Mobile vacancy in a quantum antiferromagnet: Effective Hamiltonian

Boris I. Shraiman
AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, New Jersey 07974

Eric D. Siggia
Department of Physics, Cornell University, Ithaca, New York 14853
(Received 20 November 1989)

A semiclassical analysis, as well as symmetry considerations, are used to explain and extend published quantum-cluster results for the ground state of a hole in a quantum antiferromagnet (AF). For the ground state with a wave vector in the face center of the reduced Brillouin zone, the spins twist into a dipolar configuration around the hole to optimize the hopping term, but remain coplanar. More complicated three-dimensional spin textures with staggered topological charge can be constructed by superimposing dipole states corresponding to distinct points in the Brillouin zone and different planes of spin twist. An effective Hamiltonian for the hole that generalizes the nonlinear sigma model is derived. The essential new term that is responsible for the textures described is a coupling between spin currents for the holes and background spins. The presence of the local antiferromagnetic correlations dictates a spinor representation of the vacancy. This description provides the foundation for the study of the phases of a quantum AF at low vacancy density.

I. INTRODUCTION

The prescient suggestion of Anderson as to the existence and importance of the copper moments in the high-T_c superconductors focused attention on the properties of the two-dimensional (2D) Hubbard model.[1] Experiments soon followed that showed, for at least one class of compounds, local moments that persisted from the insulating to the superconducting phase.[2,3]

This article, together with Ref. 4, amplify and extend Ref. 5 and are devoted to the properties of one hole in a quantum antiferromagnet as described by the model,

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

where $c_{r,\sigma}$ is the electron annihilation operator constrained to single occupancy. $\mathbf{s}=\frac{1}{2}c^{\dagger}\hat{\boldsymbol{\tau}}c$ is the spin. The sums are over all sites r on one sublattice of a 2D square lattice and $\hat{\mathbf{a}}=\pm\hat{\mathbf{x}},\pm\hat{\mathbf{y}}$ are the nearest neighbors. Various arguments have been advanced as to why (1.1) is a reasonable model for the Cu-O planes.[1,6–8] Reference 4 was devoted to a numerical study of an 18-site cluster described by (1.1). In this article we derive and explain those aspects of the one-hole problem that are present as long wavelengths and formalize our understanding in terms of an effective Hamiltonian. When one hole is properly understood, the various new phases that we[9,10] and others[11] have proposed for the normal state of (1.1) at low hole density follow readily. An effective Hamiltonian is useful in this regard since it clarifies the symmetries and, even if treated on a mean-field level, allows one to parametrize various strong-coupling corrections to the short-distance properties of (1.1).

Our principal points are the following. Holes carry with them transverse, dipole distortion (i.e., a twist) in the Néel order-parameter field; therefore, all three angles of SU(2) are needed to describe the spins. The spins twist to minimize the hole's kinetic energy just as in the Nagaoka problem[12] with the essential difference being where in the Brillouin zone the ground state occurs. In the effective Hamiltonian the spin twist originates as a coupling between spin currents. A spin configuration with topological charge, which in the far field is described by a skyrmion, can be created by superimposing two dipole states. Holes must be represented by a spinor wave function whose spin represents both physical angular momentum and a sublattice pseudospin. There is complete continuity in the long-wavelength properties of (1.1) from $t/J\ll 1$ up to $t/J\gtrsim O(10)$ when Nagaoka polarons form. Lastly, a semiclassical Born-Oppenheimer analysis is useful and appropriate at long wavelengths.

In Sec. II we summarize relevant facts about the low-lying states of (1.1) with no holes and then recapitulate the numerical results of Ref. 4. The dipole moment is exhibited using simple semiclassical or Born-Oppenheimer variational wave functions in both the small- and large-t/J limits in Sec. III. These results are reformulated in terms of a "gauge-invariant" phenomenological Hamiltonian in Sec. IV. Both a CP^1 spinor description with respect to the local order parameter and a vector spin representation are presented. Finally, in Sec. V we use just quantum mechanics and symmetries to explore the relation between the hole ground states with and without an infinitesimal symmetry-breaking field in order to clarify the quantum meaning of the dipole moment.

II. BACKGROUND PRELIMINARIES

A. Heisenberg and nonlinear σ model

A variety of theoretical techniques have been used to show that the spin-$\frac{1}{2}$ antiferromagnetic (AF) Heisenberg

model is Néel ordered in two dimensions on a square lattice.[13–17] Given sufficient Néel order, it is highly plausible[18] that the appropriate continuum theory for scales larger than the lattice is the NLσ model,

$$H_{\mathrm{NL}\sigma}=\tfrac{1}{2}\int d^2r[\chi^{-1}\mathbf{m}^2+\rho(\partial_a\hat{\Omega})^2]\ , \tag{2.1a}$$

where

$$\begin{aligned}&[m^{\alpha}(x),m^{\beta}(x')]=i\epsilon^{\alpha\beta\gamma}m^{\gamma}(x)\delta(x-x')\ ,\\&[m^{\alpha}(x),\Omega^{\beta}(x')]=i\epsilon^{\alpha\beta\gamma}\Omega^{\gamma}(x)\delta(x-x')\ ,\end{aligned} \tag{2.1b}$$

and the commutator of $\hat{\Omega}$ with itself is zero. (When employing the summation convention on products in physical space $a=x,y$, whereas lattice sums run over $a=\pm x,\pm y$.)

The unit vector, $\hat{\Omega}$, gives the direction of the staggered magnetization order parameter and the conjugate variable is the magnetization density $\mathbf{m}$. Equation (2.1) still contains quantum fluctuations which further renormalize the "bare" values of the magnetic susceptibility χ and the stiffness ρ, which are the only dimensional constants in the theory. The ratio of their renormalized values is the spin-wave velocity, $c^2=\rho_R/\chi_R$. To evaluate χ_R and ρ_R quantitatively and in a controlled manner for spin $\frac{1}{2}$ and a square lattice, it is necessary to work directly from the microscopic Hamiltonian (1.1).[19–21] Both ρ_R and the c are within 20% of their semiclassical values. If we recall the moderate reduction in the magnitude of the order parameter from its Néel value, $\frac{1}{2}$, due to quantum fluctuations, then all these numbers suggest that $S=\frac{1}{2}$ in two dimensions is indeed large.

In other terms, if we were to represent the 2D quantum ground state as a 3D classical partition function, then the latter would be well into the order regime and have a short correlation length.[22] Once this correlation length was exceeded, the remaining renormalization of ρ and χ could be calculated from nonlinear spin-wave theory, i.e., (2.1). It will occasionally clarify approximations to realize that the validity of (2.1) can be pushed further towards lattice scales by imagining a next-nearest-neighbor ferromagnetic exchange added to (1.1).

Clearly (2.1) is rotationally invariant so that the total spin $\int\mathbf{m}dx$ is conserved. A less obvious constant of the motion is $\mathbf{m}(x)\cdot\hat{\Omega}(x)$, which, in fact, commutes with all operators in the theory, and can therefore be eliminated directly. Its physical interpretation is as a generator of rotations about $\hat{\Omega}$. Clearly when the sole "coordinate"-like variable is a unit vector, rotations about it are physically meaningless.

Another important quantity in the following will be the current $\mathbf{J}_a$ for the conserved magnetization $\mathbf{m}$; which suppressing a constant ρ is

$$\mathbf{J}_a=\hat{\Omega}\times\partial_a\hat{\Omega}\ . \tag{2.2}$$

The equation of motion for $\mathbf{m}$ is just $\partial\mathbf{m}/dt=-\rho\partial_a\mathbf{J}_a$.

The presence of Néel order makes any topological correction to (2.1) unlikely.[23] The other ostensible difference between (2.1) and the finite-lattice Hamiltonian, namely that the lattice ground state is a singlet[24] while the thermodynamic ground state of (2.1) is ordered for comparable parameters, is a subtlety of the thermodynamic limit and not the representation. The dichotomy disappears if either a staggered field, vanishing with the volume, is applied to the quantum model or an average over the uniform mode is done in the classical case.[25] A more extensive discussion of the quantum case is left for Sec. V.

B. Numerical results

Determining the exact ground state of (1.1) for an 18-site cluster and one hole is, presently, the most convincing route to finding the band energy and spin distortion around the hole.[4] We work for $t/J\lesssim 4$ where finite-size effects are not too serious, and we found, in addition, that nothing qualitative changes as t/J decreases even if it becomes much less than one. A good understanding of the energy has been obtained by a variety of analytic methods (cf. Ref. 4), sometimes only rigorously justified for $t/J\ll 1$. Here, too, we will frequently exploit the small-t/J limit to make the physics of the spin distortion most transparent and then do more ponderous calculations in the physically relevant limit.

It is important to realize that the exact strongly coupled ground state of (1.1) for one hole may be put into Bloch form because the underlying Hamiltonian is translationally invariant. Specifically,

$$\psi_k=\sum_{r,\{\sigma\}}e^{ikr}\phi_k(r,\{\sigma_\rho\})|r,\{\sigma_\rho\}\rangle\ , \tag{2.3}$$

where r is the hole location, which is summed over the entire lattice, and $\{\sigma_\rho\}$ denote a complete set of spin eigenstates at all sites $\rho\neq r$. The amplitude ϕ obeys, of course,

$$\phi_k(r+a,\{\sigma_{\rho+a}\})=\phi_k(r,\{\sigma_\rho\})\ .$$

Corresponding to (2.4) is the energy dispersion $E(k)$ and a Brillouin zone which, in the presence of AF order, is reduced to the diamond defined by $(\pi,0),(0,\pi)$, $(-\pi,0),(0,-\pi)$ (Fig. 1).

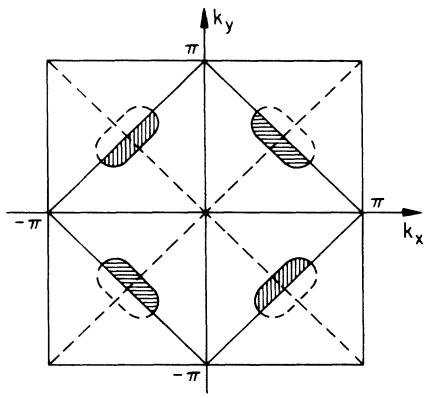

FIG. 1. The reduced Brillouin zone appropriate for an AF ordered system. The constant energy surfaces near the ground state $(\pm\pi/2,\pm\pi/2)$ are shown as semiellipses. Note that by using the reciprocal-lattice vector (π,π) the correct count of states includes only two complete ellipses.

The other quantum number characterizing the quantum cluster is the total spin which is always the minimum possible, i.e., $\frac{1}{2}$, so long as finite-size effects play no role. The square of the order parameter is not greatly reduced by the hole but its direction fluctuates, and the associated subtleties of interpretation are deferred to Sec. V when they were not already discussed in Ref. 4.

The energy $E(k)$ is conveniently parametrized by

$$E(k)=-c_1+c_2(\cos k_x+\cos k_y)^2-c_3(\sin^2 k_x+\sin^2 k_y) \tag{2.4}$$

with $c_i>0$ and $c_2>c_3$. The second terms favor the zone face over the zone center while the last term places the energy minimum at $(\pm\pi/2,\pm\pi/2)$ rather than at the zone corners $(\pi,0)$, etc. Near the minimum energy, the mass perpendicular to the face is lighter than the parallel mass.

The symmetry of the bond spin currents $\mathbf{s}_r\times\mathbf{s}_{r+a}$ allows one to deduce the structure of the spin distortion[4] even though its far-field behavior is not directly accessible in the small cluster study. In the continuum limit (as we shall argue below), the spin distortion defines the dipole moment $\mathbf{P}_b$ according to

$$\hat{\Omega}\times\partial_a\hat{\Omega}=(\delta_{ab}-2\hat{\mathbf{r}}_a\hat{\mathbf{r}}_b)\frac{\mathbf{P}_b}{r^2}\ . \tag{2.5}$$

The k dependence of the dipole moments has the same symmetry as $\sin k_a$ as it must, and so vanishes at the zone corners and center. Finally, ferromagnetic polarons, which occur in our simulations for large t/J as a finite-size effect, change the ground state to $k=0$ and its spin from $\frac{1}{2}$ to $\frac{17}{2}$ (i.e., the maximal value).

