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Spiral phase in a doped antiferromagnet

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The coherent motion of a hole in an antiferromagnetic described by the *t-J* model is discussed assuming that the spins show a spiral correlation function. The results are obtained from an ansatz for the wave function and no kind of mean-field approximation has to be made. When the resulting band is filled up for a low concentration of holes the total energy of the system can be estimated and it is found that for any finite concentration of holes a state with spiral spin configuration is energetically favorable compared to a state with Néel order.

I. INTRODUCTION

The problem of describing the motion of a hole in an antiferromagnetic has received considerable attention during the last years.[1-5] This is because one can hope to gain some insight into the nature of the carriers responsible for high-temperature superconductivity. One model Hamiltonian which is frequently studied in this context is the *t-J* Hamiltonian:[6]

$$H_{t-J}=-t\sum_{\langle i,j\rangle,\sigma}(\hat{c}^{+}_{i\sigma}\hat{c}_{j,\sigma}+\hat{c}^{\dagger}_{j,\sigma}\hat{c}_{i,\sigma})+J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ . \tag{1}$$

Here the $\mathbf{S}_i$ are the electronic spin operators, n_i is the total electron number operator at site i, and the sum over $\langle i,j\rangle$ stands for a summation over all pairs of nearest neighbors on a two-dimensional square lattice. The operators $\hat{c}^{\dagger}_{i,\sigma}$ can be expressed in terms of ordinary fermion operators as $c^{\dagger}_{i,\sigma}(1-n_{i,-\sigma})$.

One of the questions which has been raised is that of the modification of the spin correlation function due to a low concentration of holes.[7-9] There is by now general agreement that the ground state of the two-dimensional Heisenberg antiferromagnetic (HAF) has long-range antiferromagnetic order.[10,11] From the Mermin-Wagner theorem, however, one can conclude that in any finite range of energies above the ground state there must be a number of excited states of the order of the system size that do not have any long-range antiferromagnetic order. It might very well be the case that due to the introduction of mobile holes some of the these excited states are lowered in energy to the extent that the ground state with holes may have qualitatively different spin correlations than the ground state of the HAF.

If one assumes that the antiferromagnetic order in the spin system is kept fixed one can provide a simple physical picture for the coherent motion of the hole. A hole created at some site j in an antiferromagnetically ordered spin system will experience an effective potential due to the formation of "strings."[4,12] This effective potential increases roughly linear with the number of hops the hole has taken away from the place where it was created and the (localized) ground state $|\Phi_j\rangle$ can be determined by solving a one-dimensional Schrödinger equation. The *t-J* Hamiltonian however, allows for a number of processes by which the hole can "escape" from the string potential. The most important one is the truncation of the strings by the spin-flip part of the Heisenberg exchange. Other possibilities are hole hopping along a spiral path such that the hole itself can absorb the spin defects it has created[3,13] or absorb a ground-state spin fluctuation of the HAF while "emitting" another one at the same time. All these processes give rise to nonvanishing matrix elements of the *t-J* Hamiltonian between localized states $|\Phi_j\rangle,|\Phi_{j'}\rangle$ centered on neighboring sites j,j' leading to an "effective" tight-binding model.[14,15] It turns out that the energies and wave functions obtained in this way can reproduce many details of results from exact diagonalizations of small clusters[16-18] and other numerical methods[3,5] with remarkable accuracy.

This picture of hole motion can be transferred easily to a state with a different spin correlation function provided there is still something like a "string potential." This certainly the case when there is a "spiral" spin correlation as long as the wavelength of the spiral is much larger than the lattice constant and it is the purpose of this work to study this case.

II. ENERGY OF THE UNDOPED SYSTEM

We begin by defining the following two basis states at site n:

$$|\chi_n\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix} e^{-i\mathbf{q}\cdot\mathbf{R}_n/2} \\ e^{i\mathbf{q}\mathbf{R}_n/2}\end{bmatrix}, \tag{2}$$

$$|\tilde{\chi}_n\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix} e^{-i\mathbf{q}\cdot\mathbf{R}_n/2} \\ -e^{i\mathbf{q}\cdot\mathbf{R}_n/2}\end{bmatrix}. \tag{3}$$

These two states form a complete set of orthonormal states at site n. Then one obtains by straightforward algebra

$$\langle\chi_n|\mathbf{S}_n|\chi_n\rangle=\frac{1}{2}\begin{bmatrix}\cos(\mathbf{q}\cdot\mathbf{R}_n) \\ \sin(\mathbf{q}\cdot\mathbf{R}_n) \\ 0\end{bmatrix}, \tag{4}$$

$$\langle \tilde{\chi}_n | \tilde{S}_n | \tilde{\chi}_n \rangle = \frac{1}{2} \begin{pmatrix} -\cos(\mathbf{q}\cdot\mathbf{R}_n) \\ -\sin(\mathbf{q}\cdot\mathbf{R}_n) \\ 0 \end{pmatrix} , \tag{5}$$

$$\langle \chi_n | \mathbf{S}_n | \tilde{\chi}_n \rangle = \frac{1}{2} \begin{pmatrix} -i\sin(\mathbf{q}\cdot\mathbf{R}_n) \\ i\cos(\mathbf{q}\cdot\mathbf{R}_n) \\ 1 \end{pmatrix} . \tag{6}$$

To define a state with a "spiral" spin correlation function one first has to divide the lattice into two sublattices, denoted by A and B. Then one can define[20]

$$|\Phi_{\mathbf{q}}\rangle = \left[\prod_{n\in A} |\chi_n\rangle \right] \otimes \left[\prod_{m\in B} |\tilde{\chi}_m\rangle \right] . \tag{7}$$

