Semiclassical spin polarons

M. J. Godfrey
Department of Pure and Applied Physics, University of Manchester Institute of Science and Technology, P.O. Box 88, Manchester M60 1QD, United Kingdom

J. M. F. Gunn
School of Physics and Space Research, University of Birmingham, Birmingham B15 2TT, United Kingdom
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The observed properties of the higher-spin analogs of the lanthanum cuprates motivate a study of charge carriers in a classical two-dimensional antiferromagnet. Even for classical spins there is a remarkable dependence on the position of the carrier wave vector in the magnetic Brillouin zone. At the zone center, there is a tendency toward ferromagnetic alignment of the spins, while at the zone boundary this tendency is suppressed and a more complex spin polaron can be formed.

I. INTRODUCTION

The absence of superconductivity[1,2] in the spin-1 and spin-$\frac{3}{2}$ analogues of the lanthanum cuprates (La_2NiO_4 and La_2CoO_4, respectively) is striking. In contrast to the cuprates, the cobaltates do not even become metallic upon doping, and the nickelate only approaches the metallic state when doped with 50% Sr.[1]

Enhanced trapping, or localization, of the carriers would seem to be an obvious interpretation, although its origin is unclear. There are at least two simple explanations based on effective-mass enhancement. First, the energy levels of the transition-metal ion are less closely degenerate with the oxygen p states, leading to a narrower bandwidth, facilitating localization. Second, the coupling of the charge carriers to the spins may lead to different types of magnetic (spin) polarons when the spins have different magnitudes, and hence perhaps to different effective masses.

A single-band model, appropriate to the nickelates and cobaltates, was derived in Ref. 3. The principal feature is that only *one* d orbital is itinerant—the $d_{x^2-y^2}$ orbital as in the cuprate. The other orbitals have either zero (because of symmetry) or reduced matrix elements for hopping, and so are in the "insulating" local moment regime. The magnetic moment comes from both the itinerant and localized states, as has been demonstrated by neutron scattering.[4,5]

The Hamiltonian of Ref. 3 is

$$H=-t\sum_{\langle i,j\rangle}\phi_i^\dagger\phi_j+\frac{J}{S^2}\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+\frac{j}{S}\sum_i\phi_i^\dagger\sigma\phi_i\cdot\mathbf{S}_i\ . \quad (1)$$

We will neglect the Hubbard U term for the itinerant electrons, which is consistent with the decline in U in moving from Cu to the left across the transition metals.

Any differences in physics as the spin of the ions is increased should be most dramatically revealed in the classical limit of large spin, $S\to\infty$. This is the opposite limit to the cuprates. Happily this limit is also mathematically tractable, as the Holstein-Primakoff transformation simplifies there. The classical limit has a long history, starting with the work by de Gennes,[6] reviewed in Refs. 7 and 8, where the nature of the spin polarons formed due to the coupling between the spins and the charge carriers is discussed. In this paper we will focus on how the nature of the distortion in the spin system depends on the wave vector of the polaron. In the spin-$\frac{1}{2}$ case[9] there is a striking distinction between a tendency to maximize the spin within the polaron when the polaron momentum is near the Brillouin-zone center, and to minimize the spin when the momentum is at the (magnetic) zone boundary. This has a quantum-mechanical origin, as it is due to a difference in sign of the superpositions of spins states. In the *classical* limit it is not clear what result will be obtained.

A convenient feature of the classical limit $S\to\infty$ is that it coincides with the adiabatic limit for the carrier-spin system. This is demonstrated in Appendix A. We can therefore regard the spins as a set of classical angular momentum variables that provide a spin-dependent potential for the carrier. The spins adopt a Néel configuration in the absence of the carrier; whereas in its presence the total energy can be reduced by distorting the Néel state with the carrier bound to the potential well created. Because a quantum-mechanical particle will bind to any attractive potential $U(r)$ in two dimensions $[\int dr\, rU(r)<0]$ it might be supposed that the carrier will be bound to the spin system whatever the strength of interaction j. As the strength of the potential is reduced the particle binds only weakly and the wave function has a correspondingly large spatial extent. Although it will turn out that a certain critical strength of coupling is required to bind the particle, it is still true that the binding energy can be small and the length scale correspondingly great compared with the lattice parameter. In this limit the antiferromagnet can be represented conveniently by the classical nonlinear σ model

$$H_{\text{spins}}=\tfrac{1}{2}J\int d^2x\,[8\mu^2+(\nabla\omega)^2]\ , \quad (2)$$

where μ is the magnetization density and ω is the sublat-

tice magnetization. The precise definitions of ω and μ are given in Appendix B. Here and elsewhere we take the unperturbed ω to lie in the z direction. Of course, the spin and space degrees of freedom are uncoupled in our model, so that ω and μ could always be subjected to a spatially homogeneous rotation.