C. Operator definition of dipole moment

We remarked in Refs. 4 and 5 and will amplify below that the dipolar distortion in the spin field around the hole resembles the incompressible flow of superfluid for a roton state in ^{4}He. This suggests that we examine the equation of motion for the local spin

$$\frac{d}{dt}c_\tau^\dagger\hat{\tau}c_r=it\sum_{\hat{\mathbf{a}}}(c_r^\dagger\hat{\tau}c_{r+\hat{\mathbf{a}}}-\text{H.c.})-i2J\mathbf{s}_r\times\sum_{\hat{\mathbf{a}}}\mathbf{s}_{r+\hat{\mathbf{a}}}\ . \tag{2.6}$$

The site occupied by the hole has a spin of zero. This should not be confused with the total spin of the many-particle ground state of (1.1) for one hole which is $\frac{1}{2}$.

The current corresponding to (2.6) is

$$\mathbf{j}_a(r)=it(c_r^\dagger\hat{\tau}c_{r+a}-\text{H.c.})+i2J\mathbf{s}_r\times\mathbf{s}_{r+a}\ . \tag{2.7}$$

Clearly the first term in (2.7) is only nonzero when either i or $i+a$ is occupied by a vacancy while the second is only nonzero in the complementary cases. The expectation value of $\mathbf{j}_a$ in any translationally invariant one-hole eigenstate of H must be along $\mathbf{k}$ by symmetry and independent of r. A more interesting quantity is, of course,

$$\mathbf{I}_a(r)=\sum_\sigma\langle\{c_{0,\sigma}c_{0,\sigma}^\dagger,\mathbf{j}_a(r)\}\rangle$$

which measures the current relative to the hole[4] ($\{\ldots,\ldots\}$ here denotes an anticommutator).

Using (2.5) we can identify the dipole moment from the Fourier transform of $\mathbf{I}_a$,

$$\mathbf{P}_a=\lim_{k\to0}\left[\frac{k_ak_b}{k^2}\mathbf{I}_b(k)\right]\ .$$

The limit should exist since, if we take the lattice divergence of $\mathbf{I}_a$, use the equation of motion (2.6) and the commutator with H to transfer the time derivative, one obtains,

$$\left\langle\left\{\frac{d}{dt}\sum_\sigma(c_{0,\sigma}c_{0,\sigma}^\dagger),c_r^\dagger\tau c_r\right\}\right\rangle\ .$$

This should decay exponentially for large r since the hole density should couple only to the magnitude of the spin order parameter, not its direction.

More naively, since the dipole moment of the hole is manifest in the far-field spin current, it makes sense to identify the first term in (2.7) as the source of this current and hence as an operator expression for the dipole moment of the hole, viz.,

$$\mathbf{P}_{r,a}=i(c_r^\dagger\hat{\tau}c_{r+a}-\text{H.c.})\ . \tag{2.8}$$

Note that (2.8) is defined on a bond and hence carries a spatial vector index. It has not proved possible to derive the effective Hamiltonian of Sec. IV merely by regrouping the lattice operators manifest in the theory and directly taking a continuum limit as Affleck did for (2.1).[26] The bare Hamiltonian is too bare and certain fluctuation effects have to be explicitly calculated.[27]

III. SEMICLASSICAL

A. Justification

We remarked in the previous section that the Heisenberg model is ordered and if one were to imagine integrating out the smallest scales one would rapidly reach a scale where the nonlinear σ model was quantitatively applicable and all subsequent renormalizations were calculable from (2.1). The influence of the hole can extend into this region since there is a broken continuous symmetry and $\hat{\Omega}$ will decay algebraically while the magnetization and whatever perturbation the hole makes to the magnitude of the order parameter decay exponentially.

In this regime a semiclassical calculation which factors in (2.3) into the product of spinors is eminently reasonable. More precisely, provided only that there is Néel order, sufficiently far from the hole there will, in general, be a $\hat{\Omega}(r)$ satisfying,

$$\nabla^2\hat{\Omega}=0\ , \tag{3.1}$$

irrespective of quantum fluctuations. In the continuum, semiclassical limit, the hole merely furnishes the boundary conditions to be imposed on (3.1) for small r and thus determines the symmetry of the state. (The same point was made in the previous subsection using the spin current.)

Spins distort around the hole to facilitate the hopping and thereby optimize the kinetic energy. With an intelligent superposition of one-particle spin states the symmetry of the hole's immediate environment can be calculated variationally for small t/J from the expectation value of the hopping term in (1.1). Isotropic exchange is now essential, i.e., Eq. (3.1), and stabilizes the twist induced by the hopping. The energy gain due to the twist is $O(t^2/J)$ after minimization with respect to the spin field and in accordance with Ref. 4.

To work in the physical $t/J \gg 1$ limit we first have to calculate the scrambling of the spins by the multiple hops the hole makes to minimize its kinetic energy[28] the spin dynamics does not play a role here and in Sec. III D we work within a Born-Oppenheimer approximation (the hopping is faster than the spin exchange) still treating the spins semiclassically.

For a plausible variational function a spin twist emerges again, now expressed in a form analogous to that emerging in the effective Hamiltonian of Sec. IV. It is explicitly shown that multiple hops do not diminish the magnitude of the twist, i.e., dipole moment, in accord with the numerical results.

B. Analytical results for $t \ll J$

We now proceed to evaluate the hopping variationally in the semiclassical approximation by factorizing ϕ in (2.3) into the product of spinors. Thus, we introduce a slowly varying spinor field $z_\sigma(r)$, $\bar{z}z=1$ (the Schwinger spin boson) corresponding to the local direction of the staggered magnetization $\hat{\Omega}$. The rapid alternation of spins from sublattice A to B is accounted for by the time-reversal operator acting on z_r for one of the sublattices. Finally, we want to allow for a small canting common to both sublattices which we parametrize by the spinor field $p_\sigma(r)$, $\mathrm{Re}(\bar{p}z)=0$. Thus, the actual spins on the two sublattices are given by spinors $w^{A,B}$ defined as

$$\begin{aligned} w_\sigma^A &= z_\sigma + \tfrac{1}{2}p_\sigma \ , \\ w_\sigma^B &= \epsilon_{\sigma\nu}(z_\nu^* - \tfrac{1}{2}p_\nu^*) \ , \end{aligned} \tag{3.2}$$

where multiplication by the antisymmetric matrix ϵ ($\epsilon_{12}=-\epsilon_{21}=1$) followed by complex conjugation implements time reversal. The spinors z,p are defined only within the AF reduced Brillouin zone so that there is no overcounting of the number of degrees of freedom in (3.2). The w's are normalized to one, and we work to first order in p, $\bar{p}p \ll 1$, and also neglect ∂p. One then finds, as desired,

$$\mathbf{s}^{A,B} = \pm \bar{z}\hat{\tau}z + \tfrac{1}{2}(\bar{z}\hat{\tau}p + \bar{p}\hat{\tau}z) \tag{3.3a}$$

and by definition[26]

$$\begin{aligned} \mathbf{m} &= \tfrac{1}{2}(\mathbf{s}^A + \mathbf{s}^B) = \tfrac{1}{2}(\bar{z}\hat{\tau}p + \bar{p}\hat{\tau}z) \ , \\ \hat{\Omega} &= \tfrac{1}{2}(\mathbf{s}^A - \mathbf{s}^B) \ . \end{aligned} \tag{3.3b}$$

The identification of $\mathbf{m}$ and $\hat{\Omega}$ can be verified by taking z and p as Bose operators and checking the commutators (2.1b) as we do in Sec. IV, Eq. (4.12).

To evaluate the hopping, all spinors will depend upon their distance from the hole, ρ, and to keep track of the up-down dependence it is necessary to split the lattice sum (2.3) into $r \in A$ and $r \in B$. One therefore has

$$\begin{aligned} |k\rangle = {} & \psi_A (2N^{-1})^{1/2} \sum_{r\in A,\{\sigma\}} e^{ikr} \prod_{\rho\neq 0} w_\sigma^{\alpha(A,\rho)}(\rho) |r,\{\sigma\}\rangle \\ & + \psi_B (2N^{-1})^{1/2} \\ & \times \sum_{r\in B,\{\sigma\}} e^{ikr} \prod_{\rho\neq 0} w_\sigma^{\alpha(B,\rho)}(\rho) |r,\{\sigma\}\rangle \ , \end{aligned} \tag{3.4}$$

where $\alpha(A/B,\rho)$ selects w^A or w^B depending on the sublattice occupied by the hole and ρ (N is the number of lattice sites and ρ is the distance measured from the hole).

Figure 2 illustrates the computation of the hopping matrix element. Due to the displacement of the hole, the inner product between spinors at $\rho=\pm\hat{\mathbf{a}}$ is drawn from opposite sublattices and therefore would be zero in the undistorted semiclassical ground state. The inner product for the remaining lattice sites involves spins from the same sublattice but whose position relative to the hole differs by $\hat{\mathbf{a}}$ (cf. Fig. 2). In the continuum limit, the results is a pure phase Δ_a of order t/J

$$e^{i\Delta_s} = \prod_{r\neq 0,\hat{\mathbf{a}}} \bar{z}(r-\hat{\mathbf{a}})z(r) \simeq \exp\left[\int \bar{z}\partial_a z d^2 r\right] .$$

The hopping matrix element then reads

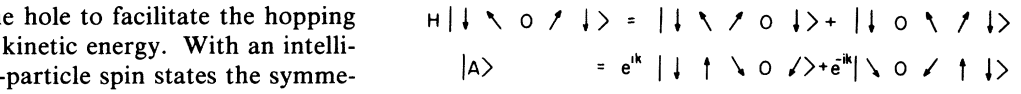

FIG. 2. Calculation of the matrix element $\langle A|(H|B\rangle)$, for a hop along $\pm\hat{\mathbf{x}}$. Only the nearest neighbors of the hole are shown distorted and in a manner appropriate to $k\sim(\pi/2,\pm\pi/2)$. Corresponding sites are displaced vertically. The phases shown on the $|A\rangle$ states are relative to the corresponding $|B\rangle$ states which appear on the line above.

$$\begin{aligned} 2\,\mathrm{Re}(\langle A|H_{\mathrm{hop}}|B\rangle) = -2t\ \mathrm{Re}\Big[& \psi_A^\dagger \psi_B \sum_a \epsilon_{\mu\nu}\{2i\sin(\mathbf{k}\cdot\hat{\mathbf{a}}+\Delta_a) z_\mu(-\hat{\mathbf{a}}) z_\nu(\hat{\mathbf{a}}) \\ & + \cos(\mathbf{k}\cdot\hat{\mathbf{a}}+\Delta_a)[p_\mu(-\hat{\mathbf{a}}) z_\nu(\hat{\mathbf{a}}) - z_\mu(-\hat{\mathbf{a}}) p_\nu(\hat{\mathbf{a}})]\}\Big] \ . \end{aligned} \tag{3.5}$$

Notice that the coupling is solely to $\hat{\Omega}$ for $k\sim(\pi/2,\pi/2)$ [N.B., $\hat{\Omega}=\bar{z}\hat{\tau}z$ from (3.3)] while for $\mathbf{k}$ near the zone center and corners the magnetization appearing in the second term becomes important. The former term is the product of two factors odd under $a\rightarrow -a$ while the latter involves even factors.

To proceed further with the minimization, we will drop Δ_a [which is $O(t/J)$], and assume (and justify in Sec. III C) that it suffices to take $\mathbf{m}$ parallel to $\hat{\mathbf{z}}$ and $\hat{\Omega}$ predominantly in the $(\hat{\mathbf{x}},\hat{\mathbf{y}})$ plane. We may then parametrize

$$z=\begin{bmatrix} e^{i\phi/2}\cos(\theta/2) \\ e^{-i\phi/2}\sin(\theta/2)\end{bmatrix} e^{i\gamma/2}\ ,$$
$$p=\epsilon\begin{bmatrix} e^{i\delta/2\cos(\theta/2)} \\ -e^{-i\delta/2}\sin(\theta/2)\end{bmatrix} e^{i\gamma/2}\ , \tag{3.6}$$

where $\epsilon\ll 1$ sets the scale of the magnetization and θ is close to $\pi/2$. Equation (3.6) explicitly makes $m_{x,y}=0$ in (3.3b) and $\mathrm{Re}(\bar{p}z)\sim O((\theta-\pi/2)^2)$. [The norm of w in (3.2) is $1+\epsilon\cos(\delta-\phi)/2$, i.e., one plus something second order in small quantities which may be neglected in the minimization.]