Using Eqs. (4) and (5) one can show that

$$\langle \Phi_{\mathbf{q}} | \mathbf{S}_m \cdot \mathbf{S}_n | \Phi_{\mathbf{q}} \rangle = \frac{\sigma_{m,n}}{4} \cos[\mathbf{q}\cdot(\mathbf{R}_m - \mathbf{R}_n)] . \tag{8}$$

Here $\sigma_{m,n}$ is equal to 1 if the sites m,n belong to the same sublattice and (-1) otherwise. One can see that the state $|\Phi_{\mathbf{q}}\rangle$ has indeed a "spiral" spin correlation function and as $\mathbf{q}\rightarrow 0$ it reduces to the Néel state polarized in the x direction. In the thermodynamic limit any two states of the type (7) with different $\mathbf{q}$ are orthogonal.[20] In the following it will be assumed that $\mathbf{q}$ is nonzero but small, so that an expansion of the energy up to $|\mathbf{q}|^2$ gives meaningful results. The expectation value of the Heisenberg Hamiltonian H_H is then found to be

$$\langle \Phi_{\mathbf{q}} | H_H | \Phi_{\mathbf{q}} \rangle = -N\frac{J}{4}(\cos(q_x)+\cos(q_y)) , \tag{9}$$

where N is the number of sites in the system. If the wave vector of the spiral $\mathbf{q}$ is parametrized as follows:

$$\mathbf{q} = \begin{pmatrix} q\cos(\theta) \\ q\sin(\theta) \end{pmatrix} , \tag{10}$$

in the limit $\mathbf{q}\rightarrow 0$ one obtains the following expansion for the energy for a state with a correlation function of the type (8):

$$E_0(\mathbf{q}) = E_0(\mathbf{q}=\mathbf{0}) + N\frac{J}{4}\frac{1}{2}q^2 \tag{11}$$

which result is independent of the angle θ. The coefficient of the term proportional to q^2 is known as the spin stiffness constant and the value obtained above is just the classical one. There have been various calculations of quantum corrections[21-23] and in general a reduction to something like 70% of the classical value is obtained. Since the precise value of the spin stiffness constant is not particularly important in the arguments to be presented below one can also continue with the classical value.

III. INFLUENCE OF HOLES

Let us consider a single hole created in the state $|\Phi_{\mathbf{q}}\rangle$ at some site i. It is well known, that a hole created in the Néel state experiences an effective potential due to the formation of "strings."[12,4] If the spiral wave vector $\mathbf{q}$ is sufficiently small, one would suspect that an analogous theory can be set up for a hole hopping in the state $|\Phi_{\mathbf{q}}\rangle$. Since the hopping hole will break bonds which are "a little bit frustrated" and creates additional bonds which are only "almost frustrated" it is immediately obvious that the "string potential" will become flatter and the binding energy of the localized states will be more negative. Whereas the formation of a spiral state *per se* requires a higher energy than the ground state of the HAF, the introduction of holes lowers the energy again. If the concentration of holes is sufficiently high this may render the spiral state energetically favorable. To make this more quantitative, the first task is to calculate the dependence of the binding energy of the localized states on the spiral wave vector $\mathbf{q}$.

If one spin is removed from the lattice this results in the breaking of four bonds. The corresponding change in the expectation value of the Heisenberg part is

$$\Delta E_0(\mathbf{q}) = 2\frac{J}{4}(\cos q_x + \cos q_y) . \tag{12}$$

Let us denote a state generated by taking out the spin at site j and moving the hole ν times in "forward direction" by $|j,\nu,\mathcal{P}\rangle$. The symbol $\mathcal{P}$ denotes a set of numbers which is some way parametrize the geometry of the path the hole has taken. Then one can make the following ansatz for the localized state centered on the site j:

$$|\Phi_j\rangle = \sum_{\nu} \alpha_\nu \left[\sum_{\mathcal{P}} |j,\nu,\mathcal{P}\rangle \right] . \tag{13}$$

The inner sum in this expression runs over all different paths of length ν and the coefficients α_ν are to be determined from the requirement of minimum total energy. If for the moment the energy of the spiral state with one hole is chosen as the zero of energy one obtains the following set of equations:

$$\begin{aligned} -zt\alpha_1 &= E_B(\mathbf{q})\alpha_0 , \\ -t[(z-1)\alpha_{\nu+1}+\alpha_{\nu-1}] &= [E_B(\mathbf{q})-V_\nu]\alpha_\nu . \end{aligned} \tag{14}$$

Here z denotes the number of nearest neighbors (i.e., $z=4$) and $E_B(\mathbf{q})$ is the "binding energy" of the localized state $|\Phi_j\rangle$. The "potential" V_ν is defined by

$$V_\nu = \frac{1}{z(z-1)^{\nu-1}} \sum_{\mathcal{P}} \langle j,\nu,\mathcal{P}|H|j,\nu,\mathcal{P}\rangle . \tag{15}$$

In the Néel state these equations are just the ones derived previously by Shraiman and Siggia.[8] Let us now calculate the quantity V_ν. Obviously in the first hop away from the site j the hole will break three "almost antiparallel aligned" bonds. The corresponding change in the expectation value of the Heisenberg part is given by

$$\frac{J}{4}(2\cos q_y + \cos q_x) . \tag{16}$$

Here it is assumed that the hole has been moved in the x direction. In the same process three "almost frustrated" bonds are generated resulting in an additional change in energy of

$$\frac{J}{4}[\cos 2q_x+\cos(q_x+q_y)+\cos(q_x-q_y)]\ . \tag{17}$$

After averaging over the four possible paths of length one, it is found that

$$V_1=\frac{J}{4}[\tfrac{3}{2}(\cos q_x+\cos q_y] +\tfrac{1}{2}[\cos 2q_x+\cos 2q_y)+\cos(q_x+q_y) +\cos(q_x-q_y)]\ . \tag{18}$$

