Skyrmion Ground States in the Presence of Localizing Potentials in Weakly Doped CuO_2 Planes

R. J. Gooding
Department of Physics, Queen's University, Kingston, Ontario, Canada K7L 3N6
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The motion of a single hole in the one-band t-t'-J model that is constrained to move over only one plaquette is shown to lead to a ground state with a three-dimensional spin texture whose topology is that of a singly charged Skyrmion. This geometry mimics the weakly doped 214 superconductors where the Sr or Ce ions locally pin the otherwise mobile holes with a pinning potential that has fourfold symmetry. The competition between t and J that leads to the novel chiral-symmetry-breaking ground states is shown to be describable via a semiclassical theory that accounts for a coupling of the hole's spin current to the magnetization current of the antiferromagnetic background.

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The interest in the doped CuO_2-plane-based antiferromagnetic (hereafter referred to as AFM) insulators, such as the Bednorz-Müller $La_{2-x}Sr_xCuO_4$ compound, or the electron-doped $Nd_{2-x}Ce_xCuO_4$ compound, is related to both their superconducting properties[1] and their unusual magnetic properties.[2] The latter is rich with the rapid depletion of AFM order with doping, possibly a reentrant spin-glass phase, and perhaps an incommensurate spin-density wave, a so-called spiral phase.[2,3]

In order to understand this complicated behavior one theoretical avenue that has been extensively explored involves doping the 2D Hubbard model away from half filling.[4] From such a model the relevant characteristics of the magnetic state may be extracted, e.g., the 2D AFM correlation length. If the reduction of AFM order is to be understood, this latter quantity suffices since the 3D magnetic ordering is a parasitic effect arising from a weak interplanar coupling, and the large correlation length of a 2D AFM at finite temperatures is the cause of the development of a nonzero T_N. Thus, one must first understand the changes of the 2D AFM state produced by the holes. In this paper we will only be concerned with the changes in the magnetic state at very small x at $T=0$. To best represent this physical system the doping must proceed in a spatially inhomogeneous manner.[5] To see this, note that upon doping the Bednorz-Müller compound the holes that are introduced go into the CuO_2 planes due to the replacement of a trivalent La^{3+} ion with a divalent Sr^{2+} ion (in the plane above a CuO_2 plane). The Sr^{2+} ions furnish an inhomogeneous electrostatic background that the holes (principally O^- in character[6]) are attracted to. To be specific, the holes will be localized in the plane in the neighborhood of a Sr^{2+} ion, and since the associated pinning potential has fourfold symmetry, each hole may only propagate over a small region with the same symmetry. A similar geometry exists in the electron-doped materials. The simplest such region is that of a single two-site-by-two-site plaquette, and the motion of a hole in such a configuration is the topic addressed here. This geometry is illustrated in Fig. 1. This leads to the observation in this Letter of ground states with a Skyrmion-type topology[7] whose stabilization may be understood using a semiclassical theory.[8]

As the Hamiltonian describing the problem of holes moving on a square lattice of $S=\frac{1}{2}$ spins we utilize the t-t'-J model given by

$$H=-t\sum_{\langle i,j\rangle}(c^\dagger_{i,\sigma}c_{j,\sigma}+\text{H.c.})-t'\sum_{\langle i,i'\rangle}(c^\dagger_{i,\sigma}c_{i',\sigma}+\text{H.c.})+J\sum_{\langle i,j\rangle}(\mathbf{S}_i\cdot\mathbf{S}_j-\tfrac{1}{4}n_in_j)\,. \quad (1)$$

In Eq. (1) the first term represents near-neighbor hopping, while the second represents diagonal next-nearest-neighbor hopping; the sums over i, j, and i' are restricted to those four sites labeled 1, 2, 3, and 4 in Fig. 1, and the summation convention is implied for the spin indices. The superexchange term involves the spin operators $\mathbf{S}=\frac{1}{2}c^\dagger_\sigma\hat{\tau}_{\sigma,\sigma'}c_{\sigma'}$, where $\hat{\tau}$ are the Pauli matrices, as well as the occupation numbers n_i for the Cu sites.