After substituting into (3.5) one observes that $\phi(a)$ is small. $\psi_A=\psi_B=1/\sqrt{2}$ without lose of generality, and ϕ may be omitted from the term involving p in (3.5) since it only occurs as the argument of a *cosine*. The third angle in the SU(2) parametrization of $\hat{\Omega}$, γ in (3.6) is an overall factor within the curly brackets of (3.5) and therefore is locked to the relative phase of ψ_A,ψ_B. The final result for the hopping is

$$E_k=-t\sum_a([\phi(a)-\phi(-a)]\sin(ka) +\epsilon\{\cos[\delta(a)/2] +\cos[\delta(-a)/2]\}\cos(ka))\ . \tag{3.7}$$

The twists implied by (3.7) are balanced by an exchange term which, with these approximations and in the continuum limit, becomes

$$H_{\mathrm{ex}}=\tfrac{1}{2}\int[\chi^{-1}m^2+\rho(\nabla\phi)^2]\ ,$$

where $m=2\epsilon\cos(\delta)$ [cf. (3.3b)], and $\chi^{-1}\sim\rho\sim J$.

Minimizing, with r the distance from the hole in lattice units,

$$\phi(r)=\mathbf{p}\cdot\mathbf{r}/r^2,\quad r\gtrsim 1\ ,$$
$$m=O(t/J)\cos(\mathbf{k}\cdot\mathbf{r}),\quad |r|\sim 1\ , \tag{3.8}$$

where the vector $p_a=O(t/J)\sin k_a$. The magnetization is always exponentially localized around the hole. It is uniform for $k\sim 0$ as expected for Nagaoka's ferropolarons and quadrapolar for k at zone corners. The order-parameter distortions are long ranged and of dipolar symmetry determined by k. They vanish only at the zone center and corners where one can no longer define a vector p_a. The actual spin arrangement around the hole is shown in Fig. 3. Note that there are actually two distinct possible states corresponding to multiplying ϕ in (3.8) by ± 1.

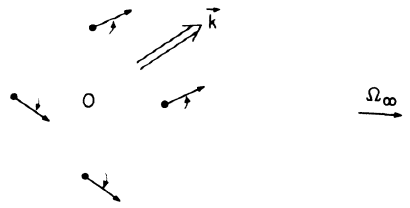

FIG. 3. Schematic of one of the two possible dipolar spin configurations around a hole for $t/J\ll 1$ according to the semiclassical treatment of Sec. III B for $k=(\pi/2,\pi/2)$. The Néel order parameter is along $\hat{\mathbf{x}}$ at infinity.

It is revealing to reexpress the order-parameter field by calculating the current (2.2), for (3.6)–(3.8).

$$\hat{\Omega}\times\partial_a\hat{\Omega}=\hat{\mathbf{z}}\partial_a\phi=\hat{\mathbf{z}}(\delta_{ab}-2\hat{\mathbf{r}}_a\hat{\mathbf{r}}_b)p_b/r^2\ . \tag{3.9}$$

Its dipolar distribution should be reminiscent of the potential flow field in a roton state of superfluid helium, with the conserved quantity now being the magnetization rather than the density. The analogy is further reinforced by the observation that both the roton and the vacancy in an AF have minimum energy for $k\neq 0$.

The meaning of the dipole moment in (3.9) and particularly its spin dependence can be further clarified by computing the expectation value of the dipole operator, (2.8), in the semiclassical ground state. Since we are interested only in $k\sim(\pi/2,\pm\pi/2)$ we ignore the uniform magnetization and find

$$\langle\mathbf{P}_{0,a}\rangle=\frac{2t}{N}\mathrm{Im}\{(2\psi_A^*\psi_B)[\epsilon_{\mu\nu}z_\nu(\hat{\mathbf{a}})\tau_{\mu\mu'}z_{\mu'}(-\hat{\mathbf{a}})e^{ika} -(\hat{\mathbf{a}}\rightarrow-\hat{\mathbf{a}})]\}\ . \tag{3.10}$$

The vector within square brackets, when evaluated from (3.6)–(3.8), becomes

$$(0,-i,1)e^{i(\gamma_a+\gamma_{-a})/2}2i\sin(\mathbf{k}\cdot\hat{\mathbf{a}})$$

plus terms of $O(\phi_{\pm a}^2)$ which is small, as is $(\gamma_a-\gamma_{-a})$. The vector is therefore, for reasons of symmetry, perpendicular to $\hat{\Omega}$ at infinity and its direction is controlled by $e^{i\gamma}$ and the other phase factors in (3.10). At the energy minimum its direction is $\hat{\mathbf{z}}$ as expected from (3.9). Its magnitude is $O(t/J)$ once one divides (2.6) by J to agree with (3.9). The volume factor disappears if we normalize to the probability of finding the hole at the origin.

It is also appropriate to note here that if we imagine the hole in a rotationally invariant state, such as would be created by a localizing impurity, then seemingly more complicated spin configurations than dipoles can be created by superimposing states from the two inequivalent valleys at $(\pi/2,\pm\pi/2)$. Specifically, we take $\hat{\Omega}=\hat{\mathbf{z}}$ at infinity and superimpose the dipole states with $\hat{\Omega}$

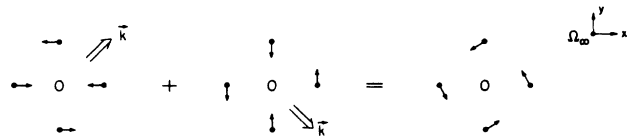

FIG. 4. The average spin field obtained by superimposing a dipole with $k\sim(\pi/2,\pi/2)$ and $\hat{\Omega}$ in the x,z plane with a $k\sim(\pi/2,-\pi/2)$ dipole and $\hat{\Omega}$ in the y,z plane. At infinity Ω is parallel to $\hat{\mathbf{z}}$.

in the x,z plane for one valley and with $\hat{\Omega}$ in the y,z plane for the other valley. The wave function is no longer strictly semiclassical since it is the sum of such wave functions, and in Fig. 4 we plot the average spin vectors on the four sites surrounding the hole or equivalently the correlation function $\langle n(0)\mathbf{s}(r)\rangle$, where n is the density operator for a hole. This will suffice to determine the symmetries of the state which is p-like when rotated around the hole.

There is a further degeneracy in Fig. 4 which is related to the sense in which the spins must be rotated around $\hat{\mathbf{z}}$ in order to bring into coincidence the spins on two sites related by a given $\pi/2$ spatial rotation. The sign of the topological charge measures this handedness,[29] i.e.,

$$\Gamma=\int\hat{\Omega}\cdot(\partial_x\hat{\Omega}\times\partial_y\hat{\Omega})\ ,$$

where we use the average spin to evaluate $\hat{\Omega}$ adjacent to the hole. Of course, Γ does not change if we rotate all spins by the same amount. Far from the hole, a semiclassical description should again apply and we have to recalculate $\hat{\Omega}$ from (3.1) with the boundary condition suggested by Fig. 4. One finds, with our conventions, the skyrmion solution[29]

$$\Omega_z=\frac{r^2-\lambda^2}{r^2+\lambda^2},\quad \Omega_x+i\Omega_r=\frac{x\pm iy}{r^2+\lambda^2}\ .$$

The scale size λ should be adjusted such that near the hole the spin deviation is $O(t/J)$ in the small t and therefore the total topological charge in the far field is $O(t^2/J^2)$. Whether a hole bound to an impurity[30] actually has a finite orbital angular momentum in the ground state requires an explicit calculation. We can only claim here that skyrmion solutions are not unexpected when dipoles are already present and from the form of the current-current coupling in Sec. IV, skyrmions favor a finite angular-momentum state for the holes. Note that if the topological charge is computed from three nearby spins drawn from the same sublattice, it will reverse sign with the sublattices.

C. Numerical minimization

We have also directly minimized the expectation value of the energy in (2.4) taking $\psi_A=\psi_B=1/\sqrt{2}$ as allowed by symmetry, but making no assumption what so ever about the spinors $w^{A,B}$. This serves as a check that the various assumptions about the symmetry of the solutions

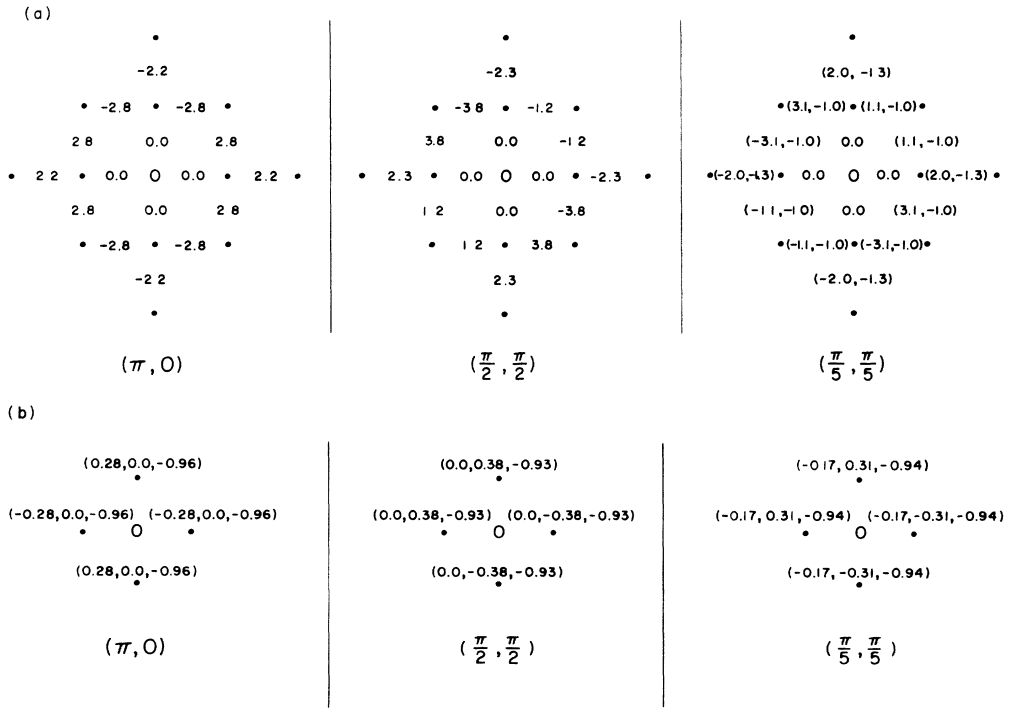

FIG. 5. Spin configuration around a hole on the A sublattice for the semiclassical variational wave function minimized numerically for the values of $\mathbf{k}$ shown and $J=t$. Lattice points are shown as circles the hole occupies the central site in all cases. In (b) we show the nonzero components [$\hat{\mathbf{y}}$, $\hat{\mathbf{x}}$, and $(\hat{\mathbf{x}},\hat{\mathbf{y}})$, respectively] of the bond spin currents, $\mathbf{s}_r\times\mathbf{s}_{r+a}$. Signs are chosen to make the currents in the second two cases invariant when reflected across the direction of $\mathbf{k}$ in physical space.

as a function of k are indeed correct. Also, we now find a quadrapolar distortion in Ω as well as $\mathbf{m}$ at $k=(\pi,0)$ which will, of course, dominate far from the hole.

We chose directions such that $\hat{\Omega}=(0,0,1)$ far from the hole (spin up on A down on B). In addition, we calculate the total magnetization for $|A\rangle$ and $|B\rangle$ separately (i.e., hole on the A sublattice or on B) and always find a component along $\hat{\mathbf{z}}$ which is negative and order 1 for $|A\rangle$ and equal but opposite for $|B\rangle$. This merely represents the loss of one spin due to the hole. The uniform canting we observe for k strictly inside the Brillouin zone is the same for both $|A\rangle$ and $|B\rangle$ and in the $\hat{\mathbf{x}}$ direction because of the various free phase factors we have assumed. To obtain a sensible approximation to the correct quantum ground state, we have to superimpose $|A\rangle$ and $|B\rangle$ and then rotate and average all spins around $\hat{\mathbf{x}}$. The net magnetization is then along $\hat{\mathbf{x}}$ and contains a contribution from the canting as well as from the separate pieces along $\pm z$ due to the superposition. We could replace $\hat{\mathbf{x}}$ with any other direction perpendicular to $\hat{\Omega}$ at infinity by including an additional relative phase between $|A\rangle$ and $|B\rangle$, i.e., by taking $\psi_A/\psi_B=e^{i\gamma}$. Further discussion of the relation between the classical and quantum solutions is deferred to Sec. V.