In the natural long-wavelength motion of the spins, μ is much smaller than ω, and the constraints $\omega^2=1$ and $\omega\cdot\mu=0$ are approximately conserved by the equations of motion. The presence of a carrier changes this situation: later we will see that μ can be of the same order as, or even greater than, the perpendicular deviations $\omega_\perp$ of the sublattice magnetization. Hence we must formulate the constraint more precisely, using the definitions in terms of spin operators. We find $\omega^2+\mu^2=1$ and $\omega\cdot\mu=0$. These constraints are preserved by the equations of motion.

II. CONTINUATION BETWEEN SUBLATTICES

Corresponding to the continuum limit for the spins we can also make a continuum approximation for the electronic degrees of freedom. Since, in general, the wave function takes a different form on the two sublattices (A and B), the continuum approximation leads us to define a four-component spinor

$$\psi_i=\begin{bmatrix}\phi_i^A\\ \phi_i^B\end{bmatrix},$$

where i belongs to the A sites and ϕ_i^B is a continuation of the B-site wave function on to the A sites. Methods for making this continuation and an estimate of its accuracy are given in Appendix B. The four-component object need only be defined on one sublattice, so that there is no doubling of the number of degrees of freedom. The same is true for the spins: the redundant spin operators introduced in Ref. 10 to help define the magnetization and sublattice magnetization of an arbitrary spin state can be replaced by interpolated quantities for the slowly varying states considered here.

Using this notation we rewrite the Hamiltonian of Eq. (1) as

$$H=-t\sum_{\langle i,j\rangle}\psi_i^\dagger\beta\psi_j+\tfrac{1}{2}J\int d^2x\,[8\mu^2+(\nabla\omega)^2]+j\int d^2x\,[\mathbf{M}\cdot\boldsymbol{\mu}+\boldsymbol{\Omega}\cdot\boldsymbol{\omega}]\ , \tag{3}$$

where

$$\mathbf{M}=\psi^\dagger\boldsymbol{\Sigma}\psi$$

and

$$\boldsymbol{\Omega}=\psi^\dagger\boldsymbol{\alpha}\psi\ .$$

Here β and $\boldsymbol{\alpha}$ are the Dirac matrices, and Σ is the 4×4 spin matrix, all in the Weyl representation.

In Eq. (3) we have preserved the lattice notation for the kinetic energy. Although the lattice expression involves variables of both sublattices, these can be understood as continuations of four-component objects of the A sublattice. Using $\mathbf{k}$, the operator conjugate to the site operator $\mathbf{R}$, we can express the kinetic energy as

$$\sum_{\langle i,j\rangle}\psi_i^\dagger\beta\psi_j=2\int d^2x\ \psi^\dagger(\mathbf{x})\beta(\cos k_x+\cos k_y)\psi(\mathbf{x})\ .$$

III. ZONE CENTER

Near $\mathbf{k}=\mathbf{0}$ the kinetic energy is of order $4t$ and the two bands are well separated. The operator $j\boldsymbol{\omega}\cdot\boldsymbol{\alpha}$ couples the two bands and consists of terms of different orders with respect to $\boldsymbol{\omega}_\perp$, the deviation from Néel order,

$$j\boldsymbol{\omega}\cdot\boldsymbol{\alpha}=j\sqrt{1-\omega_\perp^2-\mu^2}\,\alpha_z+j\boldsymbol{\omega}_\perp\cdot\boldsymbol{\alpha}\ .$$

Having adopted a four-component description of the carrier, it seems natural to apply successive Foldy-Wouthuysen transformations[11] to eliminate the interband transitions. This leads to an effective single-band Hamiltonian for the carrier. First we eliminate the effect of the uniform, unperturbed spin system. The transformed Hamiltonian is

$$H'=e^{\lambda\beta\alpha_z}He^{-\lambda\beta\alpha_z} \tag{4}$$

with $\tan2\lambda=j/\epsilon(\mathbf{k})$, or

$$H'=\beta\sqrt{\epsilon(\mathbf{k})^2+j^2}+j\boldsymbol{\alpha}_\perp\cdot\boldsymbol{\omega}_\perp-\tfrac{1}{2}j\alpha_z(\omega_\perp^2+\mu_\perp^2)+j\boldsymbol{\Sigma}'\cdot\boldsymbol{\mu}+O(\omega_\perp^3)\ ,$$

where $\Sigma_z'=\Sigma_z$ and

$$\boldsymbol{\Sigma}_\perp'=\cos2\lambda\begin{bmatrix}\boldsymbol{\sigma}_\perp & 0\\ 0 & \boldsymbol{\sigma}_\perp\end{bmatrix}+\sin2\lambda\begin{bmatrix}0 & -i\hat{\mathbf{z}}\times\boldsymbol{\sigma}\\ i\hat{\mathbf{z}}\times\boldsymbol{\sigma} & 0\end{bmatrix}.$$