In an analogous way one obtains

$$V_2=V_1+\frac{J}{4}[\cos q_x+\cos q_y+\cos(q_x+q_y) +\cos(q_x-q_y)] \tag{19}$$

and similar expressions for the other V's. Once the expansion coefficients α are known for the Néel state [e.g., from a numerical solution of Eqs. (14)] the shift in ground-state energy for small but finite vectors $\mathbf{q}$ can be found by perturbation theory:

$$E_B(\mathbf{q})=E_B(\mathbf{q}=0)+z\sum_{\nu=1}^{\infty}(z-1)^{\nu-1}\alpha_\nu^2[V_\nu(\mathbf{q}) -V_\nu(\mathbf{q}=0)]\ . \tag{20}$$

Using the parametrization (10) of $\mathbf{q}$ one finds

$$\epsilon=-\left.\frac{\partial^2\Delta E_B}{\partial q^2}\right|_{q=0} \sim -z\sum_{\nu=1}^{\infty}(z-1)^{\nu-1}\alpha_\nu^2\frac{\partial^2 V_\nu(\mathbf{q})}{\partial q^2}\ . \tag{21}$$

The quantity ϵ which is defined by the above equations can be evaluated numerically once the derivatives of the potential V_ν are known. From Eqs. (18) and (19) one obtains

$$\frac{\partial^2 V_\nu(\mathbf{q})}{\partial q^2}=-\frac{J}{4}[\tfrac{11}{2}+3(\nu-1)]\ . \tag{22}$$

Again this result is independent of the angle θ. It should be noted that whereas the expression (21) for the second derivative of the binding energy with respect to q is only an approximation, the fact that the first derivative vanishes follows rigorously from the Hellman-Feynman theorem.

IV. HOLE MOTION

Having thus constructed localized states one can proceed to evaluate the dispersion relation for coherent motion of the hole. In a state with antiferromagnetic order of the spins the hole can propagate because the transverse part of the Heisenberg exchange can truncate the "strings" thus shifting their "starting point" to a second or third nearest neighbor.[2,24] Thus there will be nonvanishing matrix elements of the t-J Hamiltonian between localized states centered on second or third nearest neighbors which can be expressed in terms of the expansion coefficients α_ν.[14,15] Let us try to set up an analogous theory for a state with a "spiral" spin correlation function. One can make the following ansatz for a Bloch-type wave function:

$$|\Psi(\mathbf{k})\rangle=\frac{1}{\sqrt{N}}\sum_j e^{i\mathbf{k}\cdot\mathbf{R}_j}|\Phi_j\rangle\ . \tag{23}$$

The dispersion relation for coherent motion can be obtained from the following ansatz:

$$E(\mathbf{k})=\frac{\langle\Psi(\mathbf{k})|H_{t-J}|\Psi(\mathbf{k})\rangle}{\langle\Psi(\mathbf{k})|\Psi(\mathbf{k})\rangle}\ . \tag{24}$$

To evaluate this expression one needs to know the quantities

$$n_\delta=\langle\Phi_{j+\delta}|\Phi_j\rangle\ , \tag{25}$$

$$h_\delta=\langle\Phi_{j+\delta}|H_{t-J}|\Phi_j\rangle\ , \tag{26}$$

which are actually independent of the site j. Let us first concentrate on the overlap integrals n_δ. One can assume that the states $|\Phi_j\rangle$ are normalized i.e., $n_{\delta=0}=1$. Making use of the expansion (13) one realizes that for $\delta\neq 0$ one needs the scalar products of individual "string states" with a different starting point:

$$\langle j',\nu',\mathcal{P}'|j,\nu,\mathcal{P}\rangle\ . \tag{27}$$

Strictly speaking for $\mathbf{q}\neq 0$ the only condition for such a scalar product to be different from zero is that the hole must sit on the same site in both states. However, the value will be proportional to rather high powers of q unless certain requirements are fulfilled. Let us assume that $\nu'>\nu$. Then the largest contribution to the overlap integral will come from those paths where the "string" in $|j',\nu',\mathcal{P}'\rangle$ goes from j' to j on the shortest way possible and then follows the string in $|j,\nu,\mathcal{P}\rangle$. For quantitative calculations one needs the following scalar products:

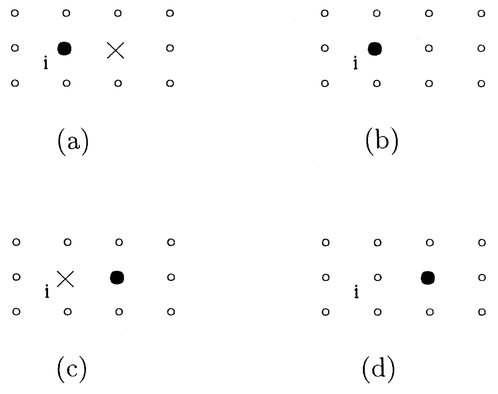

FIG. 1. States which contribute to the overlap $\langle\Phi_{j+\hat{x}}|\Phi_j\rangle$ and the matrix element $\langle\Phi_{j+\hat{x}}|H_H|\Phi_j\rangle$. Here a cross denotes a displaced spin, a small circle denotes an undisplaced spin, and the big circle denotes the hole. The states shown in (a) and (d) are included in $|\Phi_{j+\hat{x}}\rangle$, the states shown in (b) and (c) are included in $|\Phi_j\rangle$.