Figures 5(a) and 5(b) permit one to verify the symmetries noted above (which are independent of t/J). The bond spin currents $\mathbf{s}_i\times\mathbf{s}_{i+a}$, are a particularly useful way to display the gradients of $\hat{\Omega}$ as was done in Ref. 4.

One unphysical feature of these results is that the energies near $k=0$ are lower than at $(\pi,0)$, though $(\pi/2,\pi/2)$ remains the ground state. This can be understood if one remembers that the energy splitting between $k=0$ and the zone boundary is mostly due to spin fluctuations, more precisely, two hops followed by a spin exchange, and thus absent in a semiclassical wave function.

D. Large t/J

In this limit we follow Brinkman and Rice[28] and represent the ground-state wave function of the hole as a "string," a sequence of hops through a frozen spin background. This is reasonable because the hopping is more rapid than the spin dynamics (yet t is not so large as to favor the formation of a ferropolaron).[28,31] The hops scramble the spins in the AF background and the cost in exchange energy is Jl, where l is the number of hops. The kinetic-energy gain is of order $-t/l^2$ implying a mean $\bar{l}\sim(t/J)^{1/3}$ and the energy is

$$E_0=-2\sqrt{3}t+2.7J^{2/3}t^{1/3}\ . \tag{3.11}$$

Note that both terms are much larger than the energy scales described by the σ model, i.e., J times gradients. The core region where the hopping suppresses the magnitude of the order parameter is exponentially localized.

We will show that a trial wave function incorporating the "string" dynamics gives rise to a twist in the spin background, expressed semiclassically, that does not decrease with t/J in accordance with the numerical simulations (Ref. 4). This argument is not rigorous since the absolute energy is not accurate to $O(J)$ and zero-point motion of the spins is neglected. We expect, however, quantum fluctuations merely to renormalize the magnitude of the twist in qualitatively the same way they reduce the magnitude of the order parameter or any other long-range spin distortion. Our goal in this section is merely to make plausible that large t and multiple hops are not per se inimical to a dipolar twist.

It is both calculationally convenient and physically instructive to work in this section with a vector representation for the spins rather than a spinor one. This anticipates the effective Hamiltonian in Sec. IV and yields an expression manifestly rotationally invariant in spin space in contrast to (3.7)–(3.9).

In accordance with (2.3) we make the string wave function (the quantity within large parentheses below), translationally invariant and furthermore allow for a slowly varying amplitude χ which will facilitate the interpretation of various matrix elements. We therefore define a trial function

$$|\psi_\nu(k)\rangle=\frac{1}{\sqrt{N}}\sum_r e^{ikr}\chi_\sigma(\nu,r)\left[c_\sigma(r)+\gamma_1\sum_{\hat{\mathbf{a}}'}c_{\sigma'}(r+\hat{\mathbf{a}}')c^\dagger_{\sigma'}(r)c_\sigma(r)\right.$$
$$\left.+\gamma_2\sum_{\hat{\mathbf{a}}'\neq-\hat{\mathbf{a}}'}\sum_a c_{\sigma''}(r+\hat{\mathbf{a}}'+\hat{\mathbf{a}}')c^\dagger_{\sigma''}(r+\hat{\mathbf{a}}')c_{\sigma'}(r+\hat{\mathbf{a}}')c^\dagger_{\sigma'}(r)c_\sigma(r)+\cdots\right]|\underline{R}\rangle\ , \tag{3.12}$$

where ν is a spin label for the hole and c are the usual Fermion operators constrained to single occupancy. They act on a product of single-particle spin states described by a smoothly varying rotation matrix, $\underline{R}$, acting on the Néel state. In particular, the spin density matrix is

$$2\langle\underline{R}|c^\dagger_\sigma(r)c_{\sigma'}(r)|\underline{R}\rangle=\delta_{\sigma\sigma'}+\hat{\tau}_{\sigma\sigma'}\cdot\hat{\mathbf{s}}(r) \tag{3.13}$$

with $\hat{\mathbf{s}}^2=1$ normalization. The successive products in (3.12) are build up by acting with the hopping and γ_{l+1} equals $3^{-l/2}/2$ for normalization, times an appropriate Airy function which varies with l on a scale $\sim(J/t)^{1/3}$ (Ref. 31). Note that it is the admixture of various length l "strings" that brings the ground-state energy down on an energy scale of order t.

In the matrix element $\langle\psi|E_k|\psi\rangle$, the terms we need are of the form $\gamma_l^*\gamma_l$, and we follow Brinkman and Rice in assuming that the two sums over the intermediate bond vectors $\hat{\mathbf{a}},\hat{\mathbf{a}}',\ldots,$ in the bra and ket simply collapse; that is, the hole retraces its path. Then each term in l, the number of hops, has a common factor containing the spin and k depen-

dence, while the sum over l is essentially the norm and therefore of order 1:

$$\langle\psi|E_k|\psi\rangle\sim\frac{t}{N}\mathrm{Re}\left[\sum_r\sum_{\hat{\mathbf{a}}}e^{-i\mathbf{k}\cdot\hat{\mathbf{a}}}\bar{\chi}_{\sigma_1}(\nu,r+\hat{\mathbf{a}})\chi_{\sigma_2}(\nu,r)\langle\underline{R}|c^\dagger_{\sigma_1}(r+\hat{\mathbf{a}})c_{\sigma'}(r+\hat{\mathbf{a}})c^\dagger_{\sigma'}(r)c_{\sigma_2}(r)|\underline{R}\rangle+\cdots\right]. \tag{3.14}$$

The matrix element in (3.14) can be rewritten with the aid of (3.13) in terms of $\hat{\mathbf{s}}(r)$ and $\hat{\mathbf{s}}(r+\hat{\mathbf{a}})$ and yields, to within numerical factors,

$$\langle\psi|E_k|\psi\rangle\sim\frac{t}{N}\mathrm{Re}\left[\sum_r\sum_a e^{-i\mathbf{k}\cdot\hat{\mathbf{a}}}\bar{\chi}(\nu,r+\hat{\mathbf{a}})\tau\chi(\nu,r)\times\left[\hat{\mathbf{s}}(r)+\hat{\mathbf{s}}(r+\hat{\mathbf{a}})+\frac{i}{2}\hat{\mathbf{s}}(r+\hat{\mathbf{a}})\times\hat{\mathbf{s}}(r)\right]\right]. \tag{3.15}$$

To proceed further we use the fact that χ is slowly varying on a small scale and identify $\mathbf{m}$ and $\hat{\mathbf{\Omega}}$ as in (3.3b). We assume slow varying fields: $\mathbf{m}\sim\partial\hat{\mathbf{\Omega}}$. Then (ignoring $\partial\chi$ for the moment),

$$\langle\psi|E_K|\psi\rangle\sim\frac{t}{N}\sum_r\bar{\chi}\hat{\boldsymbol{\tau}}\chi\cdot\left[(\cos k_x+\cos k_y)\mathbf{m}+\sum_{a=x,y}\sin k_a\hat{\mathbf{\Omega}}\times\partial_a\hat{\mathbf{\Omega}}\right]. \tag{3.16}$$

The similarity of (3.16) to (3.7)–(3.9) should be evident, namely the spin coupling is predominantly to $\mathbf{m}$ in the vicinity of $k\sim0$ and to the spin current near $(\pi/2,\pi/2)$. [The quadrupole behavior of $\mathbf{m}$ near $(\pi,0)$ has been lost again in the continuum limit.] The spin dependence of χ can be used to build a wave function with the total spin either parallel or perpendicular to the order parameter in accordance with our discussion in the Introduction and Sec. V.

The object multiplying $\hat{\mathbf{\Omega}}\times\partial_a\hat{\mathbf{\Omega}}$ in (3.16) should be a spin current since it multiplies another spin current [cf. (3.9)] to yield an energy. It should be interpreted as a current for the hole built from the phase velocity $\sin(k_a)$, as we discuss further in Sec. IV. An additional term analogous to a group velocity (i.e., it vanishes in the ground state) emerges when we retain gradients of χ. For $k\sim(\pi/2,\pi/2)$ the relevant, i.e., nonzero, terms in $\langle\psi|E_k|\psi\rangle$ are those in which the bra, ket, and additional hopping retrace to within two sites rather than one as in (3.14). One finds a contribution,

$$\langle\psi|E_k|\psi\rangle\sim\cdots+it\sum_{\hat{\mathbf{a}},\hat{\mathbf{a}}'}e^{-i\mathbf{k}\cdot(\hat{\mathbf{a}}+\hat{\mathbf{a}}')}(\hat{\mathbf{a}}+\hat{\mathbf{a}}')^2\times(\partial_b\bar{\chi}\hat{\tau}\chi-\mathrm{H.c.})(\hat{\mathbf{\Omega}}\times\partial_b\hat{\mathbf{\Omega}})+\cdots,$$

where $b=\hat{\mathbf{x}},\hat{\mathbf{y}}$ and is summed. The current-current form of the hopping-induced twist should now be evident.

IV. EFFECTIVE HAMILTONIAN

In this section we systematize and extend the description of the ground state of one hole to include the interaction of the hole with an imposed slowly varying Néel order parameter and magnetization. In applications, or in the presence of a low density of holes, n, the "imposed" $\hat{\mathbf{\Omega}}$ and $\mathbf{m}$ fields will obey the $NL\sigma$ model and reflect the presence of other particles. Our effective Hamiltonian will apply for wave numbers $k<k_F\sim n^{1/2}$ where it generalizes and extends the nonlinear σ model to include holes. Spin degrees of freedom $k\gtrsim k_F$ are integrated out and generate the correct one particle dispersion $\varepsilon(k)$. The dipole moment is also determined by the hole quasiparticle on short scales, i.e., locally. We will work in the small-t/J limit, which should not restrict the applicability of the effective Hamiltonian, since the most significant new term was derived for $t/J\gg1$ in the previous subsection and no qualitative change in the one-hole ground state was found as a function of t/J. In addition, when properly understood, all terms follow from symmetry and all the complexities of the local spin structure around the hole for $t/J\gg1$ are incorporated into coefficients.

One question of symmetry which the explicit calculations of Sec. III elucidated was the necessity of carrying a sublattice index for the hole creation operator. This may have appeared to be merely a convenience but is required to correctly account for the two degenerate ground states of a hole in a small cluster and the manner in which they superimpose. In the presence of local AF order the presence of a hole means the absence of a spin parallel or antiparallel to $\hat{\mathbf{\Omega}}(r)$. Irrespective of where the excess magnetization resides, it is imperative to describe the holes by a spinor in order to write the current-current coupling, which is the source of the dipolar distortion, in a basis-free manner.

