, only degenerate perturbation in $J_\perp$ is permitted even for $J_\perp \ll J_z$. In the following we shall represent the transverse term $[3]$ by its matrix elements within the basis of the eigenstates of the $t - J_z$ Hamiltonian that we have constructed in the previous subsection. A typical example illustrating how the spin fluctuations generate quasiparticle hopping is shown in Fig. [4]. Exchanging the first two spins on a string cuts off its length by two lattice units. Since the location of the quasiparticle is determined by the common starting point of the strings inside $[3]$ and $[8]$, this process moves the quasiparticle to a nearby site in the same sublattice. Similarly, exchanging two spins near the starting point but outside a string increases the string length by two lattice units and also generates quasiparticle hopping. We note that a quasiparticle cannot hop to the other sublattice simply because the quasiparticle spin directions are opposite in different sublattices. To obtain the effective hopping amplitude of the quasiparticle, we construct the propagating quasiparticle state

$$|k\rangle = \frac{1}{\sqrt{N_k}} \sum_{r \in A} \exp(i \mathbf{k} \cdot \mathbf{r}) |r\rangle, \quad (15)$$

where $1/\sqrt{N_k}$ is the normalization factor. Then we calculate the quasiparticle dispersion according to the tight-binding approximation $[2]$

$$\epsilon_k = \frac{1}{N_k} (k H |k\rangle, \quad (16)$$
where $H$ is the full $t - J$ Hamiltonian. Using the fact that the string state $| \mathbf{r} \rangle$ is an exact eigenstate of the Hamiltonian

$$H_{r} = -t \sum_{<i,j>} [(1 - n_{i,-\sigma})c_{i\sigma}^{\dagger}c_{j\sigma}(1 - n_{j,-\sigma}) + \text{h.c.}] + \sum_{l} \epsilon_{l} | r, l \rangle \langle r, l |,$$

we can rewrite

$$\epsilon_{k} = \text{const} + \frac{1}{N_{k}} \sum_{\mathbf{R}\in\mathcal{A}} \exp(ik\mathbf{R}) \langle \mathbf{r} + \mathbf{R} | H - H_{r} | \mathbf{r} \rangle.$$

The normalization factor can be expanded in a power series,

$$\frac{1}{N_{k}} \simeq 1 - 4 \langle \mathbf{r} + \mathbf{x} + \mathbf{y} | \mathbf{r} \rangle \cos k_{x} \cos k_{y}.$$

For $J_{z}/t = 0.2$, 0.3, 0.4, 0.5, and 0.6, we have found $\langle \mathbf{r} + \mathbf{x} + \mathbf{y} | \mathbf{r} \rangle = 0.065$, 0.041, 0.027, 0.018, and 0.012 respectively. The direct overlap $\langle \mathbf{r} + 2\mathbf{x} | \mathbf{r} \rangle$ is neglected in (19) because it is too small even compared to $\langle \mathbf{r} + \mathbf{x} + \mathbf{y} | \mathbf{r} \rangle$. Similarly, the matrix element $\langle \mathbf{r} + 2\mathbf{x} | (J_{z} \sum_{<i,j>} S_{i}^{x} S_{j}^{y} - \sum_{l} \epsilon_{l} | r, l \rangle \langle r, l |) | r \rangle$, which appears in the calculation of Eq. (18), can also be neglected because the nonvanishing contributions to this matrix element have the same origin as in the direct overlap $\langle \mathbf{r} + 2\mathbf{x} | \mathbf{r} \rangle$. After some straightforward algebra, we obtain from Eq. (18)

$$\epsilon_{k} = \text{const} + 4 \alpha_{1} \cos k_{x} \cos k_{y} + 2 \alpha_{2} (\cos 2k_{x} + \cos 2k_{y}) + \mathcal{O}(\cos k_{x} \cos 3k_{y}, \cos 2k_{x} \cos 2k_{y}),$$

