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### Ground state of a mobile vacancy in a quantum antiferromagnet: Small-cluster study

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The ground state of a mobile vacancy in a square-lattice spin- $\frac{1}{2}$  Heisenberg antiferromagnet described by the  $t$ - $J$  Hamiltonian is investigated numerically for an 18-site cluster. The ground state has spin  $1/2$ , and the bottom of the vacancy band is at momentum  $k = (\pm\pi/2, \pm\pi/2)$ , for  $t/J < 4$ , which is consistent with the spin-wave perturbation theory. The structure of the spin configuration in the vicinity of the vacancy is examined using a number of correlation functions. The latter reveal the existence of a dipolar distortion of the staggered magnetization, as suggested by the semiclassical theory.

#### I. INTRODUCTION

This paper will discuss the properties of the ground state of a single mobile vacancy (or "hole") in a quantum antiferromagnet (AF) governed by the " $t$ - $J$ " Hamiltonian

$$H = -t \sum_{r,\mu,\sigma} (c_{r+\mu,\sigma}^\dagger c_{r,\sigma} + \text{H.c.}) + J \sum_{r,\mu} \mathbf{s}_{r+\mu} \cdot \mathbf{s}_r, \quad (1.1)$$

where  $c_{r,\sigma}$  is the electron annihilation operator;  $\mathbf{s} \equiv \frac{1}{2} c^\dagger \hat{\tau} c$  is the spin; the sums are over all sites  $r$  on one sublattice of the square lattice, all nearest-neighbor vectors  $\mu$ , and two spin states  $\sigma$ . All sites are either singly occupied or empty, the latter representing the vacancies. To the extent that this model corresponds to the large on-site repulsion limit of the Hubbard model,<sup>1</sup> one expects the hopping rate  $t$  to be large compared with the spin exchange  $J$ . It will however prove profitable to examine the limit of small  $t/J$  as well.

The vacancy state has been investigated recently by a number of authors<sup>2-14</sup> both analytically and numerically. Below, after reviewing briefly the physics of the problem in Sec. II we present the exact numerical analysis of the ground state of a single vacancy in the 18-site [ $3 \times 3$  on each sublattice, see Fig. 1(a)] cluster with periodic boundary conditions. An attempt is made to extract the dependence of the lowest-lying state's energy on the wave vector and to understand the nature of the spin distortions introduced by the mobile vacancy. In agreement with the perturbation theory we find (Sec. III) that the bottom of the vacancy band lies on the magnetic zone boundary and

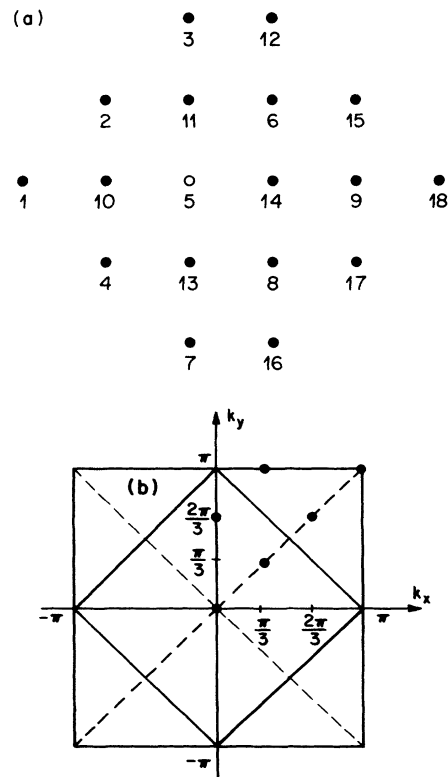


FIG. 1. (a) The 18-site cluster used here. The open circle represents the vacancy. The periodic boundary conditions identify vectors  $(\pm 3, \pm 3)$  and zero. (b) Brillouin zone of the 18-site cluster with six distinct wave numbers unrelated by symmetry.

is located at the zone face<sup>15</sup> centers  $k = (\pm\pi/2, \pm\pi/2)$ , at least for  $t/J < 4$ . As the main focus of the paper, in Sec. IV we examine a number of spin correlation functions for the ground state and conclude that the mobile vacancy generates a transverse spin distortion with dipolar symmetry. This distortion can be interpreted semiclassically as a “twist” in the direction of the staggered order parameter of the spin background leading to a dipolar backflow of magnetization. Combined with the fact that the minimum energy state of the vacancy is at finite momentum, this suggests an amusing analogy between the AF vacancy state and the *roton* excitation of He II. The key results of this paper have been summarized in Ref. 5 which also outlined the semiclassical analysis; more detailed discussions of the latter can be found in Ref. 16.

## II. ASPECTS OF VACANCY DYNAMICS

The nature of the coupling between the vacancy and the spin degrees of freedom is most evident in the Ising limit where only the diagonal part  $J_z s_{r+\mu}^z s_r^z$  of the spin exchange term in Eq. (1.1) is kept. Consider the case of the fully Néel-ordered spin background (which is clearly the ground state in the absence of vacancies) compared with saturated ferromagnetic order. It was observed by Brinkman and Rice<sup>2</sup> and Bulaevskii, Nagaev, and Khomskii<sup>3</sup> that while for the ferromagnet the vacancy behaves as a free particle with the energy minimum  $E_0 = -4t$  at  $k = 0$  and bandwidth  $\Delta E = 8t$  for the Néel antiferromagnet the vacancy motion is hindered by the scrambling of the spin order which is caused by hopping. This presents a non-trivial many-body problem. It appears however that for large (but not too large)  $t/J_z$  the bulk of the vacancy kinetic energy is accounted for by the virtual excursions, where the hole creates a “string” of overturned spins and then retraces its path back.<sup>2,3</sup> The length of the string scales as  $(t/J_z)^{1/3}$  and the energy of the string state is approximately<sup>4,14</sup>  $E_0 = -t2\sqrt{3} + 2.7J_z^{2/3}t^{1/3}$ . This energy has to be compared to the energy of a ferromagnetic polaron which is the state where the spin background is polarized ferromagnetically in a region with an area scaling as  $(t/J_z)^{1/2}$ . While the latter is clearly favorable in the Nagaoka<sup>17</sup> case  $J_z/t = 0$ , the crossover between these two regimes appears to occur<sup>14</sup> only in the rather extreme<sup>18</sup> limit  $J_z/t < 10^{-2}$ . Here we concentrate only on larger values of  $J/t$ .