We note the inclusion of the second-neighbor hopping

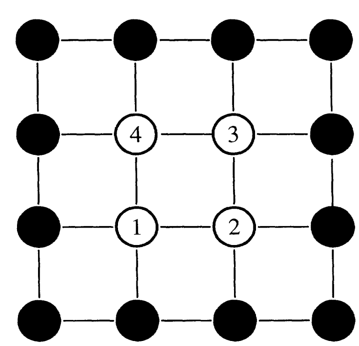

FIG. 1. The geometry of the cluster used in this study. The circles represent Cu sites, and the hole is constrained to only move over the numbered sites.

term t'. This can be thought of as arising from the projection of the three-band CuO extended Hubbard model's ground state for a single hole onto the Hilbert space relevant to the one-band model.[9] This renormalization is possible owing to the fact that the quantum numbers describing the ground state of the single hole in the strong-correlation limit of both the single- and three-band models are the same.[10] Further, as shown by Zhang and Rice,[11] the O^- hole can locally form a singlet state with the Cu spins, from which the t-J model may be argued to give the essential physics. However, the strong O-site correlation limit of the extended Hubbard model makes clear[12] the necessity of including t' hopping terms in addition to the near-neighbor t-hopping term. Thus, we include the t' term throughout our considerations of this model.

It will be instructive to begin our study of this model by first considering the motion of a single hole in a ferromagnetic (referred to by FM) background. Denoting the state with the hole located at site i in the FM background by $|i\rangle$, the four eigenstates are

$$\begin{aligned} |\omega=1\rangle &= \tfrac{1}{2}(|1\rangle+|2\rangle+|3\rangle+|4\rangle)\,,\\ |\omega=-1\rangle &= \tfrac{1}{2}(|1\rangle-|2\rangle+|3\rangle-|4\rangle)\,,\\ |\omega=i\rangle &= \tfrac{1}{2}(|1\rangle+i|2\rangle-|3\rangle-i|4\rangle)\,,\\ |\omega=-i\rangle &= \tfrac{1}{2}(|1\rangle-i|2\rangle-|3\rangle+i|4\rangle)\,, \end{aligned} \tag{2}$$

with energies,

$$\begin{aligned} &E(\omega=1)=-2t-t',\quad E(\omega=-1)=2t-t',\\ &E(\omega=\pm i)=t', \end{aligned} \tag{3}$$

where the eigenstates are labeled[13] by the orbital-angular-momentum index $\omega=\pm 1,\pm i$. The spatial functions which generate the irreducible representations under which these eigenstates transform are thus clear: x^2+y^2, x^2-y^2, and $x\pm iy$. Observe that the $\omega=\pm i$ states have circulations associated with them, while the other two states do not. This will prove to be important in understanding how the obtained Skyrmion ground state is stabilized.

Quantum cluster exact diagonalization studies on a 4×4 lattice of spins with a single vacancy were performed for the Hamiltonian defined by Eq. (1) with the values believed[9] to describe the $LaCuO_4$ system: $J/t=0.29$, and $t'/t=-0.136$. One may show that periodic boundary conditions frustrate the $\omega=\pm i$ states, and from now on only results obtained from open boundary conditions will be displayed.