where the high order trigonometric functions corresponding to longer range quasiparticle hopping are neglected. The coefficients in the dispersion are given by

$$\alpha_{1} = \langle \mathbf{r} + \mathbf{x} + \mathbf{y} | H - H_{r} | \mathbf{r} \rangle - \langle \mathbf{r} | H_{1} | \mathbf{r} \rangle + \langle \mathbf{r} + 2\mathbf{x} | H_{1} | \mathbf{r} \rangle \langle \mathbf{r} + \mathbf{x} + \mathbf{y} | \mathbf{r} \rangle,$$

$$\alpha_{2} = \langle \mathbf{r} + 2\mathbf{x} | H_{1} | \mathbf{r} \rangle - 2 \langle \mathbf{r} + \mathbf{x} + \mathbf{y} | \mathbf{r} + \mathbf{x} + \mathbf{y} | H - H_{r} | \mathbf{r} \rangle.$$

This quasiparticle dispersion can be described by a tight-binding Hamiltonian

$$H_{f} = \frac{1}{2} \sum_{\mathbf{r} \in \mathcal{A}, \sigma = \pm} \left[ \alpha_{1} \sum_{a = \pm x, \pm y} + \alpha_{2} \sum_{a = \pm 2x, \pm 2y} \right] (f_{r,\sigma}^{\dagger} f_{r+a,\sigma} + \text{h.c.}),$$

where $\mathbf{r} \in \mathcal{A}$ denotes summation over only one sublattice. The summation over $\mathcal{A}$ and $\mathcal{B}$ sublattices is converted into the spin index $\sigma$ summation.

To obtain the coefficients $\alpha_{1}$ and $\alpha_{2}$, we need to calculate the matrix elements of the type $\langle \mathbf{r}_{2} | \hat{O} | \mathbf{r}_{1} \rangle$ for several different operators $\hat{O}$. We employ the following approximation when calculating these matrix elements: $\langle \mathbf{r}_{2} | \hat{O} | \mathbf{r}_{1} \rangle = \sum_{l_{1} + l_{2} \leq 10} u_{l_{1}} u_{l_{2}} (\mathbf{r}_{2}, l_{2}) | \hat{O} | \mathbf{r}_{1}, l_{1} \rangle$. Each matrix element in the sum is then computed straightforwardly. By investigating how fast the eigenvector $u_{l}$ decreases as a function of the string length, one can be convinced that the approximation $l_{1} + l_{2} \leq 10$ is sufficient for $J_{z}/t \geq 0.2$. The values of $\alpha_{1}$ and $\alpha_{2}$ for different $J_{z}/t$ ratios are listed in Table II.

The spin fluctuation term $H_{1}$ exchanges two neighboring spins. For most cases, this pair of exchanged spins is far away from the hole. If so, the situation is completely same as in the undoped case. Thus, the Hamiltonian describing long wavelength spin excitations using the Holstein-Primakoff bosons has the familiar form $^{21}$ upon neglecting the spin wave interactions,

$$H_{b} = 2J_{z} \left[ \sum_{i \in \mathcal{A}} b_{i,1}^{\dagger} b_{i,1} + \sum_{i \in \mathcal{B}} b_{i,2}^{\dagger} b_{i,2} \right] + \frac{J_{z}}{2} \sum_{i \in \mathcal{A}, a = \pm x, \pm y} \left( b_{i,1}^{\dagger} b_{i+a,2}^{\dagger} b_{i,1} b_{i+a,2} + b_{i,1} b_{i+a,2} \right).$$

In principle, the summation over the nearest neighbors in (24) should avoid a small region surrounding the hole to prevent double counting. However, this restriction only results in interaction vertices involving four operators of the type $f^{\dagger} f b^{\dagger} b$ or $f^{\dagger} f b b^{\dagger}$. These interactions are neglected in this paper. Physically, these interactions occur because the quasiparticle has a finite spatial extent of a few lattice spacing. But for long wavelength spin excitations the quasiparticle can be viewed as a point particle.