$$\begin{aligned} \langle \chi_n | \tilde{\chi}_{n+\hat{x}} \rangle &= -i \sin(q_x/2) \ , \\ \langle \chi_n | \tilde{\chi}_{n+\hat{y}} \rangle &= -i \sin(q_y/2) \ . \end{aligned} \tag{28}$$

Now let us evaluate the overlap $\langle \Phi_{j+\hat{x}} | \Phi_j \rangle$. From the scalar product of the states shown in Figs. 1(a) and 1(b) and 1(c) and 1(d), respectively, one gets a contribution of

$$\delta \langle \Phi_{j+\hat{x}} | \Phi_j \rangle = 2i \sin(q_x/2) \alpha_0 \alpha_1 \ . \tag{29}$$

The additional factor of (-1) arises from fermion commutation relations as can be easily checked by writing down explicit expressions for the states $|j,\nu,\mathcal{P}\rangle$. Adding the contributions from the longer paths one obtains

$$\begin{aligned} \langle \Phi_{j+\hat{x}} | \Phi_j \rangle &= n_{(1,0)} \\ &= 2i \sin(q_x/2) \sum_{\nu=0}^{\infty} (z-1)^\nu \alpha_\nu \alpha_{\nu+1} \ . \end{aligned} \tag{30}$$

In an entirely analogous fashion one obtains

$$\begin{aligned} \langle \Phi_{j+2\hat{x}} | \Phi_j \rangle &= -2 \sin^2(q_x/2) \sum_{\nu=0}^{\infty} (z-1)^\nu \alpha_\nu \alpha_{\nu+2} \ , \\ \langle \Phi_{j+\hat{x}+\hat{y}} | \Phi_j \rangle &= -4 \sin(q_x/2) \sin(q_y/2) \sum_{\nu=0}^{\infty} (z-1)^\nu \alpha_\nu \alpha_{\nu+2} \ . \end{aligned} \tag{31}$$

One can see that these latter overlap integrals are proportional to q^2 as $\mathbf{q} \to \mathbf{0}$. Obviously the overlap integrals between localized states centered on more distant sites will be of even higher order in $\sin(q_x), \sin(q_y)$. In addition their expansions in terms of the α's will begin with even higher indices so due to the rapid decay of this function they will be small, too. In the following quantities which are $O(q^2)$ as $q \to 0$ will be referred to as "higher-order terms" and they will be ignored throughout the remainder of the calculation of the dispersion relation.

Let us now turn to the evaluation of matrix elements of the Hamiltonian. To that end it is advantageous to introduce a few definitions:

$$\begin{aligned} \varepsilon(j,\nu,\mathcal{P}) &= \langle j,\nu,\mathcal{P} | H_{t-J} | j,\nu,\mathcal{P} \rangle \ , \\ P_{j,\nu,\mathcal{P}} &= |j,\nu,\mathcal{P}\rangle \langle j,\nu,\mathcal{P}| \ . \end{aligned} \tag{32}$$

Also let us decompose the Heisenberg part H_H of H_{t-J} in two parts:

$$\begin{aligned} H_H &= H_H^{\mathrm{diag}} + H_H^{\mathrm{res}} \ , \\ H_H^{\mathrm{diag}} &= \sum_{\nu,\mathcal{P}} \varepsilon(j,\nu,\mathcal{P}) P_{j,\nu,\mathcal{P}} \ . \end{aligned} \tag{33}$$

Then it is easy to see that up to higher-order terms

$$\begin{aligned} \langle \Phi_{j+\delta} | (H_t + H_H^{\mathrm{diag}}) | \Phi_j \rangle &= \sum_{\nu,\nu',\mathcal{P}'} \alpha_{\nu'} \sum_{\mathcal{P}} \{ -t[(z-1)\alpha_{\nu+1} + \alpha_{\nu-1}] \\ &\qquad + \varepsilon(j,\nu,\mathcal{P}) \alpha_\nu \} \\ &\qquad \times \langle j',\nu',\mathcal{P}' | j,\nu,\mathcal{P} \rangle \ . \end{aligned} \tag{34}$$

If higher-order terms are neglected the scalar product on the right-hand side of the above equation will actually depend only on j,j'. Then one can make use of Eqs. (14) to obtain

$$\begin{aligned} \langle \Phi_{j+\delta} | (H_t + H_H^{\mathrm{diag}}) | \Phi_j \rangle &= [E_0(\mathbf{q}) + \Delta E_0(\mathbf{q}) + E_B(\mathbf{q})] \langle \Phi_{j+\delta} | \Phi_j \rangle \ . \end{aligned} \tag{35}$$

Neglecting higher-order terms one can also show that

$$\begin{aligned} \langle j',\nu',\mathcal{P}' | H_H^{\mathrm{res}} | j,\nu,\mathcal{P} \rangle = \sum_{\langle m,n \rangle} (&\langle j',\nu',\mathcal{P}' | \mathbf{S}_n \cdot \mathbf{S}_m | j,\nu,\mathcal{P} \rangle \\ &- \langle j',\nu',\mathcal{P}' | j,\nu,\mathcal{P} \rangle \langle j,\nu,\mathcal{P} | \mathbf{S}_n \cdot \mathbf{S}_m | j,\nu,\mathcal{P} \rangle) \ . \end{aligned} \tag{36}$$