To facilitate the derivation let us formally separate the spin and charge degrees of freedom by factorizing the electron operator constrained to single occupancy

$$c_\sigma(r)=\bar{\psi}(r)w_\sigma(r), \tag{4.1}$$

where $\bar{\psi}(r)$ creates a fermionic vacancy on site r and $w_\sigma(r)$ annihilates a Schwinger spin boson ($\bar{w}w=1$ for spin-$\frac{1}{2}$). Next we separate the spin field $w_\sigma(r)$ into a slowly varying semiclassical background and spin-wave fluctuations about it. This can be accomplished by introducing a SU(2) rotation matrix $\underline{R}$ relating the local semiclassical spin orientation to a fixed basis Néel state and then expressing the deviations away from the local Néel state in terms of Bose operators a_r,b_r:

$$w_A(r)=\underline{R}_A(r)\begin{bmatrix}1-\frac{1}{2}a_r^\dagger a_r\\ a_r\end{bmatrix},$$
$$w_B(r)=\underline{R}_B(r)\begin{bmatrix}b_r\\ 1-\frac{1}{2}b_r^\dagger b_r\end{bmatrix}. \tag{4.2}$$

We will parametrize the rotation matrix $\underline{R}$ in essentially the same way as in the semiclassical calculation of Sec. III B, namely with two slowly varying orthogonal spinors z_σ and p_σ obeying $\bar{z}z=1$ and $\mathrm{Re}(\bar{z}p)=0$. The local order parameter and magnetization are $\hat{\Omega}=\bar{z}\tau z$ and $\mathbf{m}=\frac{1}{2}(\bar{p}\hat{\tau}z+\bar{z}\hat{\tau}p)$. Note that the $\mathrm{Re}(\bar{z}p)=0$ constraint corresponds to $\mathbf{m}\cdot\hat{\Omega}=0$. When we restore the quantum dynamics to the long-wavelength fields, p and z will be canonically conjugate and express the $NL\sigma$ Hamiltonian in CP^1 variables. We therefore write

$$\underline{R}_A=\begin{bmatrix}z_1+\frac{1}{2\kappa}p_1 & -\bar{z}_2-\frac{1}{2\kappa}\bar{p}_2\\ z_2+\frac{1}{2\kappa}p_2 & \bar{z}_1+\frac{1}{2\kappa}\bar{p}_1\end{bmatrix},$$
$$\underline{R}_B=\begin{bmatrix}z_1-\frac{1}{2\kappa}p_1 & -\bar{z}_2+\frac{1}{2\kappa}\bar{p}_2\\ z_2-\frac{1}{2\kappa}p_2 & \bar{z}_1-\frac{1}{2\kappa}\bar{p}_1\end{bmatrix}, \tag{4.3}$$

where κ is the magnitude of the staggered moment. The quantity κ will play no substantive role in the following but serves to formally adsorb the reduction in the local moment due to quantum fluctuations (recall that now $\hat{\Omega}$ and $\mathbf{m}$ refer only to long wavelengths). It occurs in $\underline{R}$ but not $\mathbf{m}$ since $\underline{R}$ must be expressible as the exponential of the real angular momentum or spin along a certain direction (cf. Ref. 5). The sign of p in (4.3) must change from A to B since the magnetization density is uniform from sublattice to sublattice [cf. (3.3b)].

The hopping term in (1.1) becomes

$$\begin{aligned}H_h&=-t\sum_{r\in A,\mu}\bar{\psi}^B_{r+\mu}\psi^A_r\bar{w}^A_r w^B_{r+\mu}+\mathrm{H.c.}\\&=-t\sum_{r\in A,\mu}\bar{\psi}^B_{r+\mu}\psi^A_r[(a_r^\dagger+b_{r+\mu})-iA_\mu(a_r^\dagger-b_{r+\mu})]-t\sum_{r\in A,\mu}\bar{\psi}^B_{r+\mu}\psi^A_r[f_\mu(r)+h(r)][1-\tfrac{1}{2}(a_r^\dagger a_r+b^\dagger_{r+\mu}b_{r+\mu})]\\&\quad-t\sum_{r\in A,\mu}\bar{\psi}^B_{r+\mu}\psi^A_r[f^*_\mu(r)+h^*(r)]a_r^\dagger b_{r+\mu}+\mathrm{H.c.}\end{aligned} \tag{4.4}$$

with the slow fields

$$\begin{aligned}&iA_\mu\equiv\bar{z}\partial_\mu z\ ,\\&f_\mu\equiv-\epsilon_{\sigma\nu}\bar{z}_\sigma\partial_\mu\bar{z}_\nu\ ,\\&h\equiv\kappa^{-1}\epsilon_{\sigma\nu}\bar{z}_\sigma\bar{p}_\nu\ ,\end{aligned} \tag{4.5}$$

arising from the gradient expansion of $\underline{R}^\dagger_A(r)\underline{R}_B(r+\mu)$. (In this section only, we denote the lattice vector $a=x,y$ in scalar products and $a=\pm x,\pm y$ in lattice sums by μ to avoid confusion with operator a.) We assume both p and ∂z to be small (in accordance with the $NL\sigma$ Hamiltonian) and keep only the leading order.

The exchange part of the Hamiltonian has the form

$$\begin{aligned}H_{\mathrm{ex}}&=J\sum_{r\in A,\mu}|f_\mu+h|^2+J\sum_{r\in A,\mu}[a_r^\dagger a_r+b_{r+\mu}b^\dagger_{r+\mu}+a_r^\dagger b^\dagger_{r+\mu}+b_{r+\mu}a_r-2iA_\mu(a_r^\dagger b^\dagger_{r+\mu}-b_{r+\mu}a_r)]\\&\quad+J\sum_{r\in A,\mu}[(a_r^\dagger a_r+b^\dagger_{r+\mu}b_{r+\mu})|f_\mu+h|^2+a_r^\dagger b_{r+\mu}(f^*_\mu+h^*)^2+b^\dagger_{r+\mu}a_r(f_\mu+h)^2]\ .\end{aligned} \tag{4.6}$$

The original Hamiltonian and thus (Eqs. (4.4)–(4.6) admit a local gauge symmetry corresponding to rotations about the local lattice spin, $\mathbf{s}_{A,B}$, direction,

$$\begin{aligned}&w_{A,B}(r)\to e^{\pm(i/2)\chi(r)}w_{A,B}(r)\ ,\\&\psi^{A,B}(r)\to e^{\pm(i/2)\chi(r)}\psi^{A,B}(r)\ ,\end{aligned} \tag{4.7}$$

which arises from the redundancy of the factorized representation Eq. (4.1) and leaves the physical electron operator invariant. This gauge symmetry can never be broken although at times it is convenient to carry non-gauge-invariant quantities at intermediate steps of a calculation.

The induced transformation of the a,b,z,p fields is

$$\begin{aligned}&z\to e^{(i/2)\chi}z,\quad p\to e^{(i/2)\chi}p\ ,\\&a\to e^{i\chi}a,\quad b\to e^{-i\chi}b\ ,\end{aligned} \tag{4.8}$$

which leaves the two physical continuum vectors $\hat{\Omega}$ and $\mathbf{m}$ invariant. The assumed continuity of the z,p fields reduces the gauge transformation to that described by a slowly varying χ, and A_μ acts as a gauge field:

$$A_\mu\to A_\mu+\tfrac{1}{2}\partial_\mu\chi\ . \tag{4.9}$$

Finally,

$$f_\mu \to e^{-i\chi} f_\mu, \quad h \to e^{-i\chi} h \ . \tag{4.10}$$

Although the gauge invariance is more apparent in the continuum limit, (4.6) is an expansion up to third order in slow gradients or magnetization and it is properly gauge invariant to the same order. In particular, note that the transformation of $a_r^\dagger b_{r+\mu}^\dagger$ involves a $\partial_\mu \chi$ and so is gauge invariant when combined with A_μ.

The exchange Hamiltonian (4.6) describes spin waves in a slowly varying background field and is essentially equivalent to Polyakov's formulation of the renormalization group for fixed-length spins.[32] Instead of doing the integration over small scales iteratively, it is sufficient for our purposes to do it in one step by standard Holstein-Primakoff spin-wave theory. The $NL\sigma$ model with renormalized susceptibility and stiffness constant emerges in the following equivalent forms:

$$H_{NL\sigma} = 4J\rho \sum_r (|h|^2 + \tfrac{1}{2}|f_\mu|^2) \tag{4.11a}$$

$$= 4J\rho \sum_r [\kappa^{-2}(\bar{p}p - \bar{p}z\bar{z}p) + \tfrac{1}{2}(\partial_\mu + iA_\mu)\bar{z}(\partial_\mu - iA_\mu)z] \tag{4.11b}$$

$$= 4J \sum_r [\chi^{-1}\mathbf{m}^2 + \rho(\partial_\mu \hat{\Omega})^2] \tag{4.11c}$$

with κ, ρ, χ calculated in spin-wave theory.[33]

It is not surprising in view of the gauge freedom (4.7)–(4.10) that a covariant derivative appears in (4.11b), and higher-order gradients should take the form of $F_{\alpha\beta}^2$, where $\alpha,\beta=0,1,2$ (0 being time) and $F_{\alpha\beta} \equiv \partial_\alpha A_\beta - \partial_\beta A_\alpha$.[32] It may be reassuring to certain readers that the classical p,z Hamiltonian can be converted into the classical Lagrangian, $|(\partial_\alpha + iA_\alpha)\bar{z}|^2$, by the usual manipulations provided one imposes on $p, \mathrm{Re}(\bar{z}p)=0$ (Appendix A).

As anticipated in the introduction to this section, the standard σ-model commutation relation (2.2b) in $\mathbf{m}, \hat{\Omega}$ variables can be reproduced within the spinor formulation by taking as nonzero solely the commutators

$$[z_\nu, \bar{p}_\sigma] = \delta_{\sigma\nu} - z_\nu \bar{z}_\sigma \ , \qquad [\bar{p}_\nu, p] = z_\sigma \bar{p}_\nu + p_\sigma \bar{z}_\nu \ . \tag{4.12}$$

The constraints $\bar{z}z=1$ and $\bar{p}z + \bar{z}p = 0$ are explicitly preserved by (4.12). One should also be able to verify from (4.12) that the conventional Lagrangian path integral is obtained from the quantum Hamiltonian. Various commutation relations induced by (4.12) for the composite operators in (4.5) are collected in Appendix B.

The three terms in the hopping Hamiltonian, (4.4), describe the coupling of hole motion to the spin fluctuations the interaction of the hopping with the slow gradients, and finally a fluctuation correction to the same that we will ignore. Integrating out the spin fluctuations gives rise to a self-energy, diagonal in the sublattice index, whose $\omega=0$ part is just the band energy $\varepsilon(k)$ discussed in Sec. II B and it will be incorporated into the effective Hamiltonian as a term $\varepsilon(k)\bar{\psi}_k^\alpha \psi_k^\alpha$. In the small-$t/J$ limit a Hartree-Fock calculation suffices and the numerical coefficients in (2.4) were calculated in Ref. 4. For $t/J \gg 1$ a more careful self-consistent calculation of the self-energy is required.[34]

The elimination of the fluctuations can be done neglecting the slow fields since the coupling of a,b to f_μ, h leads to corrections of order $O(\partial^2)$ and the coupling to A_μ can be correctly deduced *a posteriori* simply by replacing $k_\mu \to k_\mu \pm A_\mu$ [where $+(-)$ refers to $A(B)$, respectively] as required by the gauge symmetry (note that vacancies on opposite sublattices have opposite "pseudo"-charge).[35,36]

The direct coupling of the vacancy fermion to the background field, H_h^{dir}, can be further rewritten if we recall that f_μ is odd in μ and h even. We also have to provisionally define a lattice difference operator $\Delta_\mu \psi_r \equiv \psi_{r+\mu} - \psi_r$ to act on the fermion fields since they are not slowly varying until we expand around the minimum energy wave vectors $(\pm\pi/2, \pm\pi/2)$. One then has with

$$\zeta = 1 - \tfrac{1}{2}\langle a_r^\dagger a_r \rangle - \tfrac{1}{2}\langle b_r b_r^\dagger \rangle \ ,$$

$$\begin{aligned} H_h^{\mathrm{dir}} &\equiv -\zeta t \sum_{r,\mu} \bar{\psi}_{r+\mu}^B \psi_r^A (f_\mu + h) + \mathrm{H.c.} \\ &= -4\zeta t \sum_{r,\mu} \tfrac{1}{2}(\Delta_\mu \bar{\psi}_r^B \psi_r^A f_\mu + \bar{\psi}_r^A \Delta_\mu \psi_r^B \bar{f}_\mu) \\ &\quad + (\bar{\psi}_{r+\mu}^B \psi_r^A h + \bar{\psi}_r^A \psi_{r+\mu}^B \bar{h}) \\ &= -\zeta t \sum_r [(i\Delta_\mu \bar{\Psi} \underline{K}_\mu \Psi + \mathrm{H.c.}) + 4\bar{\Psi} \underline{M} \Psi] \ , \end{aligned} \tag{4.13}$$

where

$$\underline{M} \equiv \begin{bmatrix} 0 & h^* \\ h & 0 \end{bmatrix}, \quad \underline{K}_\mu \equiv \begin{bmatrix} 0 & -if_\mu \\ if_\mu^* & 0 \end{bmatrix} , \tag{4.14}$$

and we defined a spinor

$$\Psi \equiv \begin{bmatrix} \psi^B \\ \psi^A \end{bmatrix} . \tag{4.15}$$

The definition of the sublattice spinor here is dictated by our earlier choice of ψ^+ as a vacancy creation operator and future convenience [cf. (4.17) and above].