A further transformation to eliminate the remaining odd parts gives [$\epsilon_0=\epsilon(\mathbf{0})=4t$]

$$H''=\beta\sqrt{\epsilon^2+j^2}+j\frac{\epsilon_0}{\sqrt{\epsilon_0^2+j^2}}\boldsymbol{\mu}_\perp\cdot\boldsymbol{\Sigma}\ . \tag{5}$$

The spatial derivatives in (5) appear at second order; second derivatives of the perpendicular spin deviations have been neglected. The effective Hamiltonian describing the carrier and its interaction with the spin system is finally

$$H_{\text{carrier}}+H_{\text{int}}=\beta\sqrt{\epsilon_0^2+j^2}+\frac{1}{4}\frac{\epsilon_0^2}{\sqrt{\epsilon_0^2+j^2}}\beta\nabla^2+j\frac{\epsilon_0}{\sqrt{\epsilon_0^2+j^2}}\boldsymbol{\mu}_\perp\cdot\boldsymbol{\Sigma}\ . \tag{6}$$

There is no remaining interaction with the sublattice magnetization ω. The effect of the carrier is to polarize the antiferromagnetic background. Since $\boldsymbol{\mu}\cdot\boldsymbol{\omega}=0$, $\mu_z\ll\mu_\perp$, and the polarization is effectively perpendicular to $\hat{\mathbf{z}}$. For a stationary carrier this distortion minimizes the energy

$$\tfrac{1}{2}J\int d^2x\ 8\mu^2+\frac{j\epsilon_0}{\sqrt{\epsilon_0^2+j^2}}\int d^2x\,[\psi^\dagger\boldsymbol{\Sigma}\psi]\cdot\boldsymbol{\mu}_\perp$$

so that the magnetization density at equilibrium is

$$\boldsymbol{\mu}_\perp = -\frac{j\epsilon_0}{8J\sqrt{\epsilon_0^2+j^2}}\psi^\dagger \boldsymbol{\Sigma}_\perp \psi \ . \tag{7}$$

Because the Hamiltonian (6) does not couple the upper and lower pairs of components of ψ, we can suppose that the particle remains in lower band, so that $\psi^\dagger \boldsymbol{\Sigma}_\perp \psi$ in (7) can be replaced by $u^\dagger \boldsymbol{\sigma}_\perp u$, where u is the lower pair of components of ψ. Substituting this form for the magnetization into the Hamiltonian (6) gives a two-dimensional (2D) nonlinear Schrödinger equation for the two-component spin wave function of the carrier:

$$-\frac{1}{4}\frac{\epsilon_0^2}{\sqrt{\epsilon_0^2+j^2}}\nabla^2 u - \frac{j^2}{8J}\frac{\epsilon_0^2}{\sqrt{\epsilon_0^2+j^2}}[u^\dagger \boldsymbol{\sigma}_\perp u]\cdot\boldsymbol{\sigma} u = (E+\sqrt{\epsilon_0^2+j^2})u \ . \tag{8}$$

Similarly, if the lower band was completely filled with electrons, their net polarizing effect would be zero and we could again confine our attention to a two-component wave function for a carrier added to the upper band.

The spinor equation (8) has solutions in which the spin and space degrees of freedom separate as $v(\mathbf{x})\chi$, where χ is a constant spinor with components $|\chi_1| = |\chi_2|$ and $v(\mathbf{x})$ satisfies a scalar nonlinear Schrödinger equation. If the coupling j is large enough the energy eigenvalue becomes negative. The polaron is then unstable to collapse because the energy scales as L^{-2}, where L is a lengthscale which can be chosen freely. For a rotationally invariant wave function $v(r)$ the critical value of the coupling can be found by numerical integration of the nonlinear Schrödinger equation; this gives

$$\frac{j^2}{8\pi J\sqrt{16t^2+j^2}} = 0.931\,13 \ , \tag{9}$$

which depends only on the parameters j, J, and t. Although in this section we have made no assumptions about the relative sizes of these parameters, we have nevertheless required the polarization of the spin system to be small, so that the magnetization is not saturated. We should verify that this leads to no inconsistency. For a particle wave function of spatial extent L, $u^+\boldsymbol{\sigma} u = O(1/L^2)$, so that we require

$$\mu_\perp \sim \frac{j}{J}\frac{\epsilon_0}{\sqrt{\epsilon_0^2+j^2}}\frac{1}{L^2} \ll 1 \ .$$

If the polaron is unstable we can combine this with (9) to obtain $t/jL^2 \ll 1$, which can be satisfied if the carrier wave function extends over a large enough area.

IV. ZONE BOUNDARY

A study of the problem at the zone center is useful for orientation, but in the systems of interest the states of lowest energy for the added carrier lie at the boundary of the magnetic Brillouin zone. Here the kinetic energy $t\cos k_\perp$ is small and we may treat it as a perturbation on the spin splitting induced by the background sublattice magnetization.