Obviously in this sum only those bonds (m,n) where at least one of the two spins points in different directions in the states $|j',\nu',\mathcal{P}'\rangle, |j,\nu,\mathcal{P}\rangle$ give a nonvanishing contribution. This is noting but some kind of "linked cluster theorem" in the framework of the present formalism. One can introduce the following abbreviation:

$$\begin{aligned} \langle j',\nu',\mathcal{P}' | \mathbf{S}_n \cdot \mathbf{S}_m | j,\nu,\mathcal{P} \rangle_c = &\langle j',\nu',\mathcal{P}' | \mathbf{S}_n \cdot \mathbf{S}_m | j,\nu,\mathcal{P} \rangle \\ &- \langle j',\nu',\mathcal{P}' | j,\nu,\mathcal{P} \rangle \langle j,\nu,\mathcal{P} | \mathbf{S}_n \cdot \mathbf{S}_m | j,\nu,\mathcal{P} \rangle \ . \end{aligned} \tag{37}$$

Then from the states shown in Figs. 1(a) and 1(b) and 1(c) and (1d), respectively, one obtains the following contribution:

$$\delta\langle \Phi_{j+\hat{x}}|\mathbf{S}_{i-\hat{x}}\cdot\mathbf{S}_i|\Phi_j\rangle_c = -\frac{J}{4}\alpha_0\alpha_1[\langle\tilde{\chi}_{i-\hat{x}}|\mathbf{S}|\tilde{\chi}_{i-\hat{x}}\rangle\cdot\langle\chi_i|\mathbf{S}|\tilde{\chi}_{i+\hat{x}}\rangle - \langle\chi_i|\tilde{\chi}_{i+\hat{x}}\rangle\cos(q_x)]$$

$$= -i\frac{J}{4}\alpha_0\alpha_1\left[\sin\left[\frac{3q_x}{2}\right]+\sin\left[\frac{q_x}{2}\right]\cos(q_x)\right] . \qquad (38)$$

The total contribution of the bond $(i,i-\hat{x})$ is then found to be

$$\langle \Phi_{j+\hat{x}}|\mathbf{S}_{i-\hat{x}}\cdot\mathbf{S}_i|\Phi_j\rangle_c = -i\frac{J}{4}\left[\sin\left[\frac{3q_x}{2}\right]+\sin\left[\frac{q_x}{2}\right]\cos(q_x)\right]\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+1} . \qquad (39)$$

There is a number of other bonds which contribute to $\langle\Phi_{j+\hat{x}}|H_H^{\text{res}}|\Phi_j\rangle$. Adding up all their contributions one obtains the total matrix element

$$\langle\Phi_{j+\hat{x}}|H_H^{\text{res}}|\Phi_j\rangle$$

$$=\tilde{h}_{(1,0)} = -i\frac{J}{4}\left[2\sin\left[\frac{3q_x}{2}\right]+4\sin\left[\frac{q_x}{2}\right]\cos(q_y)+\sin(q_x)\cos\left[\frac{q_y}{2}\right]+\sin\left[\frac{q_x}{2}\right]\cos(q_x)\right.$$

$$\left.-\sin\left[\frac{q_x}{2}\right]\cos\left[\frac{q_x}{2}\right]-2\sin\left[\frac{q_x}{2}\right]\cos\left[\frac{q_x}{2}\right]\right]\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+1}$$

$$-i\frac{J}{4}\left[2\sin\left[\frac{3q_x}{2}\right]+\sin\left[\frac{q_x}{2}\right]\cos(q_x)-\sin\left[\frac{q_x}{2}\right]\cos\left[\frac{q_x}{2}\right]\right]\sum_{\nu=1}^{\infty}(z-1)^{\nu-1}\alpha_{\nu}\alpha_{\nu+1} . \qquad (40)$$

In an analogous fashion one obtains other matrix elements of H_H^{res}:

$$\langle\Phi_{j+2\hat{x}}|H_H^{\text{res}}|\Phi_j\rangle = 2\frac{J}{4}\left[\cos(q_x)+\cos^2\left[\frac{q_x}{2}\right]\right]\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+2}+O(q^2) ,$$

$$\langle\Phi_{j+\hat{x}+\hat{y}}|H_H^{\text{res}}|\Phi_j\rangle = 4\frac{J}{4}\left[\cos\left[\frac{q_x+q_y}{2}\right]+\cos\left[\frac{q_x}{2}\right]\cos\left[\frac{q_y}{2}\right]\right]\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+2}+O(q^2) . \qquad (41)$$

Combining the above results one finds that the expression for the energy (24) can be rewritten as

$$E(\mathbf{k}) = E_0(\mathbf{q})+\Delta E_0(\mathbf{q})+E_B(\mathbf{q})+\frac{\sum_{\delta}\tilde{h}_{\delta}e^{i\mathbf{k}\cdot\mathbf{R}_{\delta}}}{1+\sum_{\delta}n_{\delta}e^{i\mathbf{k}\cdot\mathbf{R}_{\delta}}} . \qquad (42)$$

Here the sums in the numerator and denominator run over all nonvanishing difference vectors δ and the $\tilde{h}_{\delta}$ are the matrix elements of H_H^{res}. Since the matrix elements of H_H^{res} between second and third nearest neighbors are real, the sums of phase factors which are multiplied by them give just the usual tight binding harmonics. The matrix elements of H_H^{res} and overlap integrals between nearest neighbors however are imaginary and therefore the $\mathbf{k}$ dependence of the corresponding terms in the numerator and denominator is unusual. For example, the matrix elements of H_H^{res} between nearest neighbors give a contribution to the denominator which is given by

$$-(2|\tilde{h}_{(1,0)}|\sin k_x+2|\tilde{h}_{(0,1)}|\sin k_y) . \qquad (43)$$

Strictly speaking there are also matrix elements of H_H between sites like (0,0) and (0,3) which are of order q. However by analogy with the above calculations one can see that their expansion in terms of the α's will begin with $\alpha_0\alpha_3$ so due to the rapid decay of the function α_{ν} they will be rather small and will be neglected.