We have found that the ground state is a doubly degenerate $\omega=\pm i$ state for the above $LaCuO_4$ values. This state has total spin $S=\frac{1}{2}$. Insight into the features of this state may be obtained by evaluating three correlation functions. The first is the hole's motional current derived from the direct hopping term. The relevant operator defining this quantity is given by

$$\mathbf{j}_\mu=\tfrac{1}{2}it(c^\dagger_{i,\sigma}\hat{\tau}_{\sigma,\sigma'}c_{i+\mu,\sigma'}-c^\dagger_{i+\mu,\sigma}\hat{\tau}_{\sigma,\sigma'}c_{i,\sigma'})\,, \tag{4}$$

where $\mu=\pm(1,2),\ (2,3),\ (3,4),\ (4,1)$. For example, for the FM eigenstates defined in Eq. (2), one has

$$t^{-1}\sum_\mu\langle\omega|\mathbf{j}_\mu\cdot\hat{\mathbf{z}}|\omega\rangle=\begin{cases}0 & (\omega=\pm 1)\,,\\ \pm 1 & (\omega=\pm i)\,,\end{cases} \tag{5}$$

where $\hat{\mathbf{z}}$ is the direction of the FM polarization. For the doubly degenerate ground state obtained in our cluster study, the expectation value of the quantity in Eq. (5) is found to be ± 0.364. Clearly, the motional currents obtained in our AFM ground states are large, since they are greater than $\frac{1}{3}$ of their maximum possible value obtained in the FM state.

The second correlation functions that we have evaluated are the bond spin currents, viz., $\langle \mathbf{S}_i\times\mathbf{S}_j\rangle$, for i,j being near neighbors. This quantity has proven useful in previous studies that concerned themselves with the manner in which hole motion perturbed the ordered AFM background.[8,10,14] Here we evaluate this quantity to show that the circuital hole motion is mimicked in the spin distortions of the ground states. This quantity is displayed in Fig. 2 for the $\omega=i$ state. For the $\omega=-i$ state, the symmetry of these correlation functions is maintained, but each circulational feature is reversed. This quantity can be related[8] to the magnetization current, and used to show that it is the hole's motional current which drives the spin distortions shown in Fig. 2.

The third correlation function that is presented is the so-called topological charge, and is defined by

$$T=\sum_{(ijk)}T_{(ijk)},\quad T_{(ijk)}=\mathbf{S}_i\cdot(\mathbf{S}_j\times\mathbf{S}_k)\,. \tag{6}$$

This so-called chiral-order parameter $T_{(ijk)}$ is defined for

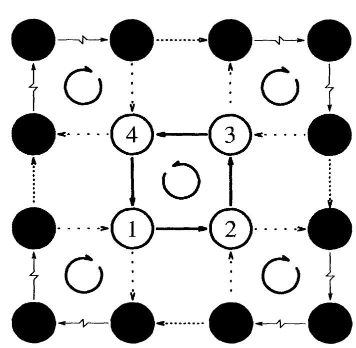

FIG. 2. The bond spin currents $\langle \mathbf{S}_i\times\mathbf{S}_j\rangle$ associated with the $\omega=i$ ground state. Similar line types indicate equal magnitudes. The arrows give the direction of the current. The circular inclusions denote the direction of the circulational magnetization current. Note the clockwise circulation of the outer edge of the cluster.

local triplets of spins. For example, in Fig. 1 two such triplets would be (123) and (134). Then, the total value of T for the single plaquette [1234] would be $T_{(123)}+T_{(134)}$. This definition is consistent with the definition of the topological charge for classical spin fields on a lattice.[15] For the $\omega=\pm1$ minimum-energy states the topological charge is found to be zero, while for the $\omega=\pm i$ ground state one finds $\langle T\rangle=\pm0.3904$. This breaking of chiral order in the lattice is explicit evidence that the $\omega=\pm i$ ground states can be thought of as topological Skyrmions with $Q=\pm1$. For example, the ground state no longer corresponds to a planar configuration, as it does for completely mobile holes.[8,10,14]

The stability of these states was studied as a function of J/t and t'/t. For open boundary conditions we find that the $\omega=\pm i$ states are always stable for $0.025\le J/t\le 4$ when $t'=0$. Allowing for $t'\neq0$ has much more profound effects, as is already suggested by Eq. (3) for a hole moving in a FM background. When $t'/t<0$, the stability of $\omega=\pm i$ states is enhanced, while for $t'/t>0$ the opposite situation arises in that the $\omega=-1$ state has its energy lowered relative to the $\omega=\pm i$ states. The effect of t' is found to be essentially perturbative:

$$E(\omega=\pm i,t'/t)\sim E(\omega=\pm i,t'/t=0)+0.316t'/t\,,$$
$$E(\omega=-1,t'/t)=E(\omega=-1,t'/t=0)-0.402t'/t\,. \tag{7}$$