It is important to realize that the exact ground state of Eq. (1.1) for one hole may be put into Bloch form because the underlying Hamiltonian is translationally invariant. Specifically, the state with total momentum  $k$  may be written as

$$\psi_k = \sum_{r, \{\sigma_\rho\}} e^{ikr} \phi_k(r, \{\sigma_\rho\}) |r, \{\sigma_\rho\}\rangle, \quad (2.1a)$$

where  $r$  is the hole location, which is summed over the entire lattice and  $\{\sigma_\rho\}$  denotes a complete set of spin eigenstates at all sites  $\rho \neq r$ , which is also summed over. The amplitudes  $\phi$  are, of course, translationally invariant:

$$\phi_k(r + \mu, \{\sigma_{\rho+\mu}\}) = \phi_k(r, \{\sigma_\rho\}). \quad (2.1b)$$

Here we focus on the lowest-energy states at each

momentum and refer to this set of  $\psi_k$  as the vacancy band and their energies as  $E(k)$ . In the presence of AF order the Brillouin zone is reduced to the diamond defined by its corners:  $(\pi, 0)$ ,  $(0, \pi)$ ,  $(-\pi, 0)$ ,  $(0, -\pi)$  as shown on Fig. 1(b).

The string state where the vacancy always retraces its path, as discussed above, is actually localized (the string being associated with a particular site). Thus in the string approximation the vacancy band  $E(k)$  is dispersionless.<sup>19</sup> However, even in the Ising limit the vacancy eigenstates have a finite bandwidth.<sup>19</sup> This bandwidth arises from the process where the hole hops around a plaquette  $1\frac{1}{2}$  times, but it is always quite small ( $\Delta E \ll t$ ) and the energy minimum remains at  $k = 0$ .

Spin dynamics is the essential factor in determining the effective mass (or bandwidth) of the vacancy, with the dominant contribution arising from the spin-exchange<sup>6</sup> part of Eq. (1.1)  $\frac{1}{2}J_\perp (s_{r+\mu}^+ s_r^- + s_{r+\mu}^- s_r^+)$ , left out in the Ising limit. The limit  $t, J_\perp \ll J_z$  can be readily treated perturbatively. While this limit is not the regime we want, the answer is illustrative of the band structure  $E(k)$  we find in the limit  $J_\perp = J_z \sim O(t)$ . This is, in fact, the first instance where we see that the small- $t$  limit of (1.1) is very useful to examine even though Eq. (1.1) is then no longer related to the Hubbard model.

Wave-vector dependence first enters the energy at order  $t^2 J_\perp / J_z^2$ . The relevant process is the one where the hole hops twice ( $t^2$ ), thereby remaining on the same sublattice, and the two scrambled spins are returned to their Néel state positions by the spin exchange ( $J_\perp$ ). There are 12 equivalent processes to consider and the energy to this order is

$$E(k) = -\frac{8t^2}{3J_z} - \frac{16}{15} \frac{t^2 J_\perp}{J_z^2} + \frac{16}{15} \frac{t^2 J_\perp}{J_z^2} (\cos k_x + \cos k_y)^2. \quad (2.2)$$

Hence the minimum energy moves from  $k = 0$  to the zone boundary, which at this level of approximation is degenerate. The bandwidth is  $O(t^2 J_\perp / J_z^2)$  which becomes  $t^2/J$  in the isotropic limit  $J_\perp = J_z$ .

Alternatively one can develop the  $t/J$  expansion for the isotropic limit ( $J_z = J_\perp = J$ ) in the framework of the Holstein-Primakoff spin-wave theory (see Appendix). The results can be expressed approximately by a three-parameter fit:

$$E(k) = -\frac{4t^2}{J} [0.54 - 0.10(\cos k_y)^2 + 0.006(\sin^2 k_x + \sin^2 k_y)]. \quad (2.3)$$

The degeneracy along the magnetic zone boundary is now lifted and the bottom of the band occurs at  $[\pm\pi/2, \pm\pi/2]$ . The band is anisotropic near the minimum with the “heavy” mass  $\mu_\parallel = 2.1Jt^{-2}$  along the magnetic zone boundary [i.e., the  $(\pi, 0), (0, \pi)$  diagonal] and the “light” mass  $\mu_\perp = 0.8Jt^{-2}$  in the direction perpendicular (toward the zone center).

There have been a number of other analytic or nearly analytic calculations that attempted to go beyond simple perturbation theory to describe the  $t \gg J$  regime. They generally agree that the ground state is at the zone face centers  $(\pm\pi/2, \pm\pi/2)$ . The effective mass is anisotropic

and for  $t/J \gg 1$  it is argued to be  $O(J^{-1})$  rather than  $O(t^{-1})$  as it would be for a free particle. Specifically we mention Trugman,<sup>6</sup> who found an energy minimum on the zone boundary (when the basis of states used in his truncation was large enough) and Sachdev<sup>8</sup> who calculated variationally and found a ground state at  $(\pi/2, \pi/2)$  and bandwidth scaling with  $J$ . Self-consistent diagrammatic spin-wave calculations have been done in one dimension by Schmitt-Rink, Varma, and Ruckenstein<sup>9</sup> showing that the energy minimum moved to the zone boundary. Kane, Lee, and Read<sup>7</sup> investigated the self-consistent equation for the self-energy of the hole in 2D in the  $t/J \gg 1$  limit, observed that the band minimum is most likely to be at the zone face centers, and argued that the quasiparticle pole is suppressed by a factor  $J/t$  and that the effective mass scales as  $J^{-1}$ .

Another question of interest is the effect of the mobile vacancy on the spin background. Above we have already brought up the possibility of a local ferromagnetic polarization appearing in the vicinity of the hole. On the other hand, in Ref. 5 on the basis of the semiclassical analysis it was pointed out that in addition to coupling to local net magnetization (which is responsible for Nagaoka ferromagnetism<sup>16</sup> and ferropolarons<sup>2,3</sup>), the vacancy kinetic energy term implicitly contains a coupling to the "twist" of the local staggered magnetization  $\hat{\Omega}$ . (The staggered magnetization is defined by the difference of local sublattice magnetizations, and the order parameter  $\hat{\Omega}$ , here is a unit vector.) A twist, or transverse distortion of  $\hat{\Omega}$ , has the effect of making neighboring spins not strictly antiparallel, which facilitates the hopping, just like the canting of sublattices introduced by the ferromagnetic polarization. However unlike a net magnetization, which contributes predominantly to  $k=0$  states, the effect of a twist dominates near  $k=(\pm\pi/2, \pm\pi/2)$  and hence one expects it to be important for the vacancy ground state.