In order to pass to the continuum limit we introduce a valley index $v \equiv 1,2$ which enumerates the energy minima at $k^v = (\pi/2, \pm\pi/2)$. The two other degenerate energy states are joined to these valleys through a shift by (π,π) [cf. Fig. 1]. The lattice derivative Δ_μ which is odd in μ then separates into a piece proportional to the dipole moment of the valley in question, $\sin(k^v)/\sqrt{2} = \hat{\mathbf{n}}^v$ plus a slow gradient which we will make gauge invariant by defining it to be $D_\mu = \partial_\mu - iA_\mu \tau_z$. The coupling to the magnetization is actually zero to this order, as we found in Sec. III B, since to make Δ_μ odd, the sum in (4.13) is really over ψ^A, ψ^B displaced by μ which vanishes at $(\pi/2, \pm\pi/2)$.[37] We will nevertheless continue to carry this term so that the effective Hamiltonian is not invalid at other points of the Brillouin zone.

At this stage of the calculation we have basically factored out the symmetry under sublattice interchange

$(\psi_A \to \psi_B, \psi_B \to -\psi_A)$ and $k \to k+(\pi,\pi)$ and restrict our attention to an elliptical region in k space about $(\pi/2, \pm\pi/2)$. Equation (4.13) is properly invariant since the f_μ term behaves like $\sin k_\mu$ while the h term is zero.

We finally have the effective continuum hopping Hamiltonian analogous to (4.11)

$$H_h^{\text{eff}} = \sum_{r,v} \bar{\Psi}^v \varepsilon_v(D_\mu)\Psi^v + g_1 \sum_{r,v} \hat{n}_\mu^v (\bar{\Psi}^v \underline{K}_\mu \Psi^v + \text{H.c.}) + g_2 \sum_{r,v} (iD_\mu \bar{\Psi}^v \underline{K}_\mu \Psi^v + \text{H.c.}) + g_3 \sum_{r,v} \bar{\Psi}^v M \Psi^v , \tag{4.16}$$

where $\varepsilon_v(D_\mu)$ is the operator valued 2×2 matrix, diagonal in sublattices, obtained from the band energy $\varepsilon_v(k)$ by expanding about $k = k_v$. Because certain higher-order terms have been included, H_h^{eff} is explicitly gauge invariant under $\Psi \to G\Psi$ with $G \equiv \exp[-(i/2)\chi\tau^z]$ under which $D_\mu \to D_\mu$, $\underline{K}_\mu \to G\underline{K}_\mu G^{-1}$, $\underline{M} \to G\underline{M}G^{-1}$, and $\underline{R} \to \underline{R}G^{-1}$. [The transformation of $\underline{R}$ follows from (4.3) and will be used below.]

The phenomenological couplings $g_{1,2}$ are $O(\zeta t)$ for $t/J \ll 1$ while in the opposite limit we expect values of $O(J)$; g_3 should be much smaller or zero. The exchange J also sets the scale of the one-particle band width and effective mass because of the reduction of the spectral weight of the quasiparticle by the incoherent stringlike excitations.[34]

The spinor Ψ in (4.16), by virtue of the definitions (4.1) and (4.2), is referred to an "intrinsic" basis fixed by the local $\hat{\Omega}$ direction. It is very useful for purposes of interpretation, though not necessarily for explicit calculations, to refer Ψ to a fixed uniform "lab" reference frame. This can be done by defining $\Phi = \underline{R}\Psi$. Noting that $\underline{R}\underline{K}_\mu \underline{R}^\dagger = \frac{1}{2}(\hat{\Omega}\times\partial_\mu\hat{\Omega})\cdot\hat{\tau}$, $\underline{R}\underline{M}\underline{R}^\dagger = \kappa^{-1}\mathbf{m}\cdot\hat{\tau}$ and[38]

$$\underline{R}D_\mu\underline{R}^\dagger = \partial_\mu + \underline{R}\partial_\mu\underline{R}^\dagger + iA_\mu\underline{R}\tau^2\underline{R}^\dagger = \partial_\mu - \frac{i}{2}(\hat{\Omega}\times\partial_\mu\hat{\Omega})\cdot\hat{\tau} , \tag{4.17}$$

one arrives at the effective Hamiltonian (with a factor of $\frac{1}{2}$ absorbed into $g_{1,2}$ and κ^{-1} into g_3),

$$H_h^{\text{eff}} = \sum_{r,v} \bar{\Phi}^v \varepsilon_v \left[\frac{1}{i}\partial_\mu - \tfrac{1}{2}\hat{\Omega}\times\partial_\mu\hat{\Omega}\cdot\hat{\tau}\right]\Phi^v + g_1 \sum_{r,v} (n_\mu^v \bar{\Phi}^v \hat{\tau}\Phi^v)\cdot(\hat{\Omega}\times\partial_\mu\hat{\Omega}) + g_2 \sum_{r,v} i(\partial_\mu\bar{\Phi}^v\hat{\tau}\Phi^v - \bar{\Phi}^v\hat{\tau}\partial_\mu\Phi^v)\cdot(\hat{\Omega}\times\partial_\mu\hat{\Omega}) + g_3 \sum_r \bar{\Phi}\hat{\tau}\Phi\cdot\mathbf{m} . \tag{4.18}$$

The second and third terms in (4.18) are just the dipole-current and current-current coupling terms found in Sec. III. They clearly cannot be written unless the holes are described by a spinor. Since these same terms are responsible for the appearance of the dipole moment of the hole, the small cluster diagonalizations indirectly point to a spinor description for the holes. This pseudospin may be related to a real spin, i.e., an angular momentum in the presence of Néel order as we do quite generally in the next section.

Recall that in the original microscopic variables, the particle spin current in the $g_{1,2}$ terms in (4.18) is constructed from $\partial\Phi$, i.e., the phase velocity and not the group velocity. This "current" therefore need not vanish in the ground state, where, in fact, it reduces to the dipole moment, but it also does not correspond to the transport of particles. If, by contrast, one varies the $\varepsilon_v(k)$ term with respect to k, the usual group velocity would be obtained, which is zero in the ground state.

The gauge symmetry as represented by (4.8)–(4.10) becomes redundant for (4.18) since $\Phi \to (RG^{-1})(G\Psi) = \Phi$ and $\hat{\Omega} \to \hat{\Omega}$.[39]

Our effective Hamiltonian first appeared in Ref. 5 with the current-current coupling and dipole moment emphasized and the gauge aspects implicit. Parallel work by Wiegman[35] emphasized the gauge aspects of the problem originating with the next-nearest-neighbor hopping term, $\varepsilon(k)$. Wen[36] has also derived an effective Hamiltonian similar to Wiegman's but he explicitly discards the current coupling which appears to us to be responsible for significant new physics.[9]

V. EXACT RESULTS FOR FINITE SYSTEMS

A. Quantum mechanics of the order parameter

In this subsection we make precise the intuitive idea that the quantum ground state can be represented as a broken-symmetry state averaged over the direction of $\hat{\Omega}$. Such a connection is essential if we are to use semiclassical ideas to understand the quantum problem. The situation is very analogous to superfluid ^{4}He if the Heisenberg ground state is likened to a superfluid wave function with a fixed number of particles. The phase is then undefined, which, unnecessarily, complicates any calculation involving superfluid flow.

Understanding the quantum mechanics of the uniform mode is also important for interpreting numerical simulations of small clusters. It would be exceedingly awkward to apply a small staggered field to define the order parameter, so, as a result, certain interesting matrix elements vanish by symmetry while others are nonzero precisely because there is no order parameter. Among important issues that can be simply resolved by understanding the quantum mechanics of the order parameter are the scaling of the singlet-triplet gap or the symmetry-breaking field with system size, and the relation of the one-hole eigenfunctions in the extended versus reduced Brillouin zones. Finally, in reference to the previous two sections, the additional angle necessary to orient the dipole moment, its relation to the relative phase between sublattices, and the conjugate relation between the dipole operator and the component of magnetization along $\hat{\Omega}$ all emerge naturally again here.

B. Undoped Heisenberg model

To define the wave function of the uniform mode it is useful to consider the minimum energy state with given

values of the total spin S and its z component S_z which both commute with H. These states are readily accessible numerically since it is simple to control S_z and the Lieb-Mattis theorem[24] then implies that S assumes the minimum value possible consistent with S_z. However, the commutators (2.1b) imply that the order parameter and total spin are conjugate variables completely analogous to the unit vector defining the configuration of a symmetrical top and its angular momentum. Hence, both cannot be simultaneously specified. To extract the wave function of $\hat{\Omega}$ in a given many-body $|S,S_z\rangle$ state we follow the Lee-Yang construction for superfluid ^{4}He and consider the one spin-density matrix for two widely separated spins.[40] This factors into the square magnitude of the order parameter times the spherical harmonic $Y_{SS_z}(\hat{\Omega})$ and its complex conjugate.

Several results follow immediately from the expression for the spin dependence of the total energy for an even lattice of N sites in the presence of a uniform field H,[19,41]

$$E(S,S_z)-E(0,0)=-gHS_z+S(S+1)/(2\chi N)\ . \qquad (5.1)$$

The lowest-energy state of given S is $Y_{SS}(\hat{\Omega})$ while implies that $\hat{\Omega}$ is in the xy plane, more precisely $\langle\Omega_z^2\rangle=O(1/S)$. This is the quantum version of the well-known result that an antiferromagnet adjusts to a uniform field by canting. In order to define the order parameter with an accuracy $1/\Lambda$, i.e., $\langle\hat{\Omega}\rangle=[1-O(\Lambda^{-1})]\hat{\mathbf{z}}$, $\langle\Omega_z^2+\Omega_y^2\rangle\sim\Omega(\Lambda^{-1})$, the uncertainty relation $\langle\Omega_z^2\rangle\langle m_y^2\rangle\geq\langle\Omega_z\rangle^2$ (derived from the corresponding commutator in analogy to the order-parameter number commutator in ^{4}He), require that total spin states up to $S\sim\Lambda^{1/2}$ have to be superimposed.[14] The energy cost is $\sim\Lambda/N$ which implies a staggered field of order $\sim\Lambda/N^2$ to achieve this degree of alignment.

Lastly, we mention that the estimates above and those to follow could be obtained from a model for the AF consisting of two equal and large spins representing two fully polarized sublattices coupled together into a singlet.

C. Heisenberg model with a vacancy

For one-hole and sufficiently small hopping the Lieb-Mattis theorem implies that the ground state is $S=\frac{1}{2}$ (on an even-size lattice). Numerically this persists until t becomes large enough to favor the formation of a ferropolaron. When there is no imposed staggered field and a small nonzero t, $\langle\hat{\Omega}\rangle=0$ in the ground state even though formally the Wigner-Eckart theorem allows a vector operator to have a nonzero expectation value in a spin-$\frac{1}{2}$ state. For a finite system, there is a nonzero matrix element connecting the states with the hole on the A and B sublattice. Therefore, both will be equally populated. Then the symmetry, true even for the ordered state, with respect to a shift by one lattice site followed by a time reversal of the spins implies $\langle\hat{\Omega}\rangle=0$ in the ground state. The periodicity allows us to define the ground state as a function of k, which lives in the full Brillouin zone $-\pi\leq k_x<\pi$, $-\pi\leq k_y<\pi$, and which is twofold degenerate because of spin. (In what follows, we will also make reference to the ground states for higher total spin.)

In contrast, imagine that we impose an order parameter Ω_z on the system which can be done in two ways (up, down) with respect to the sublattice structure which we regard as tied to the lattice not the spin. The total spin is no longer a good quantum number, and once $S_z=\pm\frac{1}{2}$ is specified, the hole resides preferentially on one sublattice, i.e., if Ω_z is up on A then the hole for $S_z=-\frac{1}{2}$ is also predominantly on A. This result is obvious perturbatively when $J_\perp<J_z$ and once Ω_z is defined there is no symmetry operation which makes A and B equivalent, without, at the same time, reversing all the spins. A spin-wave calculation has also been done[42] for $t=0$ which shows that some of the "missing" spin is localized around the hole and therefore assigning the total spin is equivalent to establishing a preference for one sublattice over the other. This preference should decrease smoothly as t/J increases and a "string" state is formed which tends to establish uniform weight on the two sublattice. The numerical simulations of Ref. 4 actually show this effect.

To understand the relation between the broken-symmetry states in the reduced Brillouin zone and the exact eigenstates, consider adding a zone-boundary magnon. The following lemma is useful.