Thus, for the La_2CuO_4 values quoted by Hybertsen *et al.*,[9] the stability of the $\omega=\pm i$ states does not seem to be in question (for finite lattices[16]). However, for systems for which t'/t is positive, the stability of the Skyrmion is something that one must be concerned with.

Last, we note that an alternate description of the hole motion around a single plaquette is to place the hole in the lattice as an O^- site. An effective Hamiltonian representing this system in the strong-correlation limit was employed,[10] and the same spin texture as in the ground state described above was obtained for parameters believed to describe the La_2CuO_4 system. Thus, regardless of whether the holes are completely or only partially mobile, the one-band description seems to suffice.[9-12]

In order to display an interpretation of the correlation functions found above we begin with the spatially varying AFM order parameter corresponding to $Q=\pm1$ Skyrmions:[7]

$$\Omega_x=\frac{2\lambda x}{r^2+\lambda^2},\quad \Omega_y=\pm\frac{2\lambda y}{r^2+\lambda^2},\quad \Omega_z=\frac{r^2-\lambda^2}{r^2+\lambda^2}\,, \tag{8}$$

where λ is some constant. This is a solution of the chiral field ($\hat{\Omega}^2=1$) equation, viz.,

$$\nabla^2\hat{\Omega}=0\,, \tag{9}$$

obtained from the nonlinear σ model.[17] The latter is believed to describe the long-wavelength hydrodynamic spin waves[8] of the 2D quantum AFM. Quite simply, the solution of Eq. (9) that corresponds to the ground state of a doped system is that which satisfies the "boundary conditions" imposed by the hole. For a hole moving on a single plaquette, the boundary condition imposed by the $\omega=\pm i$ states are that the spin part of the AFM order parameter behave in the same manner as $\mathbf{r}$. To be specific, for these states one requires that Ω_x and Ω_y should transform like $x\pm iy$; note from Eq. (8) that $\Omega_x+i\Omega_y\propto x\pm iy$. Further, note that the bond spin currents $\langle\mathbf{S}_i\times\mathbf{S}_j\rangle$ predicted by Eq. (8) reproduce Fig. 2.

We now utilize the semiclassical theory of Shraiman and Siggia,[8,14] who previously postulated the Skyrmion ground state for this problem,[8] to show why the hole and magnetization currents couple in a fashion that stabilizes the $Q=\pm1$ Skyrmion states. Within this theory, the classical interaction between the hole's motional current and the magnetization current, viz., $\hat{\Omega}\times\partial_\mu\hat{\Omega}$, is given by, $\mu=x,y$,

$$H_{\rm int}=-g\mathbf{j}_\mu\cdot(\hat{\Omega}\times\partial_\mu\hat{\Omega})+\tfrac{1}{2}J(\hat{\Omega}\times\partial_\mu\hat{\Omega})^2\,, \tag{10}$$

where $g>0$ is some phenomenological coupling constant. From Fig. 1 one sees that what is required to obtain the coupling is the magnetization current along the lines $y=0$ and $x=0$, which corresponds to hole motion along $\pm\hat{\mathbf{y}}$ and $\mp\hat{\mathbf{x}}$, respectively. In the association of the magnetization current we have used that for the $Q=1$ Skyrmion, when $x>0$ along the line $y=0$, the hole moves in the positive y direction, etc. From Eq. (8) one finds that for the $Q=\pm1$ Skyrmions, the z component[18] of the magnetization current is given by

$$\hat{\Omega}\times\partial_x\hat{\Omega}\,|_{x=0}=\mp\frac{4\lambda^2y}{(y^2+\lambda^2)^2}\hat{\mathbf{z}}\,,$$
$$\hat{\Omega}\times\partial_y\hat{\Omega}\,|_{y=0}=\pm\frac{4\lambda^2x}{(x^2+\lambda^2)^2}\hat{\mathbf{z}}\,. \tag{11}$$