The physically relevant quantity associated with the twist of the staggered magnetization is the magnetization current  $\hat{\Omega} \times \partial_\mu \hat{\Omega}$  which we expect in the vacancy ground state with momentum  $k$  to have the form<sup>5</sup>

$$(\hat{\Omega} \times \partial_\mu \hat{\Omega})^\alpha = \left[ \delta_{\mu\nu} - \frac{2r_\mu r_\nu}{r^2} \right] \frac{p_\nu^\alpha(k)}{r^2} \quad (2.4)$$

for large  $r$ , where the distance  $r$  is with respect to the position of the vacancy. This pattern can be associated with the AF dipole moment  $p_\mu^\alpha(k)$  which has the quantum numbers of the spin current: it is a vector in both spin,  $\alpha$ , and lattice,  $\mu$ , spaces. The long-range nature of the distortion follows from the semiclassical analysis, which is justified far enough from the vacancy where the disturbance is sufficiently small; in fact this behavior arises from the gaplessness of the transverse spin excitations (spin waves) in the isotropic limit ( $J_1 = J_2$ ). On symmetry grounds one expects  $p_\mu^\alpha(k) \sim \sin k_\mu$  so that it vanishes at  $k=0$ ,  $(\pi, 0)$ , etc., as required by reflection symmetry. Note that the magnitude of  $p_\mu^\alpha$  is thus likely to be maximal at the zone face centers and thus for the vacancy ground state. A detailed discussion of the semiclassical analysis can be found in Ref. 16. Let us now pass on to the numerical results.

### III. NUMERICAL RESULTS

The lowest-energy state for the mobile vacancy with a given momentum  $k$  on an 18-site cluster ( $3 \times 3$  per sublattice) is readily obtained by simply iterating the action of the Hamiltonian, Eq. (1.1), on a random initial state with that momentum. Use of the translational invariance (i.e., Bloch states) reduces the Hilbert space of the 18-site cluster with one vacancy to  $\binom{17}{8} = 24\,310$  states with  $S_{\text{tot}}^z \equiv \frac{1}{2}$ ; this ( $S_{\text{tot}}^z = \frac{1}{2}$ ) is the sector we primarily examine. The Brillouin zone of this cluster contains 6 symmetry-inequivalent points<sup>20</sup> as shown on Fig. 1(b). Of these, 4 lie close to the magnetic zone boundary  $|k_x| + |k_y| = \pi$ . Over a large range of  $t/J$  (the present study covers  $t/J \leq 10$ ) the ground state was found to have spin  $\frac{1}{2}$  and  $k$  at one of these 4 magnetic zone boundary points. It is important to note that the constraint on  $S_{\text{tot}}^z$  only imposes a lower bound on the total spin (i.e., the total spin could be  $\frac{3}{2}$ ,  $\frac{5}{2}$ , etc.), and level crossing transitions to higher spin states occur with increasing  $t/J$  (the exact  $t/J$  value for level crossing depends on the wave vector  $k$  of the state and, for the small cluster, is likely to be size dependent). For  $t/J$  larger than a size dependent critical value the ground state of the vacancy shifts to a  $k=0$  state with the maximum total spin.<sup>11,13</sup> (This transition to the Nagaoka<sup>16</sup> ferromagnetic state is clearly a finite-size effect, which limits the range of  $t/J$  to be studied.)

The interpretation of the numerical results is, unfortunately, far from straightforward because, on one hand, of the finite-size effects and, on the other, the already large number of Hilbert space states which necessitates the use of correlation functions for studying the spin configuration. Below we report in some detail what we have found; the key results of this investigation have been presented briefly in Ref. 5.

Let us start with the energy dispersion of the vacancy band  $E(k)$ . Because the Brillouin zone consists of six inequivalent points, the vacancy band can be uniquely fit by

$$\begin{aligned} E(k) = & c_1 + \frac{c_2}{4} (\cos k_x + \cos k_y)^2 + \frac{c_3}{2} (\sin^2 k_x + \sin^2 k_y) \\ & + \frac{c_4}{2} (\cos 2k_x \cos k_y + \cos 2k_y \cos k_x) \\ & + \frac{c_5}{2} (\cos 3k_x + \cos 3k_y) + \frac{c_6}{2} (\cos k_x + \cos k_y). \end{aligned} \quad (3.1)$$

The coefficients  $c_j$  as a function of  $t/J$  are given in Table I (where we have subtracted out the energy of the cluster with a static,  $t=0$ , vacancy:  $E_0 = -11.173J$ ). We remark that the  $E(k)$ , given by Eq. (3.1) and the data in Table I, corresponds to the lowest energy states with fixed  $k$  and therefore must be a continuous function of  $t/J$ . This function, however, need not be smooth because of the possibility of level crossing. In particular the evolution of the  $c_{4,5}$  terms suggests a possibility of level crossing near  $t/J \approx 1$  (perhaps between even and odd parity states with  $k=0$ ). Also, we found that the lowest energy state in the  $k=0$  sector switches from  $S_{\text{tot}} = \frac{1}{2}$  for  $t/J \leq 2.5$  to  $S_{\text{tot}} \geq \frac{3}{2}$  for  $t/J \geq 5$ . Needless to say, the

TABLE I. Values of the vacancy band parameters as defined in Eq. (3.1) (in the units of  $t$ ) as a function of  $t/J$ .

$t/J$	$C_1$	$C_2$	$C_3$	$C_4$	$C_5$	$C_6$
0.1	-0.260	0.237	-0.062	0.004	$5.4 \times 10^{-4}$	0.514
0.25	-0.616	0.557	-0.145	0.021	0.003	0.493
0.5	-1.077	0.947	-0.237	0.050	0.006	0.452
1.0	-1.662	0.991	-0.161	-0.063	-0.027	0.245
2.5	-2.342	0.635	-0.008	-0.054	-0.027	0.149
5.0	-2.676	0.214	0.010	-0.018	-0.037	0.035
10.0	-2.897	0.050	-0.007	-0.021	-0.013	0.037

convergence rate of our numerical method slows down near the level crossing.

The terms appearing in Eq. (3.1) are motivated by the  $k$  dependence corresponding to different translations of the plane wave state under 1, 2, and 3 hops: e.g., in small- $t$  perturbation theory the  $c_6$  term would arise in first order,  $c_1, c_2, c_3$  in second order, and  $c_4, c_5$  in third order. Indeed, in Table I one observes that  $c_6$  quoted in units of  $t$  approaches a constant as  $t/J \rightarrow 0$ , while  $c_1, c_2, c_3$  scale linearly and  $c_4, c_5$  quadratically, with  $t/J$  for  $t/J \ll 1$ .