V. TOTAL ENERGY

It is easy to see that in the case $\mathbf{q}=0$ the dispersion relation obtained from (42) is completely flat on the surface of the magnetic Brillouin zone. There is by now general agreement that for the motion in a Néel ordered spin background this degeneracy is unphysical.[2,3,5,8,14,18,19] Rather there is an absolute minimum of the dispersion relation at the four points $\mathbf{k}=(\pm\pi/2,\pm\pi/2)$. Let us therefore accept that for $\mathbf{q}=\mathbf{0}$ the absolute minimum of the band is at the four $\mathbf{k}$ points $(\pm\pi/2,\pm\pi/2)$ and investigate the consequences of switching on a small $\mathbf{q}$. As can be seen from Eqs. (41) the matrix elements between second and third nearest neighbors will change only to second order in q. However the matrix elements and the overlap integral between nearest neighbors are linear in q. Therefore the change in the energy of the four $\mathbf{k}$ points mentioned above will be linear in q. As can be seen from (43) any nonvanishing value of $\tilde{h}_{(1,0)}$, $\tilde{h}_{(0,1)}$ will destroy the symmetry between the four $\mathbf{k}$ points $(\pm\pi/2,\pm\pi/2)$.

In the following the cases $\theta=\pi/4$ ["(1,1) spiral"] and $\theta=0$ ["(1,0) spiral"] will be discussed. In the first case the minimum at $(\pi/2,\pi/2)$ will be lowered while the one at $(-\pi/2,-\pi/2)$ will be raised in energy. The two other minima at $(\pi/2,-\pi/2),(-\pi/2,\pi/2)$ will be unaffected to linear order in q. Let us define

$$\eta_{1,1}=\frac{\partial}{\partial_q}\left[E\left(-\frac{\pi}{2},-\frac{\pi}{2}\right)-E\left(\frac{\pi}{2},\frac{\pi}{2}\right)\right]\Bigg|_{q=0,\theta=\pi/4}$$

$$=8\left[\frac{\partial|\tilde{h}_{(1,0)}|}{\partial q}-2\tilde{h}_{(1,1)}\frac{\partial|n_{(1,0)}|}{\partial q}\right]. \qquad (44)$$

All the matrix elements in this equation are to be evaluated at $\mathbf{q}=0$.

In the second case the two minima at $(\pi/2,\pi/2)$, $(\pi/2,-\pi/2)$ will be lowered while the other two minima at $(-\pi/2,\pi/2)$, $(-\pi/2,-\pi/2)$ will be raised in energy. Again we define

$$\eta_{1,0}=\frac{\partial}{\partial_q}\left[E\left(-\frac{\pi}{2},\frac{\pi}{2}\right)-E\left(\frac{\pi}{2},\frac{\pi}{2}\right)\right]\Bigg|_{q=0,\theta=0}$$

$$=4\left[\frac{\partial|\tilde{h}_{(1,0)}|}{\partial q}-2\tilde{h}_{(1,1)}\frac{\partial|n_{(1,0)}|}{\partial q}\right]. \qquad (45)$$

So far we have only considered one single hole. Let us assume that for a low concentration of holes the ground state is given by filling up the band calculated above.[25] One can give arguments[15] that this is a reasonable assumption provided that there is no clustering of holes (phase separation)[26] and no real-space pairing of holes into pairs. A clustering of holes would probably be prevented by the Coulomb repulsion between the holes which is not included in the *t-J* model.[27] In addition the numerical work by Trugman[3] has shown that a composite object of two holes has a very large effective mass and therefore is energetically unfavorable. So the assumption that the quasiparticle band is simply filled up for low concentration is at least not completely unreasonable.

Then for $\mathbf{q}=0$ one has four pockets around the four absolute minima. This can be seen in Fig. 2 where a contour map of the energy dispersion is shown as calculated with the "effective" matrix elements given in the Appendix. As a nonzero $\mathbf{q}$ is switched on some of the pockets will be depopulated while others are filled up. For example, in Fig. 3 a contour map is shown for the dispersion relation of one hole in a (1,1) spiral background and in Fig. 4 for one hole in a (1,0) spiral background. Depending on the degree of redistribution of "quasiparticles" the gain in energy will have a different dependence on the wave vector $\mathbf{q}$. After some algebra one obtains the energy gain per hole for the case of the (1,1) spiral:

$$\overline{\Delta E}=\begin{cases}-\dfrac{\sqrt{2}}{2}\eta q, & 0<q<\dfrac{\sqrt{2}\,\delta}{16\eta\rho},\\[2mm] -\dfrac{3\sqrt{2}}{2}\eta q+\dfrac{\delta}{8\rho}, & \dfrac{\sqrt{2}\,\delta}{16\eta\rho}<q<\dfrac{\sqrt{2}\,\delta}{4\eta\rho},\\[2mm] 2\sqrt{2}\,\eta q+\dfrac{3\delta}{8\rho}, & \dfrac{\sqrt{2}\,\delta}{4\eta\rho}<q<\infty,\end{cases} \qquad (46)$$

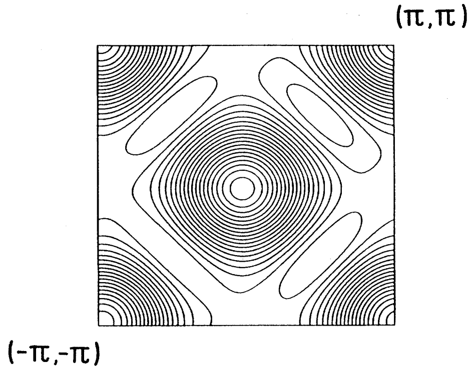

FIG. 3. Contour map showing the energy dispersion in the whole Brillouin zone for hole motion in a (1,1) spiral state. The modulus of the wave vector $\mathbf{q}$ is 0.1 and all contributions of order q^2 to the overlap integrals and matrix elements of the Hamiltonian have been discarded. The value of $t/J=3$.