If $|\frac{1}{2},\pm\frac{1}{2},k\rangle$ is the spin-$\frac{1}{2}$, $S_z=\pm\frac{1}{2}$ ground state then the state $(S_A^\alpha-S_B^\alpha)|\frac{1}{2},\pm\frac{1}{2},k\rangle$ (where $\mathbf{S}_{A,B}=\sum_{r\in A,B}\mathbf{s}_r$ and $\alpha=x,y,z$) is a mixture of spin $\frac{1}{2}$ and $\frac{3}{2}$, has a crystal momentum, $k+(\pi,\pi)$ and an energy expectation value within $O(1/N)$ of the ground state.

Even though the demonstration is trivial, this lemma is a succinct statement of what is true and it is used below. The spin quantum numbers follow from the Wigner-Eckart theorem. The momentum shifts by (π,π) since the symmetry under the sublattice interchange reverses, and the energy estimate follows from Eq. (5.1).

To construct the broken-symmetry eigenstates from those of the isotropic Hamiltonian, apply a staggered field at least of order $1/N^2$ along $\hat{\mathbf{z}}$, i.e., add $h_z(S_A^z-S_B^z)$ to H. This will mix in first order the ground state, $|\frac{1}{2},\frac{1}{2},k\rangle$, of H with $|S,\frac{1}{2},k+(\pi,\pi)\rangle$ for $S=\frac{3}{2},\frac{1}{2}$, and k in the reduced Brillouin zone. Appropriate linear combinations all with $S_z=\frac{1}{2}$ correspond to Ω_z up or down and thus the hole predominantly on A or B. Conversely, if we project from the exact ground state those basis states with the hole on a given sublattice, $\langle\Omega_z\rangle$ will be nonzero and, in accordance with our remarks several paragraphs above, decreasing as t/J increases. This accords with the numerical results in Ref. 4. The total count of states is correct since we took a doubly degenerate ($S_z=\pm\frac{1}{2}$) state in the extended zone and constructed four nearly degenerate states in the reduced zone ($S_z=\pm\frac{1}{2},\Omega_z=\pm1$).

To construct an Ω_z equal to nearly its thermodynamic value would require yet higher total spin state as in (5.1) and below. Thus, the broken-symmetry states are not simply constructed by "folding back" the extended zone states since higher spin states have to be mixed in. Their energy splitting is of order $1/N$ and the additional spin is predominately in the x,y directions (N.B., $S_z=\pm\frac{1}{2}$) (i.e., perpendicular to $\hat{\Omega}$), and spread over the entire lattice as

we argued in Sec. V A. The energy gap due to the existence of an order parameter and the doubling of the unit cell vanishes in the thermodynamic limit.

To combine the broken-symmetry states into plausible isotropic eigenstates it is most convenient to work with $\hat{\Omega}$ in the x direction and then average around $\hat{\mathbf{z}}$. By superimposing the $S_x=\pm\frac{1}{2}$ states before averaging, one makes the weights on A,B equal and puts the net spin along $\hat{\mathbf{z}}$. The properly weighted average over $\hat{\Omega}$ (described more precisely in the next section) assures that the total spin is $\frac{1}{2}$. The quantum spin-$\frac{1}{2}$ eigenstates with k outside of the reduced zone may be constructed by adding to the state a zone-boundary magnon with spin 1 and $k=(\pi,\pi)$ and projecting back onto $S=\frac{1}{2}$.

It is not, strictly speaking, meaningful to ask whether the ground state is better described by the total magnetization parallel to $\hat{\Omega}$ as would be correct for $J_z>J_\perp$ or perpendicular to $\hat{\Omega}$ as appropriate for $J_z<J_\perp$. The isotropic ground state is a mixture of both but the energy differences among all these states for $J_z=J_\perp$ are $O(1/N)$.

It is perhaps useful to contrast our problem with polyacetylene which is a dimerized system with only Ising symmetry.[43] When solitons or domain walls are introduced, the dimerization is formally lifted to an infinite system and the bands should be drawn in an extended zone. However, there remains a virtual, order 1 gap at the reduced zone edge which contains just the carrier states localized on the solitons. In our case the symmetry is continuous, and our analogue of a domain wall is a spin-1 momentum (π,π) zone-boundary magnon that is spread out over the entire system.

D. Dipole moment

In Sec. V A we observed that a wave function $Y_{S,S_z}(\Omega)$ could be defined from the one-particle density matrix for a Heisenberg ground state with quantum numbers SS_z, so that we can write schematically

$$|SS_z\rangle=Z_\Omega\int\frac{d\hat{\Omega}}{4\pi}Y_{SS_z}(\hat{\Omega})|\hat{\Omega}\rangle+|\psi_{\text{incoherent}}\rangle\ . \tag{5.2}$$

To see that (5.2) is equivalent to our earlier remark the Lee-Yang definition of the order parameter, imagine using a coherent-state basis for the spin on each site. Then (5.2) says that the quantum state where we take the staggered component of this spin and average over Y_{S,S_z} has a nonzero amplitude, $Z_\Omega<1$, in the thermodynamic limit. The spin correlations calculated in the remaining incoherent piece, which will be henceforth ignored, decay algebraically with distance.

In this section we generalize (5.2) to allow for a single hole and thereby reproduce several relations that emerged analytically in Sec. IV by using just freshman quantum mechanics. Specifically, we will see that the dipole moment is like a generalized "coordinate" on par with $\hat{\Omega}$, which fixes the angle of rotation about $\hat{\Omega}$ and is related to the phase between the sublattices.

For one hole, let us replace $|\hat{\Omega}\rangle$ by a ket labeled by a spinor z_σ and a Bloch vector k (in the reduced zone) which we further decompose as

$$|z,k\rangle\equiv\frac{1}{\sqrt{2}}(|z,k,A\rangle+|z,k,B\rangle)\ , \tag{5.3}$$

where the additional label denotes the sublattice of the hole. Under time reversal and reflection in a lattice site we merely replace z in (5.3) by $\underline{T}z\equiv-i\tau_y\bar{z}$ and leave A,B invariant while under translations, $S_{\hat{\mathbf{a}}}$, of the entire system by $\hat{\mathbf{a}}$ we have

$$S_{\hat{\mathbf{a}}}|z,k,A\rangle=e^{i\mathbf{k}\cdot\hat{\mathbf{a}}}|\underline{T}z,k,B\rangle\ . \tag{5.4}$$

The analogue of Eq. (5.2) for the two possible spin-$\frac{1}{2}$ states ($\sigma=\pm$) has the form

$$|\tfrac{1}{2},\sigma/2\rangle=Z_\Omega Z_t\int dR z_\sigma|z,k\rangle - \frac{Z_\Omega Z_t}{\sqrt{2}}\int dR\,(z_\sigma|z,k,A\rangle+\underline{T}z_\sigma|\underline{T}z,k,B\rangle)\ , \tag{5.5}$$

where $dR=(d\cos\theta d\phi d\gamma/8\pi^2)$ is an integral over SU(2) in the parametrization $z_\sigma=e^{i\gamma/2}$ $[\cos(\theta/2)e^{i\phi/2},\sin(\theta/2)e^{-i\phi/2}]$ and a simple variable change from z to $\underline{T}z$ was made in the second term in the second line. The additional renormalization factor $Z_t<1$ takes account of the tendency of the hole to average over the two sublattices as t/J increases.

An immediate consequence is that if we project the hole onto A then Ω_z has a nonzero expectation value, i.e.,

$$2\langle\delta_{r,A}\Omega_z\rangle=|Z_\Omega Z_t|^2\int dR\,|z_\sigma|^2(|z_+|^2-|z_-|^2) =\sigma|Z_\Omega Z_t|^2/3\ , \tag{5.6}$$

while the averages of $\Omega_{x,y}$ are always zero by symmetry. Therefore, with both the sublattice for the hole and S_z specified, there appears a nonzero component of $\hat{\Omega}$ extending throughout the system. It only exists, so to speak, in the hole's reference frame, i.e., if we omitted the $\delta_{r,A}$ in (5.6) the expectation value of Ω_z alone would be zero. The numerical simulations in Ref. 4 used the full translational symmetry of the isotropic ground state to reduce all basis states to those with the hole on a fixed site. A component of average staggered magnetization accordingly appeared with magnitude close to $\frac{1}{3}$ for $t/J\ll1$ since, for the 18-site cluster studied,

$$4\left\langle\left[\frac{1}{N}\sum_r(\pm1)^r\mathbf{s}_r\right]^2\right\rangle\equiv\langle\tilde{\Omega}^2\rangle$$

is very close to 1.[4] Even though, in principal, (5.6) should only apply well away from the hole, we also found numerically that $\langle\tilde{\Omega}_\alpha^2\rangle$, $\alpha=1,2,3$, were all equal for arbitrary t/J. This follows from the Wigner-Eckhart theorem and the total spin of the ground state, $\frac{1}{2}$, and nothing else.

It is apparent from the second line in (5.5) that because of $\underline{T}z_\sigma=\sigma\bar{z}_{-\sigma}$ ($\sigma=\pm1$), γ appears as the relative angle between sublattices. It is manifestly part of the SU(2) parametrization, on the same footing as θ and ϕ which fix $\hat{\Omega}$, and is therefore conjugate to the magnetization. There is clearly no dipole quantum number that can be

assigned along with the spin. However, we can define an operator in the z basis with dipole symmetry whose expectation value in the state $|\frac{1}{2},\sigma\rangle$ is nonzero, namely

$$\mathbf{P}_a=\tfrac{1}{2}(\underline{S}_{\hat{\mathbf{a}}}-\underline{S}_{-\hat{\mathbf{a}}})\times(\mathrm{Re}(\bar{z}_1^2-z_2^2),\mathrm{Im}(\bar{z}_1^2-z_2^2),-2\,\mathrm{Re}(z_1z_2))\ , \tag{5.7}$$

where $\underline{S}_{\hat{\mathbf{a}}}$ was defined in (5.4). The spin part of (5.7) equals $\mathrm{Tr}(\hat{\tau}R\tau_xR^+)$ using the definitions of Sec. IV (with $p_\sigma=0$) and just represents in the "laboratory" reference frame one of two possible vectors perpendicular to τ_z (i.e., $\hat{\mathbf{\Omega}}$), in the local reference system. Accordingly it satisfies

$$\mathbf{P}_a\cdot\hat{\mathbf{\Omega}}=0$$

and has magnitude one. It therefore precisely establishes a direction perpendicular to $\hat{\mathbf{\Omega}}$. We then have,

$$\langle\tfrac{1}{2}\sigma|\mathbf{P}_a|\tfrac{1}{2}\sigma\rangle=\frac{\sigma|Z_\Omega Z_t|^2}{6}(\sin k_a)\hat{\mathbf{z}}\ . \tag{5.8}$$

(It should not be a surprise that there exist new ordered states in the presence of holes in which the order parameter is a triad of vectors, i.e., $\mathbf{P}$ has a nonzero expectation value along with $\hat{\mathbf{\Omega}}$.[9])

As expected, only the $\hat{\mathbf{z}}$ component is nonzero since $|\frac{1}{2},\sigma\rangle$ is an eigenstate of S_z, and the dipole moment takes its sign from σ. By time reversal (and cf. Fig. 3), in enumerating states, the two values of the dipole moment for a given k serve as a surrogate for S_z. The $\hat{\mathbf{z}}$ component of $\mathbf{P}_a$ as an operator is proportional to $\sin\theta\sin\delta$ and the reader should note the resemblance with the first term on the right-hand side of (3.5) which generated the dipole moment in the semiclassical approximation. In that calculation, we assumed equal amplitudes for the hole to be on A or B and thereby put Ω in the xy plane so as to implicitly put the net spin in $\hat{\mathbf{z}}$.

Within the basis states $|z,k\rangle$ an operator for the total spin can be defined in terms of derivatives with respect to z_σ and $\bar{z}_\sigma$. One can then verify, in accordance with Secs. III and IV, that both $\mathbf{P}_a$ and $\hat{\mathbf{\Omega}}$ transform as vectors under spin rotation. We are unable to go further along the lines of Sec. IV and reproduce the spin current relative to the hole since we have only retained here the uniform mode.

ACKNOWLEDGMENTS

The authors thank V. Elser and D. Huse for discussions and the Ecole Normale Superieure, where the part of the work was done, for its hospitality. E.D.S. acknowledges financial support from the Guggenheim foundation and the National Science Foundation (NSF) under Grant No. DMRS83114625 and the hospitality of AT&T Bell Laboratories.