Note that the first and last three terms in Eq. (3.1) differ by the parity of the number of hops: The first three are invariant under  $k \rightarrow k + (\pi, \pi)$ ; the last three change sign and therefore contribute to the energy splitting between  $k=0$  and  $(\pi, \pi)$  states. In the infinite system, however, the latter two states must be degenerate: Clearly in the broken symmetry state, i.e., in the presence of a nonzero AF order parameter, the translational symmetry is reduced to that of a single sublattice and the Brillouin zone is reduced by identification of  $k$  and  $k + (\pi, \pi)$ . The degeneracy of the  $k$  and  $k + (\pi, \pi)$  vacancy states in the infinite system is obvious intuitively, since the spin ground state of the infinite system can be thought of, simply, as the average over the broken symmetry states with different directions of the staggered magnetization order parameter  $\hat{\Omega}$ . The matrix element connecting the states with opposite staggered magnetization goes to zero with the size of the system. In the finite cluster, however, it is finite and gives rise to the splitting of  $k$  and  $k + (\pi, \pi)$  states by allowing transitions with odd number of hops combined with the flip of  $\hat{\Omega}$ , which transfer the vacancy from one sublattice to another, to contribute. In the small  $t/J$  limit this effect dominates the energy dispersion, since the single hop contribution scales with  $t$  compared to  $t^2/J$  scaling of the two hop, the same sublattice, process. The advantage of the fit used in Eq. (3.1) is that this finite-size effect can be accounted for simply by subtracting out the *odd* terms, i.e.,  $c_{4,5,6}$ , which according to the argument above vanish with the volume of the system. Thus we define the estimated vacancy band energy  $\tilde{E}(k)$  (over the magnetic Brillouin zone) by keeping only the first three terms in Eq. (3.1). Of the terms kept,  $c_1, c_2$  determine the energies at  $k=0$  and  $(\pi, 0)$  while  $c_3$  determines the splitting between the points  $k=(\pi, 0)$  and  $(\pi/2, \pi/2)$ .

Figure 2 shows the bandwidth  $\Delta E \equiv \sup_k \{\tilde{E}(k)\} - \inf_k \{\tilde{E}(k)\}$ , in units of  $t$ , as a function of  $t/(t+J)$  (the

argument here is chosen so as to emphasize the expected linearity of  $\Delta E/t$  in both  $t/J \ll 1$  and  $J/T \ll 1$  limits). For small  $t/J$ ,  $\Delta E/t$  is linear in  $t/J$  as predicted by perturbation theory. For larger  $t/J$ , the bandwidth  $\Delta E/t$  starts decreasing with  $J/t$  as anticipated. It appears that the scaling  $\Delta E \sim J$  expected on the basis of the self-consistent perturbation theory<sup>7</sup> and semiclassical<sup>5</sup> arguments provides at least an upper bound on the bandwidth for  $t/J \gg 1$ . However, the uncertainty about the finite-size effects for larger values of  $t/J$  makes it difficult to make a conclusion about the exact scaling. In particular, the fact that the  $k=0$  state for  $t/J \geq 5$  switches to  $S_{\text{tot}} = \frac{3}{2}$  may be responsible for the faster than expected reduction of the bandwidth. Also, since the  $k=(\pi, \pi)$  state remains spin  $\frac{1}{2}$ ,  $\mathbf{k} \rightarrow \mathbf{k} + (\pi, \pi)$  is not even an approximate symmetry (for  $t/J \geq 5$ ) and the  $\tilde{E}(k)$  estimate of energy dispersion in the reduced zone may be misleading. The bottom of the energy band is at  $k=(\pm\pi/2, \pm\pi/2)$  points until  $t/J \approx 4$ . For  $t/J=5$  the bottom of the energy band appears to switch to the zone corner points,  $k=(\pi, 0)$ , etc; while for  $t/J=10$  it returns to the zone face centers. However the validity of our interpolation  $\tilde{E}(k)$  in this range is in doubt for the reason we have just described. The band is strongly anisotropic near the minimum with the “heavy” mass  $\mu_{\parallel} = -c_3^{-1}$  along the magnetic zone boundary [i.e.,  $(\pi, 0), (0, \pi)$  diagonal] and the “light” mass  $\mu_{\perp} = (c_2 - c_3)^{-1}$  in the direction perpendicular. The anisotropy factor  $\mu_{\parallel}/\mu_{\perp}$  as a function of  $t/J$  is given in Table II.

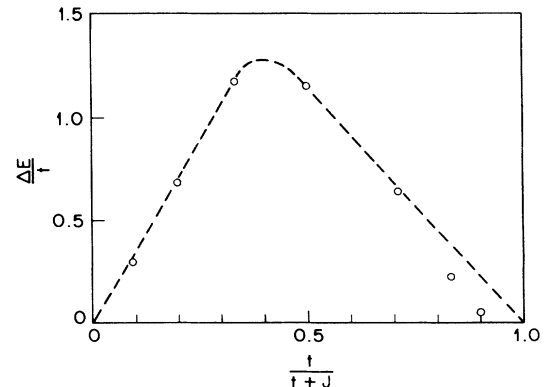


FIG. 2. Normalized bandwidth  $E(k)/t$  as a function of  $t/(t+J)$ .

TABLE II. Ratio of the masses parallel and perpendicular to the magnetic zone boundary as a function of  $t/J$ . Note that this quantity depends on the interpolation  $\tilde{E}(k)$  of the energy dispersion and may be particularly sensitive to finite-size effects for large  $t/J$ .

$t/J$	$\mu_{\parallel}/\mu_{\perp}$
0.1	4.8
0.25	4.8
0.5	5.0
1.0	7.2
2.5	80.0
5.0	-20.0
10.0	8.1

While we have attempted to correct for the finite-size effects on the energy dispersion for small  $t/J$ , the opposite limit is more difficult to control. The formation of a ferromagnetic “polaron” structure in the states at and near  $k=0$  [and  $k=(\pi,\pi)$ ] is likely to be sensitive to the cluster size. Intuitively one expects finite-size effects for any  $k$  state arising simply from the fact that for large  $t/J$  the size of the disturbance introduced by the vacancy becomes comparable with the size of the cluster. Below when we examine the spin configuration, we will see an indication of such effects becoming substantial for  $t/J > 2$ . Hence one must be cautious in interpreting the numerical results in that range.