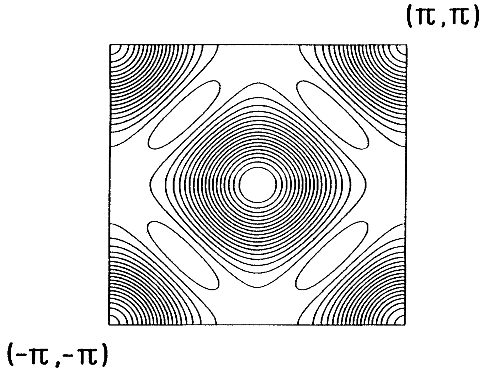

FIG. 2. Contour map showing the energy dispersion in the whole Brillouin zone for hole motion in a Néel ordered spin background. The dispersion relation has been calculated using the "effective" matrix elements given in the Appendix evaluated for $t/J=3$.

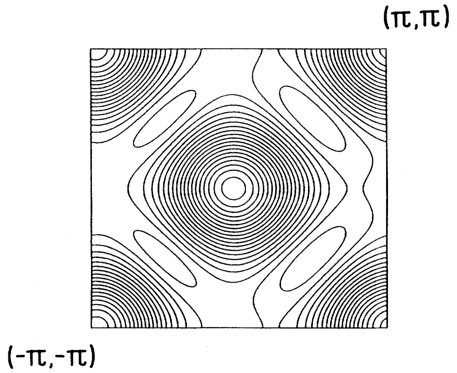

FIG. 4. Contour map showing the energy dispersion in the whole Brillouin zone for hole motion in a (1,0) spiral state. The modulus of the wave vector $\mathbf{q}$ is 0.1 and all contributions of order q^2 to the overlap integrals and matrix elements of the Hamiltonian have been discarded. Again $t/J=3$.

where ρ is the (constant) density of states per site near the minima which can be evaluated from the dispersion relation for $\mathbf{q}=0$ (Appendix A) and the quantity η is given by

$$\eta=\frac{J}{4}\left[5\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+1}+3\sum_{\nu=1}^{\infty}(z-1)^{\nu-1}\alpha_{\nu}\alpha_{\nu+1}-8\left[\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+2}\right]\left[\sum_{\nu=0}^{\infty}(z-1)^{\nu}\alpha_{\nu}\alpha_{\nu+1}\right]\right] . \tag{47}$$

In an analogous way one obtains the energy gain per hole for the case of the (1,0) spiral:

$$\overline{\Delta E}=\begin{cases}-\eta q, & 0<q<\dfrac{\delta}{8\eta\rho} ,\\ -2\eta q+\dfrac{\delta}{8\rho}, & \dfrac{\delta}{8\eta\rho}<q<\infty .\end{cases} \tag{48}$$

Equations (46) and (48) are the key results of this paper because they show that for any finite concentration of holes the derivative of the total energy with respect to q is negative, i.e., for any finite concentration of holes the Néel order in the antiferromagnet is unstable against the formation of a "spiral phase." In order to evaluate the q value that would give the minimum energy from a power series expansion in q strictly speaking one would need the terms of order q^2 in the matrix elements $\tilde{h}_\delta$ of the Hamiltonian which are very tedious to evaluate. However it seems quite reasonable to neglect them because of the smallness of the bandwidth due to the coherent motion as compared to the binding energy $E_B(\mathbf{q})$ of the localized states. For example, for $\mathbf{q}=0$ and $t/J=5$ this binding energy E_B is $13.6J$ whereas the bandwidth due to the coherent motion is only $2J$.[14] Therefore the contribution of the binding energy $E_B(\mathbf{q})$ to the second-order terms in q is likely to be much more important.

Combining all the above results one can write down the following expression for the total energy of the system with a finite concentration of holes δ:

$$E_{\mathrm{tot}}=N[aq^2+\delta(bq+c)] . \tag{49}$$

The coefficients b,c depend on the direction of the wave vector $\mathbf{q}$, on the ratio t/J, and on the concentration of holes, and can be read off from Eqs. (46) and (48). The coefficient a is independent of the direction of $\mathbf{q}$ and is given by

$$a=\frac{J}{8}-\delta\left[\frac{J}{4}+\frac{\epsilon}{2}\right] , \tag{50}$$

where ϵ is defined by (21). Within the framework of the present approximations this equation determines the phase diagram of the doped antiferromagnet. All the quantities required for the evaluation of the coefficients a,b,c can be obtained from the solution of Eqs. (14) for $\mathbf{q}=0$. By numerical evaluation it is found that for any value of the ratio t/J between 1 and 10 and for any concentration of holes δ between 0 and 0.1 the (1,1) spiral is energetically favored in agreement with the previous mean-field results.[7,28] This is basically due to the large density of states which makes sure that even for small values of q all the holes sit in the one pocket around $(+\pi/2,+\pi/2)$. It should be noted that the present approach may not be expected to give meaningful results when $t<J$, which is an unphysical range of parameters anyway.