To take into account the background we use the transformed Hamiltonian (4) with $\lambda = \pi/4$:

$$H' = j\begin{bmatrix} \omega_z+\sigma_z\mu_z & \boldsymbol{\sigma}_\perp\cdot\boldsymbol{\omega}_\perp - i\hat{\mathbf{z}}\times\boldsymbol{\sigma}\cdot\boldsymbol{\mu} - \epsilon\sigma_z/j \\ \boldsymbol{\sigma}_\perp\cdot\boldsymbol{\omega}_\perp + i\hat{\mathbf{z}}\times\boldsymbol{\sigma}\cdot\boldsymbol{\mu} - \epsilon\sigma_z/j & -\omega_z+\sigma_z\mu_z \end{bmatrix} . \tag{10}$$

The off-diagonal terms in (10) are small compared with j, so that we can perform a further Foldy-Wouthuysen transformation regarding these "odd" terms as a perturbation. The result is

$$H'' = j(\mu_z + \boldsymbol{\mu}_\perp\cdot\boldsymbol{\omega}_\perp)\sigma_z + \tfrac{1}{2}\{\boldsymbol{\mu}_\perp,\epsilon\}\cdot\boldsymbol{\sigma} + \left\{ j[\omega_z + \tfrac{1}{2}(\omega_\perp^2+\mu_\perp^2)] - \tfrac{1}{2}i[\boldsymbol{\omega}_\perp,\epsilon]\times\hat{\mathbf{z}}\cdot\boldsymbol{\sigma} + \frac{1}{2j}\epsilon^2 \right\}\beta \ ,$$

in which $[,]$ and $\{,\}$ denote the commutator and anticommutator, respectively. Using $\mu_z + \boldsymbol{\mu}_\perp\cdot\boldsymbol{\omega}_\perp \simeq \boldsymbol{\mu}\cdot\boldsymbol{\omega} = 0$ and

$$\omega_z^2+\omega_\perp^2+\mu^2 = 1$$

or

$$\omega_z + \tfrac{1}{2}(\omega_\perp^2+\mu_\perp^2) = 1 + O(\omega_\perp^4,\mu_\perp^4) \ ,$$

we find the upper (+) and lower (−) 2×2 blocks of H''

$$H''_\pm = \pm\left[j + \frac{1}{2j}\epsilon^2 - \tfrac{1}{2}i[\boldsymbol{\omega}_\perp,\epsilon]\times\hat{\mathbf{z}}\cdot\boldsymbol{\sigma} \right] + \tfrac{1}{2}\{\boldsymbol{\mu}_\perp,\epsilon\}\cdot\boldsymbol{\sigma} \ . \tag{11}$$

Note that the second-order terms in $\boldsymbol{\omega}_\perp$ and $\boldsymbol{\mu}_\perp$ have canceled exactly. This should not surprise us: if the hopping were switched off, the electron spin would align with the local spin direction, making the energy independent of $\boldsymbol{\omega}$ and $\boldsymbol{\mu}$. Hence, the terms in the Hamiltonian that do not involve the hopping integral t must reduce to a constant after the Foldy-Wouthuysen transformation.

In (11), ϵ is the differential operator $-2t(\cos k_x + \cos k_y)$, or

$$\epsilon(\mathbf{k}) = -4t\cos\tfrac{1}{2}(k_x+k_y)\cos\tfrac{1}{2}(k_x-k_y) = -4t\cos(k_n/\sqrt{2})\cos(k_t/\sqrt{2}) \ ,$$

where $k_n \simeq \pi/\sqrt{2}$ and $k_t \simeq 0$ are the components of $\mathbf{k}$ resolved parallel and perpendicular to the normal of the Brillouin-zone boundary. It is helpful to extract the rapidly oscillating factor $(-1)^{x+y}$ from the wave functions. Then $\epsilon \simeq -4t\sin(-i\nabla_n/\sqrt{2}) \simeq 2\sqrt{2}ti\nabla_n$ is an operator acting on the slowly varying envelope of the wave function. With this understanding, the Hamiltonian may be taken to be

$$H''_{+}=j-\frac{4t^2}{j}\nabla_n^2+\sqrt{2}t\boldsymbol{\sigma}\cdot[i\nabla_n\boldsymbol{\mu}_\perp+\boldsymbol{\mu}_\perp i\nabla_n+\hat{\mathbf{z}}\times(\nabla_n\boldsymbol{\omega}_\perp)] . \quad (12)$$

The appearance of gradient terms involving the magnetization and sublattice magnetization is plausible as the transfer of a carrier from one site to its neighbor involves both a spin flip (with amplitude $\sim j\mu_\perp$) and a hop ($\sim it\nabla_n$) via an intermediate state separated in energy by j. We can interpret the interaction terms as a local coupling of the spin current $i[u^\dagger\boldsymbol{\sigma}(\nabla_n u)-(\nabla_n u^\dagger)\boldsymbol{\sigma}u]$ to the magnetization density $\boldsymbol{\mu}_\perp$ and of the spin density with the gradient of the sublattice magnetization.