#### IV. SPIN CORRELATIONS

We have examined the spin structure of the ground-state wave functions by evaluating a number of correlation functions. One may start by looking at the spin-expectation values in the comoving frame, that is as a function of distance relative to the hole:

$$\langle \mathbf{s}(r) \rangle_h \equiv \langle c^\dagger(0)c(0)\mathbf{s}(r) \rangle, \quad (4.1)$$

where  $N$  is the number of sites. Only the  $z$  component of  $\langle \mathbf{s}(r) \rangle_h$  is nonvanishing and for  $t/J=0.05$  and  $2.5$  it is shown in Figs. 3(a) and 3(b). The sum  $\sum_r \langle s^z(r) \rangle_h$  equals one-half as it must. For small  $t/J$ , there is a substantial staggered component of the spin:  $\langle \Omega^z \rangle_h \neq 0$ . The latter is due to the tendency of the hole to reside on the sublattice with the spin opposite to the total spin, so that the

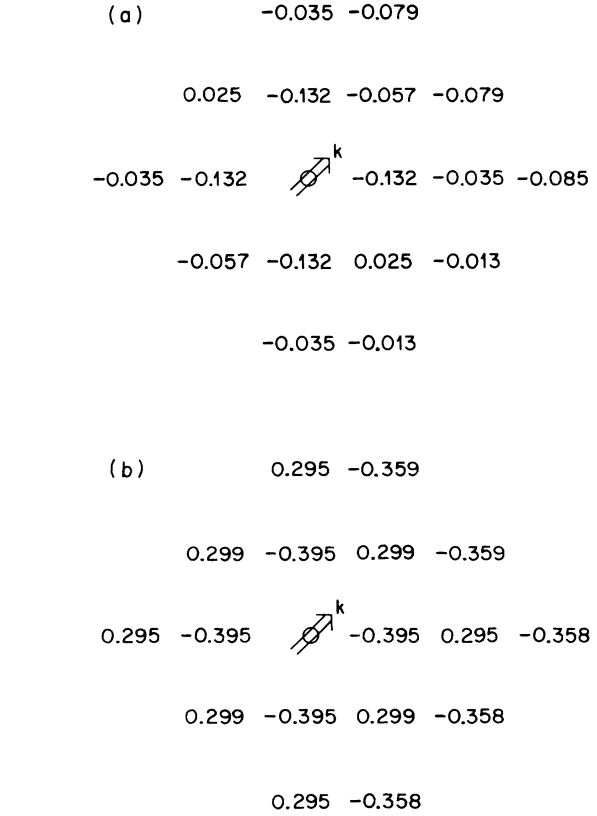


FIG. 3. Local spin expectation values  $-2\langle s_j^z \rangle_h$  in the  $k=(2\pi/3)(1,1)$  state for (a)  $t/J=0.05$ ; (b)  $t/J=2.5$ .

total spin  $s^z = \frac{1}{2}$  constraint is satisfied. Constructing a total spin- $\frac{1}{2}$  state out of two fully polarized sublattices, one of which is missing one spin, yields  $\langle \Omega^z \rangle = \frac{1}{3}$  which is quite close to the numerical value for  $t/J \ll 1$ . The  $t/J$  dependence of this quantity is given in Table III. Note that for large  $t/J$ ,  $\langle \Omega^z \rangle_h$  decreases suggesting that the vacancy resides equally on both sublattices, as might be expected. The magnitude of the staggered order parameter  $\langle \Omega^z \rangle^{1/2}$ , as shown in Table III, decreases with increasing  $t/J$  but the effect is not dramatic. It is curious that the staggered magnetization is quite isotropic:  $|\langle \Omega_z^2 \rangle^{1/2} - \langle \frac{1}{2}\Omega_1^2 \rangle^{1/2}| \leq 10^{-3}$ . The effect of the hole on AF correlations of neighboring spins can be seen by ex-

TABLE III. Different measures of the staggered magnetization in the  $k=(2\pi/3)(1,1)$  state as a function of  $t/J$ .

$t/J$	$\langle \Omega^z \rangle^{1/2}$	$\langle \Omega_z \rangle$	$\langle \Omega_z^2 \rangle^{1/2}$	$\langle \frac{1}{2}\Omega_1^2 \rangle^{1/2}$
0.05	1.03	0.34	0.597	0.597
0.1	1.03	0.33	0.596	0.596
0.25	1.03	0.29	0.592	0.591
0.5	1.0	0.22	0.583	0.582
1.0	0.98	0.12	0.57	0.57
2.5	0.91	0.035	0.525	0.525
5.0	0.83	0.0133	0.483	0.482
10.0	0.77	0.0075	0.444	0.444

aming  $\langle \mathbf{s}_j \cdot \mathbf{s}_{j+\mu} \rangle_h$  on bonds  $(j, j+\mu)$  which are shown for  $t/J=0.05$  in Fig. 4(a) and for  $t/J=2.5$  in Fig. 4(b). One may note that AF correlations on bonds close to the vacancy are enhanced for  $t/J \ll 1$ , as occurs for a static vacancy,<sup>21</sup> but they decrease with increasing  $t/J$ . The local suppression of  $\langle \mathbf{s}_j \cdot \mathbf{s}_{j+\mu} \rangle_h$  for larger  $t/J$  can be understood in terms of a Brinkman-Rice string picture as a consequence of the spin flips induced by the hopping hole. On the basis of that analysis one expects the size of the affected region to scale with  $(t/J)^{1/6}$ ; unfortunately it is impossible to explore this "string" effect numerically on this small cluster.

The semiclassical analysis however suggests that the suppression of local  $|\langle \mathbf{s}_j \cdot \mathbf{s}_{j+\mu} \rangle_h|$  magnitude is in part due to the appearance of a twist of the staggered magneti-

zation. The distortion of the staggered magnetization direction,  $\tilde{\Omega}$  can be displayed by evaluating the expectation values of the bond spin currents  $\langle \mathbf{s}_j \times \mathbf{s}_{j+\mu} \rangle_h$ , the  $z$  component of which is nonzero and is shown for  $t/J=1$  and  $k=(2\pi/3, 2\pi/3)$  in Fig. 5(a) and for  $k=(2\pi/3, 0)$  in Fig. 5(b). Note that both configurations exhibit dipolar spatial symmetry with  $\mathbf{k}$  as a reflection axis. [The symmetry corresponds to the dipolar current, see Eq. (2.4): i.e., component along  $\mathbf{k}$  is even under  $\mathbf{r} \rightarrow -\mathbf{r}$  while the component perpendicular is odd.] The spin currents vanish in the  $k=0$  and  $(\pi, \pi)$  states as required by symmetry. The same should be true of  $k=(\pi, 0), (0, \pi)$  points, which unfortunately do not exist for our cluster. As a rather arbitrary quantitative measure of the effect we display in Table IV the spin current on one of the bonds near the