The spin fluctuation term $H_{1}$ also connects the states given by Eqs. (3) and (13). A typical example is shown in Fig. II. This process allows the quasiparticle to jump over two sites, leaving behind an isolated overturned spin. We directly evaluate the following two overlap coefficients:
\[
\lambda_1(J_z/t) = \frac{1}{J_z} \langle r | H_1 | r, r + 2x + y \rangle,
\]
\[
\lambda_2(J_z/t) = \frac{1}{J_z} \langle r | H_1 | r, r + 3x \rangle.
\]  

The nonorthogonality of the approximate eigenstates \(|r\rangle\) has a negligible effect on the coefficients \(\lambda_1\) and \(\lambda_2\). The results are also listed in Table I. The corresponding part of the effective Hamiltonian is, using Eq. (14),

\[
H_{eff} = H_f + H_b + H_{fb}.
\]

Since inside \(H_{eff}\) the lattice site summation only extends within one sublattice, the corresponding momentum summation should be limited within the antiferromagnetic Brillouin zone (AFBZ). This is due to the presence of the Néel order which breaks the symmetry between the two sublattices. In the momentum space, the three parts of \(H_{eff}\) have the following forms:

\[
H_f = \sum_{\mathbf{k} \in \text{AFBZ}, \sigma = \pm} \epsilon_\mathbf{k} f^\dagger_{\mathbf{k}, \sigma} f_{\mathbf{k}, \sigma},
\]

\[
H_b = \sum_{\mathbf{q} \in \text{AFBZ}} \left[ 2J_z b^\dagger_{\mathbf{q},1} b_{\mathbf{q},1} + J_\perp (\cos q_x + \cos q_y) \left( b^\dagger_{\mathbf{q},2} b_{\mathbf{q},2} + b^\dagger_{\mathbf{q},1} b_{\mathbf{q},1} \right) \right],
\]

\[
H_{fb} = \frac{1}{N} \sum_{\mathbf{k}, \mathbf{q} \in \text{AFBZ}} \lambda_\mathbf{k} \left[ f^\dagger_{\mathbf{k}+\mathbf{q}, \sigma} b^\dagger_{\mathbf{q},1} + f^\dagger_{\mathbf{k}, \sigma} b_{\mathbf{q},1} + h.c. \right],
\]

where \(N\) is the number of sites of one sublattice. The quasiparticle-magnon interaction vertex is given by

\[
\lambda_\mathbf{k} = 2J_\perp \left[ 2\lambda_1 (\cos 2k_x \cos k_y + \cos k_x \cos 2k_y) + \lambda_2 (\cos 3k_x + \cos 3k_y) \right].
\]

The dispersion \(\epsilon_\mathbf{k}\) is given by Eq. (20).

### III. QUASIPARTICLE PROPERTIES

The quasiparticle dispersion parametrized by \(\alpha_1\) and \(\alpha_2\) (see Table I) correctly captures all qualitative features found in the numerical studies of the \(\ell - J\) model with one hole. These include (i) the right magnitude of band width given by \(4(\alpha_1 + 2\alpha_2)\) (ii) the tight-binding dispersion of the same-sublattice hopping type with the bottom of the band at \((\pi/2, \pi/2)\), and (iii) the small energy difference between the quasiparticle energies at the momenta \((\pi/2, \pi/2)\) and \((\pi, 0)\). This small energy difference results from the closeness between the values \(\alpha_1\) and \(2\alpha_2\).

In our approach, this is due to the fact that a quasiparticle can hop from the site \(r\) to \(r + x + y\) by exchanging spins either between the sites \(r\) and \(r + x\) or between \(r\) and \(r + y\). In contrast, the two spins on the sites \(r\) and \(r + x\) must be exchanged in order to move the quasiparticle from \(r\) to \(r + 2x\) as illustrated in Fig. 3. Taking \(t = 1\) and \(J_\perp = J_z = 0.4\) as an example, our dispersion is given by \(\epsilon_\mathbf{k} = 0.387 \cos k_x \cos k_y + 0.110(\cos 2k_x + \cos 2k_y)\). This is to be compared with \(\epsilon_\mathbf{k} = 0.34 \cos k_x \cos k_y + 0.13(\cos 2k_x + \cos 2k_y)\) reported in the literature.