APPENDIX A: σ MODEL LAGRANGIAN

In this section we derive the usual $NL\sigma$ Lagrangian in two ways: directly from (4.11b) by a Legendre transform, and then by reparametrizing the microscopic spin Lagrangian by introducing sublattices and the relation (3.2). In both cases we will only have to examine the kinetic or p-independent part of the Hamiltonian or Lagrangian. Note the differing meanings of p. In (4.11b) we declare it to be, modulo a constraint, the momentum conjugate to z, and therefore will arrive at the commutation relations (4.12). When employing (3.2), however, to rewrite the microscopic Lagrangian for $w^{A,B}$, both p and z label the configuration space and are to be integrated over.

To implement a Legendre transform on (4.11b) we must keep the velocity $\partial_t z,\partial_t\bar{z}$ variables manifestly on the manifold, $z\bar{z}=1$. Hence, we write from (4.11b)

$$L=\partial_t\bar{z}Tp+\bar{p}T\partial_t z-\bar{p}Tp-\cdots\ , \tag{A1}$$

where $T_{\sigma\nu}=\delta_{\sigma\nu}-z_\sigma\bar{z}_\nu$ and p and $\bar{p}$ are to be varied independently. The final result may be written

$$L=\chi|(\partial_t+iA_t)\bar{z}|^2-\rho|(\partial_a+iA_a)\bar{z}|^2 \tag{A2}$$

and a gauge field $iA_t=\bar{z}\partial_t z$ defined in analogy with (4.5).

It will be observed that (A1) involves p only in the combination $Tp=\zeta$. Hence, one is led to introduce commutators,

$$[z_\nu,\bar{\zeta}_\sigma]=T_{\nu\sigma}$$

and all others zero. These relations are compatible with (4.12) if one uses the constraint $\bar{p}z+\bar{z}p=0$ which, again, is saying that only the component of p "normal" to z is a physical operator.

The preceding manipulations implicitly involved the long-wavelength Lagrangian and an arbitrary numerical coefficient was suppressed in (A1). We now write the temporal part of the Lagrangian for the lattice spins whose coefficient is determined by the spin quantum number S as

$$L=Si\sum_r\partial_t\bar{w}w-\bar{w}\partial_t w+\cdots\ , \tag{A3}$$

which becomes, upon using (3.2) and doing various integrals by parts,

$$L=Si\sum_r[(-1)^r(\partial_t\bar{z}z-\bar{z}\partial_t z+\tfrac{1}{4}\partial_t\bar{p}p-\tfrac{1}{4}\bar{p}\partial_t p)+(\partial_t\bar{z}p-\bar{p}\partial_t z)]+\cdots\ .$$

The alternating term can be evaluated in the continuum limit by grouping terms into disjoint plaquettes and expanding to yield $\frac{1}{2}S\int\partial^2_{x,y}A_t\,dx\,dy$. This term only contributes for "singular" spin configuration corresponding to the appearance or disappearance of Skyrmions as demonstrated by Haldane.[44]

To (A3) we have to adjoin the potential energy which is just (4.11b) in the continuum limit. Note that p and z together label the configuration space, the only difference between them is that the energy is quadratic in p which can then be integrated out. Thus,

$$L=iS\sum(\partial_t\bar{z}p-\bar{p}\partial_t z)-\tfrac{1}{2}\tilde{\chi}^{-1}\sum\bar{p}Tp=-2\chi S^2\sum_r\partial_t\bar{z}T\partial_t z+\cdots$$

which is equivalent to (A2).

APPENDIX B: COMMUTATORS OF COMPOSITE OPERATORS

Having verified the commutators (Appendix A) for the microscopic fields z_σ and p_σ it is instructive to consider the induced algebra of the composite fields f_μ, h, and A_μ which can be derived in the long-wavelength limit. Using the definition Eq. (4), one finds the commutators

$$[f_a(r),\bar{h}(r')]=(\partial_a-2iA_a)\delta(r-r') ,$$
$$[h(r),\bar{h}(r')]=0 , \tag{B1}$$
$$[A_a(r),\bar{h}(r')]=i\bar{f}_a(r)\delta(r-r') .$$

Some care has to be exercised in this derivation because the expressions for $A_a(r)$ and $f_a(r)$ in terms of fundamental operator z involve spatial derivatives. The problem is circumvented by interpreting these fields in the sense of the distributions, i.e., assuming that they always appear in spatial integrals along with some smooth function decaying at infinity. [These commutators together with the Hamiltonian of Eq. (4.11a) leading immediately to the "spin-wave" excitation spectrum.]

It is important to realize that the composite operators f_a and A_a are not unconstrained. The constraints derive from the definitions (4.5) and have the form

$$\epsilon_{ab}\partial_a A_b=i\epsilon_{ab}\bar{f}_a f_b \tag{B2}$$

and

$$\epsilon_{ab}(\partial_a-2iA_a)f_b=0 , \tag{B3}$$

and can be obtained most conveniently via matrix identities

$$\delta_{\sigma\nu}\delta_{\sigma'\nu'}=\epsilon_{\sigma\sigma'}\epsilon_{\nu\nu'}+\delta_{\sigma\nu'}\delta_{\sigma'\nu}$$

and

$$\delta_{\sigma\sigma'}\epsilon_{\nu\nu'}=\tfrac{1}{2}\delta_{\sigma\nu}\epsilon_{\sigma'\nu'}-\tfrac{1}{2}\delta_{\sigma\nu'}\epsilon_{\sigma'\nu}+\tfrac{1}{2}\delta_{\sigma'\nu}\epsilon_{\sigma\nu'}-\tfrac{1}{2}\delta_{\sigma'\nu'}\epsilon_{\sigma\nu} ,$$

respectively.

Equation (B2) determines the flux associated with the gauge field A_a in terms of the gauge-invariant combination of "twist" operators f_a, while Eq. (B3) imposes the gauge-invariant transversality condition on the twist field.

[1]P. W. Anderson, Science **235**, 1196 (1987).

[2]R. J. Birgeneau *et al.*, Phys. Rev. B **38**, 6614 (1988); R. J. Birgeneau *et al.*, *ibid.* **39**, 2868 (1989).

[3]G. Shirane *et al.*, Phys. Rev. Lett. **63**, 330 (1989).

[4]V. Elser, D. Huse, B. I. Shraiman, and E. D. Siggia, Phys. Rev. B **41**, 6715 (1990).

[5]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **61**, 467 (1988).

[6]F. C. Zhang and T. M. Rice, Phys. Rev. B **37**, 3759 (1988).

[7]V. J. Emergy and G. Reiter, Phys. Rev. B **38**, 4547 (1988).

[8]D. Frenkel, R. Gooding, B. Shraiman, and E. Siggia, Phys. Rev. B **41**, 350 (1990).

[9]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989).

[10]B. I. Shraiman and E. D. Siggia, Proceedings of the Trieste Conference on Strongly Correlated Electron Systems, 1989, edited by Yu Lu (World-Scientific, Singapore, in press).

[11]C. Kane, P. Lee, T. Ng, B. Chakraborty, and N. Read (unpublished).

[12]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).

[13]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).

[14]M. Gross, E. Sanchez-Velasco, and E. D. Siggia, Phys. Rev. B **39**, 2484 (1989).

[15]N. Trivedi and D. Ceperley, Phys. Rev. B **40**, 2737 (1989); J. Carlson, *ibid.* **40**, 846 (1989).

[16]D. A. Huse and V. Elser, Phys. Rev. Lett. **60**, 2531 (1988); D. A. Huse, Phys. Rev. B **37**, 2380 (1988).

[17]S. Chakravarty, D. Nelson, and B. Halperin, Phys. Rev. Lett. **60**, 1057 (1988).

[18]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983).

[19]M. Gross, E. Sanchez-Velasco, and E. D. Siggia, Phys. Rev. B **40**, 11 328 (1990).

[20]R. Singh, Phys. Rev. B **39**, 9760 (1989).

[21]G. Gomez-Santos, J. D. Joannopoulos, and J. W. Negele, Phys. Rev. B **39**, 4435 (1989).

[22]A measure of this correlation length is shown in Ref. 14.

[23]X. G. Wen and A. Zee, Phys. Rev. Lett. **61**, 1025 (1988); F. D. M. Haldane, *ibid.* **61**, 1029 (1988); E. Fradkin and M. Stone, Phys. Rev. B **38**, 7215 (1988).

[24]E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. (N.Y.) **16**, 407 (1961).

[25]M. Fisher and V. Privman, Phys. Rev. B **32**, 447 (1985).

[26]I. Affleck, Nucl. Phys. B **257**, 397 (1985).

[27]It is of some formal interest to calculate the commutators of **P** with the operators of the $NL\sigma$ model. One finds for spin $\frac{1}{2}$

$$[\mathbf{P}^\alpha_{r,a},s^\beta_r+s^\beta_{r+a}]=2i\epsilon^{\alpha\beta\gamma}\mathbf{P}^\gamma_{r,a} ,$$
$$\{\mathbf{P}^\alpha_{r,a},s^\beta_r-s^\beta_{r+a}\}=0 ,$$
$$[\mathbf{P}^\alpha_{r,a},s^\beta_r-s^\beta_{r+a}]=-2i\delta^{\alpha\beta}(c^\dagger_{r,\sigma}c_{r+a,\sigma}+\text{H.c.}) ,$$
$$[\mathbf{P}^\alpha_{r,a},\mathbf{P}^\beta_{r,a}]=2i\epsilon^{\alpha\beta\gamma}(s^\gamma_r+s^\gamma_{r+a}) .$$

Clearly the first commutator says that **P** rotates as a vector in spin space, while the second anticommutator implies that **P** and $\hat{\Omega}$ are perpendicular, a point to be made from a different perspective in Sec. V. The last two commutators should be zero in the large-S limit (or for long wavelength for spin $\frac{1}{2}$), since, in analogy with the σ model derivation **P**, like $\mathbf{s}_r-\mathbf{s}_{r+a}$, has to be divided by S to have a sensible limit (Ref. 26).

[28]W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970); L. Bulaevskii, E. Nagaev, and D. Khomskii, Z. Eksp. Teor. Fiz. **54**, 1562 (1968) [Sov. Phys.—JETP **27**, 836 (1968)].

[29]A. A. Belavin and A. M. Polyakov, Pis'ma Zh. Eksp. Teor. Fiz. **22**, 503 (1975) [JETP Lett. **22**, 245 (1975)].

[30]R. Bhatt and K. Rabe (private communication).

[31]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **60**, 740 (1988).

[32]A. M. Polyakov, *Gauge Fields and Strings* (Harwood, New York, 1987).

[33]T. Oguchi, Phys. Rev. **117**, 117 (1960).
[34]C. L. Kane, P. A. Lee, and N. Read, Phys. Rev. B **39**, 2653 (1989).
[35]P. Wiegman, Phys. Rev. Lett. **60**, 821 (1988).
[36]X. G. Wen, Phys. Rev. B **39**, 7223 (1989).
[37]See also, S. Brazovskii (unpublished).
[38]In Ref. 5 above Eq. (5), a factor of $\frac{1}{2}$ was omitted from the transformation equation for $\underline{K}_\mu$ and an i from the analogous equation for $\underline{M}$.
[39]Although irrelevant to the question of gauge invariance as we have defined it, it is interesting to note that only $\underline{Q}_\mu = i\partial_\mu - A_\mu \hat{\mathbf{\Omega}}\cdot\boldsymbol{\tau} + \frac{1}{2}\hat{\mathbf{\Omega}}\times\partial_\mu\hat{\mathbf{\Omega}}\cdot\boldsymbol{\tau}$ is invariant under $\underline{Q}_\mu \to e^{ix\hat{\mathbf{\Omega}}\cdot\boldsymbol{\tau}/2}\underline{Q}_\mu e^{-ix\hat{\mathbf{\Omega}}\cdot\boldsymbol{\tau}/2}$.
[40]C. N. Yang, Rev. Mod. Phys. **34**, 694 (1962).
[41]D. S. Fisher, Phys. Rev. B **39**, 11 783 (1989).
[42]D. Scalapino (private communication).
[43]A. J. Heager, S. Kivelson, J. R. Schrieffer, and W. P. Su, Rev. Mod. Phys. **60**, 781 (1988).
[44]F. D. M. Haldane, Phys. Rev. Lett. **61**, 1029 (1988).