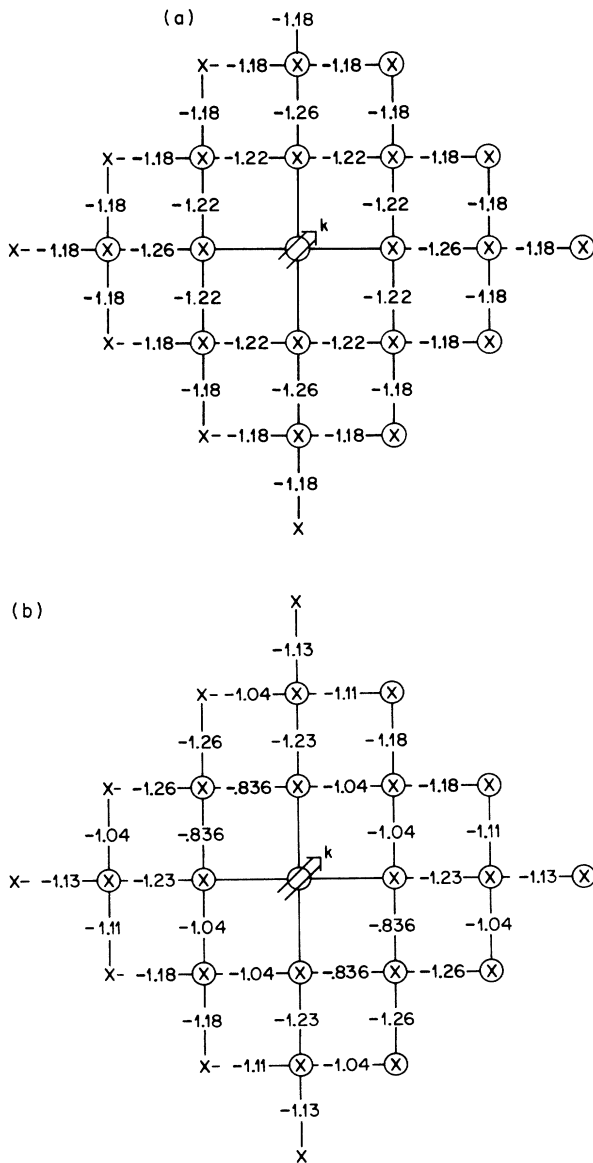


FIG. 4. Antiferromagnetic spin correlations for nearest-neighbor sites:  $2\langle \mathbf{s}_j \cdot \mathbf{s}_j \rangle - \frac{1}{2}$  in the  $k=(2\pi/3)(1,1)$  state for (a)  $t/J=0.05$ ; (b)  $t/J=2.5$ .

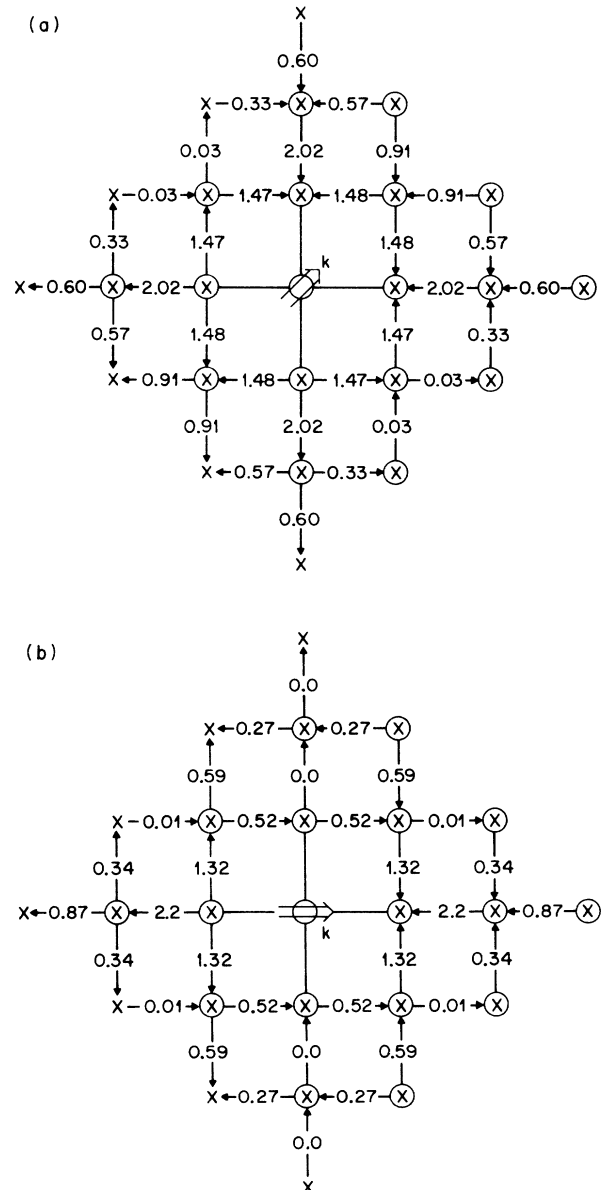


FIG. 5. The bond spin currents  $40\langle (\mathbf{S}_j \times \mathbf{S}_{j+\mu})^z \rangle$ , for  $t/J=1$  and (a)  $k=(2\pi/3)(1,1)$ ; (b)  $k=(2\pi/3)(1,0)$ .

TABLE IV. The vacancy spin current and the bond spin current (between sites 6 and 14, see Fig. 1) in the  $k=(2\pi/3)(1,1)$  state as a function of  $t/J$ .

$t/J$	$\hat{\mathbf{k}}_\mu \langle j_\mu^z \rangle$	$4 \langle \mathbf{S}_6 \times \mathbf{S}_{14} \rangle_z$
0.05	0.09	+0.018
0.1	0.16	0.035
0.25	0.36	0.077
0.5	0.56	0.12
1.0	0.68	0.15
2.5	0.40	0.16
5.0	-0.29	0.15
10.0	-1.81	0.13

vacancy [that between sites 6 and 14, see Fig. 1(a)] as a function of  $t/J$ . It can be argued<sup>16</sup> that at least for small  $t/J$  the twist of the staggered magnetization  $\hat{\Omega} \times \partial_\mu \hat{\Omega}$ , which is directly related to the bond spin currents  $\langle \mathbf{s}_j \times \mathbf{s}_{j+\mu} \rangle_h$ , correlates with spin current carried by the vacancy

$$\mathbf{j}_\mu = t \langle i(c_{r+\mu}^\dagger \hat{\tau} c_r - c_{r-\mu}^\dagger \hat{\tau} c_r) \rangle. \quad (4.2)$$

The expectation value  $\sum_{\mu=x,y} \hat{\mathbf{k}}_\mu \langle j_\mu \rangle$  is also displayed in Table IV. Note that magnitude of the bond spin current starts out linearly with  $t/J$  and then saturates. The presence of the spin twist with a dipolar symmetry near the vacancy implies a dipolar distortion of the staggered magnetization in the far field decaying as  $r^{-1}$  (since in the far field the distortion is small and the spin system is in the semiclassical regime). While our small cluster is nowhere near the far field it is not unreasonable to expect the dipole moment that is associated with the distortion to exhibit the same behavior as a function of  $t/J$  as the bond spin current  $\langle \mathbf{s}_6 \times \mathbf{s}_{14} \rangle$  displayed in Table IV. The vacancy spin current  $\mathbf{j}_\mu$  follows the same behavior at  $t/J \lesssim 1$  but then deviates. This deviation at large  $t/J$  can be attributed to the appearance of a ‘‘core’’ structure associated with the vacancy so that its spin is distributed over a finite region. The appearance of such a core is expected for large  $t/J$  on the basis of the ‘‘string’’ picture and is also indicated by the behavior of  $\langle \Omega^2 \rangle_h$  discussed earlier. At larger values of  $t/J$ , as the size of the core increases, one might expect that the bond currents near the hole also become affected, making the inference of the dipole moment from the near-field distortion unreliable.