In Fig. 5 the value of q as determined by minimizing the expression (49) is shown as a function of the concentration of holes δ for different values of the ratio t/J. One can see that for a larger concentration of holes the q values are rather large so that an expansion up to second order in q is not a good approximation any more. Obviously a more detailed calculation is required in this range of doping. On the other hand it seems doubtful whether the simple "string" picture still has much relevance for hole concentrations as large as 0.1

One can also ask for a minimum concentration required to induce spiral spin correlations. Obviously in two dimensions the modulus of the minimum wave vector compatible with periodic boundary conditions is of order $1/\sqrt{N}$ where N is the number of sites in the lattice. Then one can see from (49) that the minimum concentration which is necessary to induce a spiral with such a wave vector is proportional to $1/\sqrt{N}$. Thus in the thermodynamic limit this minimum concentration tends to zero. It should be noted however that one single hole is never sufficient to induce spiral spin correlations so there is no orthogonality catastrophe due to the formation of a spiral in the t-J model.

Finally one might ask how the present results compare with exact diagonalizations of finite clusters. One basic problem is here that for a finite system states of the type (7) with different $\mathbf{q}$ are not orthogonal any more. Thus the ground state of a finite system might be a linear combination of spirals with a different $\mathbf{q}$. When the ground-state spin correlation function

$$S(\mathbf{q})=\frac{1}{N^2}\sum_{m,n}e^{i\mathbf{q}\cdot(\mathbf{R}_n-\mathbf{R}_m)}\langle\mathbf{S}_m\cdot\mathbf{S}_n\rangle \tag{51}$$

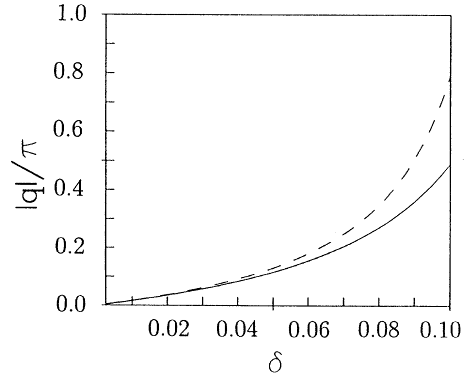

FIG. 5. The modulus of the spiral wave vector $\mathbf{q}$ in units of π as a function of the hole concentration δ for $t/J=2$ (full line) and $t/J=3$ (dashed line). The vector $\mathbf{q}$ points in (1,1) direction.

is examined for a finite system, it is found[29,30] that whereas for the undoped case there is a sharp maximum at $\mathbf{q}=(\pi,\pi)$, in the doped case the values for $\mathbf{q}$ vectors in the neighborhood of this point are of comparable magnitude. Thus the finite-size data are at least not completely inconsistent with the results of this paper.

VI. CONCLUSION

From the discussion of the coherent motion of a hole in a spin state with a spiral spin correlation function one can conclude that the change in ground-state energy as compared to the case of hole motion in a Néel state is linear in the wave vector of the spiral. Then if one makes the (reasonably justified) assumption that the "quasiparticle band" obtained in this way is simply filled up for low hole concentrations one finds that the Néel order of the spin system alone is always unstable.

One advantage of the approach outlined above is that it gives a rather simple picture of the hole motion which has given quite good results as compared to finite-size diagonalizations in the limit $\mathbf{q}=\mathbf{0}$. Also it provides the wave functions for the "quasiparticle states" which can be used to evaluate, e.g., correlation functions. It should be noted that the wave function (23) should have rather unusual physical properties. For example, the "spin of the hole" seems to be constantly rotating as the hole is moving through the lattice. Of course one cannot conclude that there is indeed a spiral spin correlation of the type (8) in a doped antiferromagnet because one also should investigate other ways of changing the "spin background." However, the method outlined above is in principle always applicable as long as there is something like a "string potential." As has been shown above this method always leads to a considerable reduction of the degrees of freedom which have to be taken into account and it is applicable whenever one can write down a wave function for the "spin background."

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APPENDIX

In the case $\mathbf{q}=\mathbf{0}$ the dispersion relation for coherent hole motion can be obtained from an "effective" tight binding Hamiltonian with two nonvanishing matrix elements between second and third nearest neighbors:[14]

$$\begin{aligned} t_{(1,1)} &= 2J \sum_{\nu=0}^{\infty} (z-1)^{\nu} \alpha_{\nu} \alpha_{\nu+2} - 2t\alpha_2\alpha_3 , \\ t_{(2,0)} &= J \sum_{\nu=0}^{\infty} (z-1)^{\nu} \alpha_{\nu} \alpha_{\nu+2} . \end{aligned} \tag{A1}$$

The terms proportional to J describe the propagation by "string truncation" whereas the other terms describe the propagation along the spiral paths where the hole can absorb its own string.[13,3] Then the two eigenvalues of the effective mass tensor at the band minimum $(\pi/2,\pi/2)$ are given by

$$\begin{aligned} m_1 &= \frac{1}{16J \sum_{\nu=0}^{\infty} (z-1)^{\nu} \alpha_{\nu} \alpha_{\nu+2}} , \\ m_2 &= \frac{1}{8t\alpha_2\alpha_3} . \end{aligned} \tag{A2}$$

The two corresponding eigenvectors are (1,1) and (1,−1), respectively, i.e., perpendicular and parallel to the surface of the so-called magnetic Brillouin zone. One can see that the effective mass in the direction parallel to the surface of the magnetic Brillouin zone is determined entirely by the tunneling processes along the spiral paths. The density of states per site is then

$$\rho = \frac{\sqrt{m_1 m_2}}{2\pi} . \tag{A3}$$

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