Again we can discuss the possibility of self-trapping of the carrier. At first sight it appears that the coupling is weakened as it depends only on gradients of the magnetization fields. This is true to an extent: the equilibrium conditions on $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ imply

$$\boldsymbol{\mu}_\perp=-\frac{\sqrt{2}t}{8J}i[u^\dagger\boldsymbol{\sigma}(\nabla_n u)-(\nabla_n u^\dagger)\boldsymbol{\sigma}u] , \quad (13a)$$

$$\boldsymbol{\omega}_\perp=-\frac{\sqrt{2}t}{8J}\int\frac{d^2x'}{2\pi}\ln|\mathbf{x}-\mathbf{x}'|\nabla'_n[\hat{\mathbf{z}}\times u^\dagger\boldsymbol{\sigma}u] . \quad (13b)$$

Since the total spin current carried by a stationary particle must be zero, the total induced magnetization given by (13a), i.e., $\int d^2x\,\boldsymbol{\mu}_\perp(\mathbf{x})$, will also be zero for a polaron exactly at the zone boundary: the effect of the particle on the magnetization is in this sense reduced compared with the zone-center case. Nevertheless, when the coupling j exceeds a certain critical value the carrier-spin system is unstable, just as before; but here the mechanism for instability can be *either* the coupling to $\boldsymbol{\mu}$ *or* to $\boldsymbol{\omega}_\perp$. The easier case to understand is the coupling of spin current to magnetization which leads to the local polarization given by (13a). We make the following variational ansatz for the envelope wave function of the carrier:

$$u(r,\theta)=\frac{re^{-r^2/L^2}}{L^2}e^{i\theta}\begin{bmatrix}1\\1\end{bmatrix} , \quad (14)$$

which represents a normalized state with a nonzero density of spin current. It is easy to see that the kinetic energy of the carrier is of order t^2/jL^2, while the magnetization energy is of order $-t^2/JL^2$, so that the total energy becomes negative when j exceeds some value of order J. A similar criterion for instability can be obtained from the relaxation of the sublattice magnetization. Both $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ will contribute to the formation of the spin polaron. This demonstrates that an instability is possible, though we cannot expect to find a quantitative result from such a simple variational function.

Equation (13b) shows incidentally that the carrier may induce a static dipolar twist at large distances in the sublattice magnetization,

$$\boldsymbol{\omega}_\perp\sim\frac{t}{J}\frac{\mathbf{x}\cdot\hat{\mathbf{n}}}{r^2}\langle\hat{\mathbf{z}}\times\boldsymbol{\sigma}\rangle ,$$

where $\langle\boldsymbol{\sigma}\rangle=\int d^2x\,u^\dagger(\mathbf{x})\boldsymbol{\sigma}u(\mathbf{x})$. This is to be contrasted with the zone-center case, where any distortion is dynamically induced (see below). The difference is simply that, at the zone center, the carrier's polarizing effect is similar on the two sublattices and results in a high-order multipolar field from a large spin polaron.[10] At the zone boundary the polarizing effect is staggered with respect to the two sublattices, maximizing the effect on the sublattice magnetization.

V. DYNAMICAL EFFECTS AT THE ZONE CENTER

The continuum Hamiltonian (6) for the coupled carrier-spin system enables us to give a microscopic derivation of the dynamical equations which were derived using general phenomenological arguments in Ref. 10. In particular, we can show how a long-range spin deformation is induced by a moving carrier.

From the results of Appendix B we have the following commutation relations for the continuum variables:

$$[\omega_x(\mathbf{x}),\mu_y(\mathbf{x}')]=[\mu_x(\mathbf{x}),\omega_y(\mathbf{x}')]=i\omega_z(\mathbf{x})\delta^2(\mathbf{x}-\mathbf{x}')/S ,$$

$$[\mu_x(\mathbf{x}),\mu_y(\mathbf{x}')]=[\omega_x(\mathbf{x}),\omega_y(\mathbf{x}')]=i\mu_z(\mathbf{x})\delta^2(\mathbf{x}-\mathbf{x}')/S .$$

In the limit of small deviations away from Néel order, $\mu_z\ll\omega_z\simeq 1$, so that $\boldsymbol{\omega}_\perp$ and $\hat{\mathbf{z}}\times\boldsymbol{\mu}_\perp$ can be regarded as canonically conjugate coordinates and momenta. Hence we can use the Hamiltonian equations of motion

$$S\dot{\omega}_x=\delta H/\delta\mu_y=8J\mu_y+gu^\dagger\sigma_y u ,$$

$$S\dot{\mu}_y=-\delta H/\delta\omega_x=J\nabla^2\omega_x ,$$

in which we have written g for the interaction strength $j\epsilon_0/\sqrt{\epsilon_0^2+j^2}$. After eliminating the magnetization $\boldsymbol{\mu}_\perp$ we find

$$S^2\ddot{\boldsymbol{\omega}}_\perp-8J^2\nabla^2\boldsymbol{\omega}_\perp=gS\frac{\partial}{\partial t}\hat{\mathbf{z}}\times u^\dagger\boldsymbol{\sigma}u . \quad (15)$$