From Table I and by setting \(J_\perp = 0\), we notice that the quasiparticle has a small dispersion compared to the \(\ell - J_z\) model and the minimum of the band is located at \(\mathbf{k} = (0, 0)\), in agreement with the previous result.

The quasiparticle spectral weight is determined by the overlap between a propagating bare hole and the quasiparticle wave function \(|\mathbf{k}\rangle\). From Eqs. (13) and (8), it is simply given by \(u^2_{2}/N_k\). For different \(t/J_z\) ratios, the quasiparticle spectral weight at the bottom of the band \((\pi/2, \pi/2)\) is listed in Table II. Within our first order degenerate perturbation in \(J_\perp\), the effect of the spin fluctuations on the internal structure of the quasiparticle is not included. The consequence is that the quasiparticle spectral weight only depends on \(J_z/t\). In the exact diagonalization study of the isotropic...
describing a string state spins. Recently, Eder and Ohta calculated the one-particle spectral function using a composite operator precisely variational calculation is that the elementary excitations can be described by a hole dressed with strings of overturned 5 the quasiparticle has the same nature as a string state. Evidence supporting this picture is abundant from early 6 the bare hole. The size of the spin bag is reduced when 7 the quasiparticle operator can be constructed at least conceptually. 8 the composite operator one will presumably reach a point where only the quasiparticle peak is left. Thus, an exact 9 peak is greatly enhanced while the incoherent part is suppressed when the composite operator is used instead of 10 will postpone the detailed discussion of this question to another publication.

Besides the effect of the quantum spin fluctuations on the quasiparticle structure, the quasiparticle motion also suffers scattering from the spin wave excitations due to the interaction terms in \( H_{fb} \). However, the second order corrections to the quasiparticle dispersion and spectral weight usually does not exceed a few percent if we use the values \( \lambda_1 \) and \( \lambda_2 \) listed in Table I. This is most due to the fact that the vertex \( \lambda_k \) given by (32) vanishes around the bottom of the band. To the accuracy of applying the first order degenerate perturbation to the isotropic \( t-J \) model, these corrections can be neglected. Strictly speaking, the spin wave excitations can mediate long range interactions between quasiparticles in the presence of Néel order. However, for the interaction vertex given by \( \lambda_k \) the disorder in real materials should localize the quasiparticles before the effect of the long range interactions becomes significant. For completeness, we include the expression for the second order self-energy of the quasiparticle here. For the one-hole problem with \( J_z = J_\perp = J \), we found

\[
\Sigma(k, i\omega_n) = \frac{1}{2N} \sum_{q \in AF BZ} \frac{\lambda_{k+q}^2 + J\lambda_{k+q}[2\lambda_{k+q} - \lambda_k(\cos q_x + \cos q_y)]/\omega_q}{i\omega_n - \omega_q - \epsilon_{k+q}},
\]

(33)

where \( \omega_n = (2n+1)\pi T \) is the Matsubara frequency and \( \omega_q = 2J\sqrt{1 - (\cos q_x + \cos q_y)^2}/4 \). We note that for the one-hole problem the chemical potential \( \mu \) is chosen such that \( \epsilon_k \geq 0 \) for all \( k \).