Close examination of the pattern of spin currents for different values of  $t/J$  [see Figs. 6(a) and 6(b) as well as Fig. 5(a)] reveals an amusing finite-size effect. While for smaller  $t/J$  the currents have a roughly dipolar pattern with the magnitude falling off away from the hole, for  $t/J > 5$  one finds the current aligned with the wave number and essentially uniform through the cluster. It appears that the system takes advantage of the periodic boundary conditions and builds up a uniform twist. While the appearance of nearly a uniform  $\langle \hat{\Omega} \times \partial_\mu \hat{\Omega} \rangle$  here is clearly a finite-size effect, which makes one concerned about various results for larger values of  $t/J$ , it also offers an insight into the physics of a finite density of vacancies.<sup>22</sup>

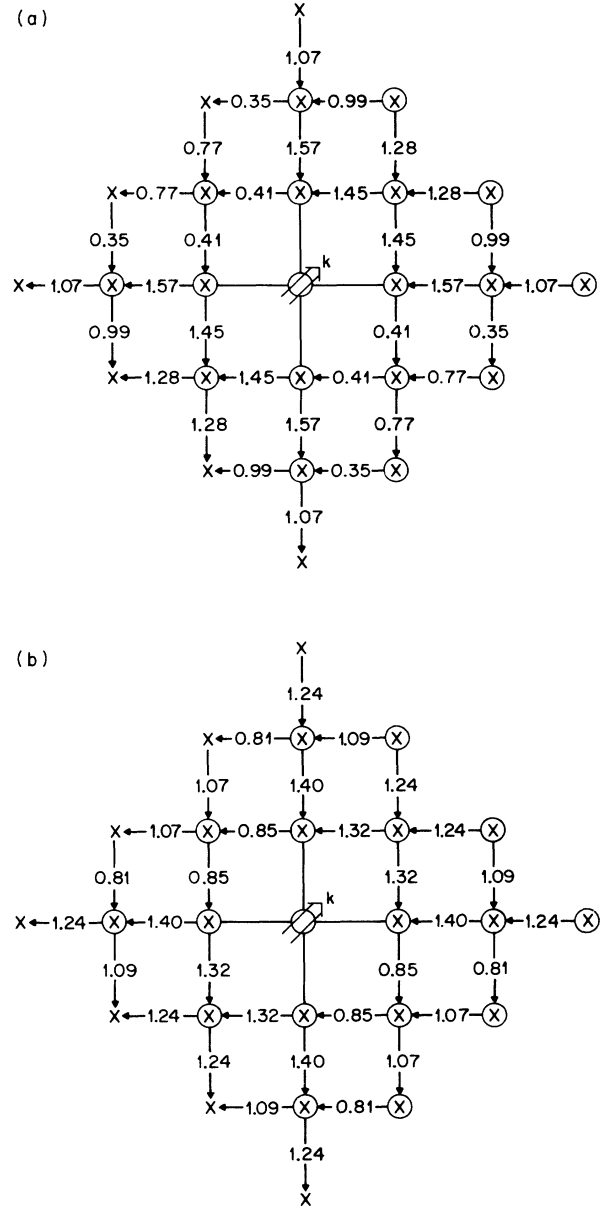


FIG. 6. The bond spin currents,  $40 \langle (\mathbf{S}_i \times \mathbf{S}_j)^z \rangle$ , for  $k=(2\pi/3)(1,1)$  and (a)  $t/J=5$ ; (b)  $t/J=10$ .

Finally, we have investigated a three-spin correlation function  $\langle \mathbf{s}_i \cdot (\mathbf{s}_j \times \mathbf{s}_k) \rangle$  defined on pairs of neighboring bonds and corresponding to the topological charge density.<sup>23</sup> We found it to be nonvanishing locally, which indicates the three-dimensional nature of the spin distortion. The topological charge density however changes sign when reflected about the direction of the  $k$  vector and hence the total topological charge averages exactly to zero.

## V. CONCLUSIONS

We have presented results for the vacancy band structure and examined the spin correlations in vacancy

ground states. It is evident that above and beyond the local suppression of the root mean square staggered magnetization (for the range of  $t/J$  studied this suppression remains less than 25%), the presence of the mobile hole causes a transverse distortion of the spins. The latter necessarily must be long ranged, because of the gaplessness of the spin-wave modes in the isotropic Heisenberg AF. While in this small cluster study it is not possible to directly see the far-field behavior, the dipolar symmetry of the near-field distortion evident on the small cluster dictates an  $r^{-2}$  falloff of the magnetization current  $\hat{\Omega} \times \partial_\mu \hat{\Omega}$ . Because the semiclassical expression Eq. (2.4) is only valid in the far field, an attempt to determine the numerical value of the "dipole moment"  $p_\mu^\alpha$  from the near-field bond spin currents may be misleading, however, it appears that this quantity increases linearly with  $t/J$  for small  $t/J$  and may saturate for  $t/J > 1$ . An interesting related and quantum mechanically well-defined quantity is the spin current of the vacancy,  $j_\mu$ . Finally, the nature of the spin distortion is different for states with different wave vectors: The dipolar twist of the staggered magnetization is dominant near zone face centers (where the ground state at least for  $t/J < 4$  is) while the "canting" distortion and local ferromagnetic polarization appear in the states with wave numbers near the zone center.

The antiferromagnetic dipole moment of the vacancy is induced by the hopping and is associated with the finite momentum of the ground state. One may expect however that the long-range distortion of the staggered magnetization will persist for a localized state of the vacancy, provided that the latter is not localized on a single site. It is natural to expect that in the absence of translational invariance, instead of finite momentum the ground state will have a finite angular momentum. The symmetry however may depend on the localizing potential<sup>24</sup> (i.e., whether it is site, bond, or plaquette centered).