For the carrier wave function, Hamilton's equations lead directly to Schrödinger's equation,

$$i\frac{\partial u}{\partial t}=\frac{\delta H}{\delta u^\dagger}=H''_{-}[\boldsymbol{\mu}_\perp]u , \quad (16)$$

where the effective single-band Hamiltonian operator $H''_{-}[\boldsymbol{\mu}_\perp]$ is the lower 2×2 block of Eq. (5). We can find uniformly translating solutions of the dynamical equations (15) and (16) together by applying the usual formulas of the Galilean transformation. We express the wave function as

$$u(\mathbf{x},t)=u(\mathbf{x}-\mathbf{v}t)\exp i[m_0\mathbf{v}\cdot\mathbf{x}-\tfrac{1}{2}m_0v^2t-Et] ,$$

where m_0 is the unrenormalized mass $2\sqrt{\epsilon_0^2+j^2}/\epsilon_0^2$. Similarly expressing the classical fields $\boldsymbol{\omega}_\perp$ and $\boldsymbol{\mu}_\perp$ in the form $f(\mathbf{x}-\mathbf{v}t)$, we obtain

$$Eu=H''_{-}[\boldsymbol{\mu}_\perp]u ,$$

$$[(S\mathbf{v}\cdot\nabla)^2-8J^2\nabla^2]\boldsymbol{\omega}_\perp=-gS\mathbf{v}\cdot\nabla[\hat{\mathbf{z}}\times u^\dagger\boldsymbol{\sigma}u] , \quad (17)$$

$$8J\boldsymbol{\mu}_\perp+gu^\dagger\boldsymbol{\sigma}_\perp u=-S(\mathbf{v}\cdot\nabla)\hat{\mathbf{z}}\times\boldsymbol{\omega}_\perp .$$

Note that for small v the sublattice magnetization is proportional to v and the change in the wave function u is proportional only to v^2. For any v less than the spin-

wave speed $c=2\sqrt{2}J/S$, (17) implies that $\omega_\perp$ has a (distorted) dipolar from at large distances,

$$\omega_\perp \simeq \frac{gS}{2\pi J^2}\frac{\gamma^3 \mathbf{v}\cdot(\mathbf{x}-\mathbf{v}t)}{[\gamma \mathbf{v}\cdot(\mathbf{x}-\mathbf{v}t)]^2+[\mathbf{v}\times\mathbf{x}]^2}\langle \hat{\mathbf{z}}\times\boldsymbol{\sigma}\rangle ,$$

where γ is the velocity-dependent factor $1/\sqrt{1-v^2/c^2}$.

Finally, the effective mass of the spin polaron can be estimated from the $O(v^2)$ change in the energy of the spin system,

$$\begin{aligned}\tfrac{1}{2}mv^2 &\sim J\int d^2x\ \omega_\perp \nabla^2 \omega_\perp \\ &\sim \frac{gS}{J}\int d^2x\ \omega_\perp\cdot\hat{\mathbf{z}}\times[(\mathbf{v}\cdot\nabla)u^\dagger \sigma u]_x \\ &\sim \frac{g^2S^2}{J^3L^2}v^2\end{aligned}$$

or $m\sim g^2S^2/J^3L^2$.

VI. CONCLUSIONS

We have investigated the dependence on wave vector of the spin distortion around a carrier in a classical two-dimensional antiferromagnet. At the zone center there is a tendency towards ferromagnetic distortion, which is similar to what happens in the extreme quantum limit $S=\frac{1}{2}$. This leads to self-trapping of the carrier if the exchange coupling j is large enough. Motion of the carrier causes a long-range, dipolar distortion of the sublattice magnetization.

At the zone boundary the induced magnetization density is proportional to the spin current due to the carrier. Surprisingly, this does not necessarily conflict with the results for $S=\frac{1}{2}$. The *total* magnetization induced is proportional to the *integrated* spin current of the carrier, and this will vanish for a stationary carrier. There remains the possibility of self-trapping and the formation of a complex spin polaron in which the magnetization and sublattice magnetization are both involved. Neutron-scattering results from the nickelate[12] suggest that there is a magnetic superlattice whose nature changes with the degree of doping. This perhaps corresponds to a spin spiral whose pitch correlates with the concentration of carriers. It remains to be seen if the pitch is related to spin distortion calculated in this paper, evaluated at the "Fermi surface" of a gas of such polarons.