IV. CONCLUSION

We have developed a degenerate perturbative treatment of the \( t-J_z-J_\perp \) model based on the observation that the quasiparticle has the same nature as a string state. Evidence supporting this picture is abundant from early variational calculations 6 to the more recent exact diagonalization studies 22. A prerequisite for the success of the variational calculation is that the elementary excitations can be described by a hole dressed with strings of overturned spins. Recently, Eder and Ohta calculated the one-particle spectral function using a composite operator precisely describing a string state \( |r \rangle \) given by (8) except with optimized coefficients \( u_l \). They found that the quasiparticle peak is greatly enhanced while the incoherent part is suppressed when the composite operator is used instead of the bare hole operator. This unambiguously reveals the nature of the quasiparticle since by progressively improving the composite operator one will presumably reach a point where only the quasiparticle peak is left. Thus, an exact quasiparticle operator can be constructed at least conceptually.

Is the quasiparticle discussed in this paper related to the so-called spin bag, introduced by Schrieffer et al. 32 We will postpone the detailed discussion of this question to another publication. 22 The original spin bag was introduced in connection with the Hubbard model, and the bag is a local reduction of the Néel order parameter associated with the bare hole. The size of the spin bag is reduced when \( U \) is increased, whereas the quasiparticle of the \( t-J \) model, discussed here, is increasing in size, when \( J \) is decreased, i.e., when \( U \) is increasing. In fact, we shall argue, that in the limit of large \( U \) Hubbard model the spin bag will become the bare hole in the \( t-J \) model. We shall present a unified treatment of the Hubbard model in the future publication.

With finite doping, it is known that the long range antiferromagnetic order is destroyed. If the quasiparticle is still formed and stable, the propagation of the quasiparticle will suffer frustration at the length scale of the magnetic correlation length because of the fluctuations of the local spin directions. Traveling along a closed path, the quasiparticle will pick up a Berry phase, resulting in a loss of phase coherence. These issues will also be discussed in the future publication.
ACKNOWLEDGMENTS

The authors acknowledge useful discussions with Dung-Hai Lee and thank D. Poilblanc for providing the exact diagonalization results used for comparison in Table I.

* Permanent address: Ørsted Laboratory, Niels Bohr Institute, Universitetsparken 5, DK-2100 Copenhagen, Denmark. Email: hedegard@fys.ku.dk.

1. P. W. Anderson, Science 235, 1196 (1987).
2. F. C. Zhang and T. M. Rice, Phys. Rev. B37, 3759 (1988).
3. E. Dagotto, Rev. Mod. Phys. 66, 763 (1994), and references therein.
4. S. Chakravarty, B. I. Halperin, and D. R. Nelson, Phys. Rev. B39, 2344 (1989).
5. S. A. Trugman, Phys. Rev. B37, 1597 (1988).
6. S. A. Trugman, Phys. Rev. B41, 892 (1990).
7. E. Dagotto, R. Joynt, A. Moreo, S. Bacci and E. Gagliano, Phys. Rev. B41, 9049 (1990).
8. Z. Liu and E. Manousakis, Phys. Rev. B45, 2425 (1992); ibid. B51, 3156 (1995).
9. D. Poilblanc, H. J. Schulz, and T. Ziman, Phys. Rev. B47, 3268 (1993).
10. D. Poilblanc, T. Ziman, H. J. Schulz, and E. Dagotto, Phys. Rev. B47, 14267 (1993).
11. B. Su, Y. M. Li, W. Y. Lai, and L. Yu, Phys. Rev. Lett. 63, 1318 (1989).
12. S. Schmitt-Rick, C. M. Varma, and A. E. Ruckenstein, Phys. Rev. Lett. 60, 2793 (1988). F. Marsiglio, A. E. Ruckenstein, S. Schmitt-Rick, and C. M. Varma, Phys. Rev. B43, 10882 (1991).
13. T. Holstein and H. Primakoff, Phys. Rev. 58, 1098 (1940). P. W. Anderson, Phys. Rev. 86, 694 (1952).
14. R. Eder, O. Otta, and T. Shimozato, Phys. Rev. B50, 3350 (1994).
15. S. Haas, A. Moreo, and E. Dagotto, Phys. Rev. Lett. 74, 4281 (1995).
16. A. Moreo, S. Haas, A. Sandvik, and E. Dagotto, Phys. Rev. B51, 12045 (1995).
17. A. Moreo and D. Duffy, J. Low Temp. Phys. 99, 311 (1995).
18. P. Aebi, J. Osterwalder, P. Schwaller, L. Schlapbach, M. Shimoda, T. Mochiku, and K. Kadowaki, Phys. Rev. Lett. 72, 2757 (1994).
19. J. Callaway, Quantum Theory of the Solid State, section 4.5, (Academic Press, New York, 1976).
20. J. Gan, D.- H. Lee, and P. Hedegård, to be published.
TABLE I. Average energies of the string configurations of different lengths \( l \).