It is important to understand the meaning of the vacancy spin. To the extent that the ground state of an even site lattice without a vacancy is a singlet, and with a vacancy has total spin  $\frac{1}{2}$ , there is no problem. However, the thermodynamic limit, with a finite density of holes and no total spin constraint is more difficult to interpret. It is evident, though, that in the presence of local staggered order the ground state of the vacancy is twofold degenerate, the degeneracy arising from the symmetry under time reversal and translation by one site. These states correspond to a particular superposition of the vacancy states with wave numbers  $\mathbf{k}$  and  $\mathbf{k} + (\pi, \pi)$  for the background with unbroken translational invariance. One naturally considers the two eigenstates of  $S_{\text{tot}}^z$ , the  $S_{\text{tot}}^z = \frac{1}{2}$  states having the vacancy more on one sublattice, while the  $S_{\text{tot}}^z = -\frac{1}{2}$  states have it more on the other. One may also take two orthogonal linear combinations of the  $S_{\text{tot}}^z$  eigenstates, even and odd under sublattice interchange. This would produce an expectation value of the spin in the plane perpendicular to the direction of local  $\hat{\Omega}$  (assumed to be along the  $z$  axis). It can be argued<sup>16</sup> that the dipole direction and staggered magnetization together define a SU(2) order parameter, and hence a triad of vectors. In the quantum sense these are conjugate to the lo-

cal magnetization and hence the spin. Still, it would be interesting to study in more detail the magnetization associated with the vacancy (i.e., the amount of net magnetization "bound" to the vacancy as opposed to excess magnetization spread over the whole volume of the system) as well as the vacancy  $g$  factor. One may expect that the latter depends on  $k$  and may actually vanish on the magnetic zone boundary and hence in the ground state.

The difficulty with interpreting the finite cluster results is due to the finite-size effects of which we can identify two types: one associated with the finiteness of the spin- $\frac{1}{2}$ -to-spin- $\frac{3}{2}$  gap, another with the large spatial size of the vacancy state for large  $t/J$ . We have attempted to account for (and subtract out) some of the more obvious manifestations of the effect of the first type. While in the range of  $t/J$  studied the size of the Brinkman-Rice string "core" of the vacancy state appears to be limited to only few sites,<sup>14</sup> we observed that the transverse "twist" distortion (associated with bond spin currents) for larger values of  $t/J$  extends over the whole cluster, making any interpretation of the  $t/J \gtrsim 5$  results questionable. A careful comparison of the results for different size clusters is needed to properly estimate the extent of the finite-size effects.

Finally, we note that the qualitative features of the vacancy state in the " $t$ - $J$ " model reported here are shared<sup>25</sup> by the O hole state in the more realistic three-band model of CuO layers.<sup>26</sup> In the latter case the issue of locating the band minimum using a 16-site cluster study is resolved by the presence of the direct O-O hopping process, which for realistic values of the parameters quite unambiguously places the minimum at the zone face centers. It is also worth noting that the current consensus places the "reasonable" values of effective  $t/J$  to be in the 2–5 range.

## ACKNOWLEDGMENTS

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## APPENDIX

Here we will briefly set up the  $t/J \ll 1$  perturbative calculation of the vacancy band in the context of the Holstein-Primakoff spin wave theory.<sup>27</sup> To facilitate the derivation let us formally separate the spin and charge degrees of freedom by factorizing the electron operator constrained to single occupancy:

$$c_\sigma(r) = \psi^\dagger(r) w_\sigma(r), \quad (\text{A1})$$

where  $\psi^\dagger(r)$  creates a fermionic vacancy on site  $r$  and  $w_\sigma(r)$  annihilates a Schwinger spin boson ( $\bar{w}w = 1$  for spin  $\frac{1}{2}$ ). In the spin-wave approximation the spins are represented by



$$w_r^A = \begin{pmatrix} 1 - \frac{1}{2} a_r^\dagger a_r \\ a_r \end{pmatrix}, \quad w_r^B = \begin{pmatrix} a_r \\ 1 - \frac{1}{2} a_r^\dagger a_r \end{pmatrix}, \quad (\text{A2})$$

where the superscripts  $A$  and  $B$  denote the sublattice and the spin-wave fluctuations away from the Néel state are represented by Bose operators  $a_r$ .

To the lowest order in spin-wave theory the hopping part of the Hamiltonian has the form

$$H_h = t \sum_{r \in A, \mu} \bar{\psi}_{r+\mu} \psi_r \bar{w}_r^A w_{r+\mu}^B + \text{H.c.}, \quad (\text{A3})$$

while the exchange part of the Hamiltonian Eq. (1.1) determines the magnon dispersion<sup>27</sup>  $\omega_k = 4J(1 - \gamma_k^2)^{1/2}$  where  $\gamma_k \equiv \frac{1}{2}(\cos k_x + \cos k_y)$ . (The exchange term also describes the interaction of spin waves with the static vacancy,<sup>21</sup> induced by the *absence* of the spin at the vacancy site.)

Clearly, the integration out of the spin fluctuations generates a self-energy,<sup>7,9</sup>  $\Sigma(\omega, k)$  term for the vacancy fermions. Within  $t/J \ll 1$  perturbation theory its  $\omega=0$  part generates the vacancy energy band. The straightforward spin-wave calculation then yields

$$E(k) = (4t)^2 \sum_q \omega_q^{-1} (u_q \gamma_{k-q} - v_q \gamma_k)^2 \quad (\text{A4})$$

with  $u_k^2 \equiv \frac{1}{2}[(1 - \gamma_k^2)^{-1/2} + 1]$  and  $v_k^2 \equiv \frac{1}{2}[(1 - \gamma_k^2)^{-1/2} - 1]$ , and the  $q$  summation runs over the Brillouin zone. The three-parameter fit to this expression is given in Eq. (2.3).

While this simple perturbative calculation gives the correct order of magnitude for the energy dispersion  $E(k)$  and appears to incorporate the correct physics, the approximation is uncontrolled. Aside from the general problem of applying the spin-wave approximation to the spin- $\frac{1}{2}$  case, there are a number of other difficulties related to inadequate description of the spins in the vicinity of the hole. As a result, the Ising-anisotropic limit ( $J_\perp \ll J_z$ ) of Eq. (A4) does not reduce to the appropriate perturbative result given in Eq. (2.2). This can be overcome by doing a variational calculation ( $t/J \ll 1$ ) using the Brinkman-Rice string wave function<sup>4,5</sup> for the vacancy in the spin-wave ground state. However the approximation remains uncontrolled. (Note that the variational nature of the wave function still does not allow to put any firm bounds on the bandwidth  $\Delta E$  since different  $k$  states may not be approximated uniformly.)

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level crossing transition to a ferropolaron (higher total spin) state happens (Refs. 11 and 13) at a value of  $t/J$  smaller than that for the infinite system.

<sup>19</sup>Here and below the bandwidth  $\Delta E$  is defined as  $\sup_k \{E(k)\} - \inf_k \{E(k)\}$ . This “coherent” bandwidth should not be confused with an “incoherent” bandwidth, which would include excited states with fixed  $k$  and therefore can be much larger.

<sup>20</sup>The choice of the 18-cluster was motivated by the accidental symmetry of the 16-site cluster (with nearest-neighbor interactions only) which makes states with  $k = (\pi/2, \pi/2)$  and  $k = (\pi, 0)$  degenerate.

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