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APPENDIX A: ADIABATIC APPROXIMATION FOR SPINS

We would like to show that the classical limit for spins, $S\to\infty$, leads directly to the adiabatic approximation for the carrier-spin system. For simplicity we consider only the stationary states of our starting Hamiltonian:

$$H=T_{\text{carrier}}+\frac{j}{S}\sum_i \boldsymbol{\sigma}_i\cdot\mathbf{S}_i+\frac{J}{S^2}\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j .$$

We follow the usual derivation of the Born-Oppenheimer approximation for molecules and solids. One significant modification is necessary owing to the noncommutativity of the components of the spin operators, so that we cannot use a representation in which they are diagonal. Instead we shall exploit the smallness of the spin fluctuations about a classical equilibrium configuration to help us define a classical effective potential for the carrier.

We seek a solution of Schrödinger's equation

$$H\Psi=E\Psi$$

in the form

$$\Psi=\sum_m \chi_m\phi_m(\{\hat{\mathbf{n}}_i\}) . \tag{A1}$$

Here the χ_m are multicomponent spinors describing spin configurations close to a classical configuration defined by unit vectors $\hat{\mathbf{n}}_i$. The functions ϕ_m are the orthonormal solutions of

$$\left[T_{\text{carrier}}+j\sum_i \boldsymbol{\sigma}_i\cdot\hat{\mathbf{n}}_i\right]\phi_m=U_m(\{\hat{\mathbf{n}}_i\})\phi_m \tag{A2}$$

and have amplitudes ϕ_{mi} on the lattice sites. Equation (A2) describes the carrier moving in a rigid background of classical spins with directions $\hat{\mathbf{n}}_i$ The wave functions and the eigenvalues U_m depend parametrically on these directions. If we substitute the form (A1) for the wave function into Schrödinger's equation we find

$$\left[\frac{J}{S^2}\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j+U_m(\{\hat{\mathbf{n}}_i\})+\frac{j}{S}\sum_i \phi^\dagger_{mi}\boldsymbol{\sigma}\phi_{mi}\cdot(\mathbf{S}_i-S\hat{\mathbf{n}}_i)-E\right]\chi_m=-\frac{j}{S}\sum_{m'\neq m}\sum_i \phi^\dagger_{mi}\boldsymbol{\sigma}\phi_{m'i}\cdot(\mathbf{S}_i-S\hat{\mathbf{n}}_i)\chi_{m'} . \tag{A3}$$

So far we have made no approximation. Let us write (A3) in the abbreviated form

$$(H_m-E)\chi_m=\sum_{m'\neq m}K_{mm'}\chi_{m'} \tag{A4}$$

and expand the functions χ_m, $m\neq 0$, in terms of the eigenfunctions of the operator H_m,

$$\chi_m=\sum_v c_{mv}\eta_{mv} ,$$

where

$$H_m\eta_{mv}=E_{mv}\eta_{mv} .$$

In the inhomogeneous equation (A4) we suppose that all the χ_m in (A1) are small compared with χ_0 so that we can neglect all but one of the terms on the right-hand side; then

$$\sum_v (E_{mv}-E)c_{mv}\eta_{mv}\simeq K_{m0}\chi_0 . \tag{A5}$$

What is the significance of the functions η_{mv}? If the directions $\hat{\mathbf{n}}_i$ correspond to an equilibrium configuration of the classical spin system in the presence of the carrier, the η_{mv} are the few-magnon states when the carrier is in an excited state of the potential provided by the spins. If the ground state of the carrier is separated from the others by a gap Δ, the difference $(E_{mv}-E)$ in (A5) is approximately constant, only slightly exceeding Δ. Therefore, we can approximate the left-hand side by $\Delta\sum_v c_{mv}\eta_{mv}=\Delta\chi_m$, so that

$$\chi_m \simeq \frac{1}{\Delta}K_{m0}\chi_0 = -\frac{j}{\Delta S}\sum_i \phi^\dagger_{mi}\boldsymbol{\sigma}\phi_{0i}\cdot(\mathbf{S}_i - S\hat{\mathbf{n}}_i)\chi_0 \ .$$

The operator $(\mathbf{S}-S\hat{\mathbf{n}})$ is approximately $\mathbf{S}_\perp$, the spin-deviation operator, and is of order $\sqrt{S}$. It follows that

$$\chi_m \simeq -\frac{j}{\Delta S}\sum_i \phi^\dagger_{mi}\boldsymbol{\sigma}\phi_{0i}\cdot\mathbf{S}_{\perp i}\chi_0 \sim \frac{j}{\Delta\sqrt{S}}\chi_0 \ .$$

This is consistent with our earlier assumption that χ_m was small for $m\neq 0$. The states of the carrier satisfy a Schrödinger equation (A2) which does not involve S, so that Δ is independent of S.