| \( l \) | \( \epsilon / J_z \) | \( \epsilon' / J_z \) for \( r_s - r = 2x + y \) | \( \epsilon' / J_z \) for \( r_s - r = 3x \) |
|---|---|---|---|
| 0 | 1 | 3 | 3 |
| 1 | 2.5 | 4.5 | 4.5 |
| 2 | 3.5 | 5.375 | 5.4583 |
| 3 | 4.3889 | 6.0139 | 6.2639 |
| 4 | 5.1296 | 6.7454 | 6.963 |
| 5 | 5.8704 | 7.412 | 7.6142 |
| 6 | 6.5535 | 8.0828 | 8.286 |
| 7 | 7.2531 |  | |

TABLE II. The parameters of effective Hamiltonian evaluated using the string state approximation. \( Z_h(k) \) is the quasi-particle spectral weight. The values of \( Z_h \) in the parentheses are the exact diagonalization results of the 26 site cluster at the ground state wave vector \( k^* \) for the \( t - J_z \) model from Refs. 9, 10. Note that, in Ref. 10, \( Z_h \) increases with the cluster size for the \( t - J_z \) model at \( J_z / t = 0.3 \) while \( Z_h \) at \( k^* \) decreases with the cluster size for the isotropic \( t - J \) model at \( J / t = 0.3 \).

| \( J_z / t \) | \( Z_h(\pi / 2, \pi / 2) \) | \( \alpha_1 \) | \( \alpha_2 \) | \( \lambda_1 \) | \( \lambda_2 \) |
|---|---|---|---|---|---|
| 0.2 | 0.160 (0.213) | 0.308J_+ - 0.077J_z | 0.157J_+ + 0.010J_z | 0.348 | 0.124 |
| 0.3 | 0.220 (0.285) | 0.293J_+ - 0.047J_z | 0.147J_+ + 0.004J_z | 0.297 | 0.101 |
| 0.4 | 0.275 | 0.272J_+ - 0.030J_z | 0.135J_+ + 0.002J_z | 0.253 | 0.083 |
| 0.5 | 0.324 (0.395) | 0.250J_+ - 0.020J_z | 0.124J_+ + 0.001J_z | 0.218 | 0.070 |
| 0.6 | 0.370 | 0.230J_+ - 0.013J_z | 0.114J_+ | 0.188 | 0.060 |
FIG. 1. An example with a winding path showing the nonorthogonality of the approximate ground states $|r\rangle$ of the $t - J_z$ Hamiltonian. The configuration is generated by successively moving the hole in the perfect Néel configuration through the sites 012301. But this is a configuration with a string of length 1 from site 2 to 1.
FIG. 2. The upper configuration has a hole separated from a pair of overturned spins by only one lattice site. The lower configuration has a hole separated from one isolated overturned spin by two lattice sites. Three hops of the hole in the lower configuration generate the upper configuration.
FIG. 3. This is a configuration with a string of length four starting from the site 1. Spin exchange between sites 1 and 2 transforms it to a configuration with a string of length 2 starting from site 3.
FIG. 4. Same configuration as in Fig. 3. Spin exchange between sites 2 and 3 transforms it to a configuration with a string of length 1 starting from site 4 and an isolated overturned spin at site 1.