Further, the $\omega=\pm i$ state which generates the $Q=\pm1$ Skyrmion has hole motional currents given by (again, in the z direction)

$$\mathbf{j}_x\cdot\hat{\mathbf{z}}=\mp|j|y/|y|,\quad \mathbf{j}_y\cdot\hat{\mathbf{z}}=\pm|j|x/|x|\,, \tag{12}$$

for $|j|$ being some constant determined by J and t. Clearly, the coupling of the magnetization and motional currents given by Eqs. (11) and (12) always yields $\mathbf{j}_\mu\cdot\hat{\Omega}\times\partial_\mu\hat{\Omega}>0$ for both the $Q=\pm1$ Skyrmions *if* the $\omega=\pm i$ state's motional current is associated with it. Thus, Eq. (10) amply describes the stabilization of the singly charged Skyrmion by hole motion around a single plaquette.

We now discuss an issue raised by Eq. (7), viz., when t'/t is sufficiently positive the singly charged Skyrmion $\omega=\pm i$ state is unstable with respect to the $\omega=-1$ state. The question then arises as to what is a simple semiclassical description of the latter state. As discussed in relation to Eq. (2), this latter state has a symmetry mirrored by x^2-y^2. Alternatively, in terms of the circuital current analogy described above, suppose that currents of the form $(x+iy)^2$ were attempted to be set up in this state. This function also transforms like the $\omega=-1$ irreducible representation of the fourfold rotation group. However, so does $(x-iy)^2$, which has the opposite circulation; why should one of these be chosen over the other?

To be specific, the issue is how can we utilize the current coupling analogy to understand the nature of the $\omega=-1$ ground state? To restore the left- and right-handed biases that the $(x\pm iy)^2$ states have, note that a linear combination of these states yields states with the correct symmetry, *vis-à-vis* $(x+iy)^2\pm(x-iy)^2$. Thus, we can consider obtaining the spin texture of the $\omega=-1$ state by superimposing $Q=\pm 2$ Skyrmions, each of which are each generated by $(x+iy)^2$ motional currents, respectively. The resulting spin texture is given by

$$\Omega_x=\frac{2\lambda^2(x^2-y^2)}{(r^4+\lambda^4)},\quad \Omega_y=0,\quad \Omega_z=\frac{(r^4-\lambda^4)}{(r^4+\lambda^4)}. \tag{13}$$

By comparing the expectation values discussed earlier for now the $\omega=-1$ quantum-mechanical ground state, with those obtained[18] from Eq. (13), we see that indeed the planar spin texture in Eq. (13) describes both the topology and symmetry of the $\omega=-1$ ground state. It is interesting to note that this disturbance of the ordered Néel state is planar, as well as shorter ranged. In fact, if the magnetization channel of the nonlinear σ model is included, one finds that the fall-off spin texture is actually short ranged[19] in that an exponential decay must append Eq. (13).

In summary, we have shown that the ground state of a weakly doped AFM insulator, where each hole has a localizing potential with fourfold symmetry, should be a three-dimensional spin texture that has the topology of a singly charged Skyrmion. This ground state is a chiral spin state. The stability of this state does depend on the ratio of t'/t, and this leads to different topologies, symmetries, and ultimately spin distortions of the AFM spin texture.

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[18]As is usual in studies that have utilized the semiclassical approximation (see Refs. 8, 10, and 14) in order to compare to the quantum cluster studies, rotational symmetry about the axis of quantization must be restored; for the cluster studied here this means a rotation around the z direction.

[19]See the discussion of the $(\pi,0)$ states for completely mobile holes in Ref. 8.