So far we have estimated the matrix elements for transitions between the states of a carrier in a classical spin configuration. At the next order with respect to $1/\sqrt{S}$ we should try to include the effect of the slow spin fluctuations. If S_{xi} and S_{yi} are spin components perpendicular to $\hat{\mathbf{n}}_i$ we can use a representation in which one of these is diagonal; for example, $S_{xi}\simeq\sqrt{S}X_i$ and $S_{yi}\simeq -i\sqrt{S}\,\partial/\partial X_i$. After we have included the terms $j\sigma_{xi}X_i/\sqrt{S}$ in the Schrödinger equation (A2) for the carrier, the wave functions ϕ_m will contain corrections that are functions of the coordinates X_i. The only significant change to the wave equation (A3) for the spins is that the right-hand side will involve only the components S_{yi} of the spins: the argument can be carried through as before to show that the functions χ_m for $m\neq 0$ are of order $1/\sqrt{S}$ compared with χ_0.

To summarize, if the carrier's state is separated from the others by a gap, the ground-state wave function of the carrier-spin system separates as a product of spin and carrier parts:

$$\Psi=\chi_0\phi_0+O(1/\sqrt{S}) \ .$$

Note that this result for the wave function is different from the more usual one for molecules in that it fails at first order in the adiabaticity parameter $1/\sqrt{S}$, compared with failure of the Born-Oppenheimer approximation at third order in the adiabaticity parameter $(m/M)^{1/4}$.

APPENDIX B: CONTINUATION OF FUNCTIONS AND OPERATORS

When can dynamical variables f_n, defined at the points n of a lattice, be replaced by field variables defined throughout space? To simplify matters we first suppose that the f_n can be obtained by sampling a smooth, slowly varying function, so that $f_n=f(n)$, where $f(x)$ varies smoothly over many lattice spacings. The problem is then to find equations of motion for the continuum variable, given the equations for the discrete variables. In fact, if the analytical expression representing the rate of change of a lattice variable can be derived by sampling some expression involving continuum variables, then we can be sure that this variable will remain smooth under the dynamics of the system, and we will also have a representation of the dynamics of the corresponding continuum variable.

We must at the very least show that *some* smooth, slowly varying function $\tilde{f}(x)$ can be obtained directly from the lattice quantities $f(n)$. (There is, of course, no reason to expect this representation to be unique.) This is easy for functions containing only spatial frequencies less than π: the well-known formula

$$f(x)=\sum_n w(x-n)f(n)=\sum_n \frac{\sin\pi(x-n)}{\pi(x-n)}f(n) \qquad \text{(B1)}$$

exactly reproduces $f(x)$ from the discrete set of values $f(n)$. This is a little too restrictive, in practice, so we consider instead a class of smooth, slowly varying functions $f(x)=h(t/L)$, where h is infinitely differentiable and L is a lengthscale, $L\gg 1$. We then define an *approximate* interpolation using the same weights as in (B1),

$$\tilde{f}(x)=\sum_n w(x-n)f(n) \ .$$

How far does $\tilde{f}(x)$ deviate from $f(x)$? We have, using Poisson's summation formula,

$$\begin{aligned}\tilde{f}(x)&=\sum_n w(x-n)h(n/L)\\ &=\sum_k \int dp\, e^{2\pi i k p}h(p/L)w(x-p)\\ &=\sum_k \int_{-\pi}^{\pi}\frac{d\omega}{2\pi}e^{i\omega x}Lh_{L(\omega-2\pi k)} \ ,\end{aligned}$$

where the subscript on h denotes the Fourier component. In this way we find

$$\begin{aligned}\tilde{f}(x)=f(x)&-\int_{|\omega|>\pi L}\frac{d\omega}{2\pi}e^{i\omega x/L}h_\omega\\ &+\sum_{k\neq 0}\int_{-\pi L}^{\pi L}\frac{d\omega}{2\pi}e^{i\omega x/L}h_{\omega-2\pi kL} \ .\end{aligned} \qquad \text{(B2)}$$

The correction terms to $f(x)$ depend on the nature of the function $h(x)$. For infinitely differentiable $h(x)$, h_ω vanishes for large $|\omega|$ faster than any negative power of ω; it follows that the corrections in (B2), which involve h_ω for $|\omega|>\pi L$, vanish faster than any negative power of L. We shall denote equality to within such rapidly vanishing terms by

$$\tilde{f}(x)\approx f(x), \quad L\to\infty \ .$$

We can extend the method explained here to any two- or three-dimensional crystal lattice. The weights used in (B1) have a natural generalization

$$w(\mathbf{x}-\mathbf{R})=\int_{\mathrm{BZ}}\frac{d^2k}{(2\pi)^2}e^{i\mathbf{k}\cdot\mathbf{x}}$$

in which the $\mathbf{k}$ integral is taken over the first Brillouin

zone. The continuation

$$\tilde{f}(\mathbf{x})=\sum_{\mathbf{R}} w(\mathbf{x}-R)f(\mathbf{R})\approx f(\mathbf{x}), \quad L\to\infty$$

is exact if $f(\mathbf{x})$ has Fourier components only within the first Brillouin zone of $\mathbf{k}$ space, but otherwise provides an interpolation formula for smooth, slow functions of lengthscale L. The weights used here for illustration are particularly simple but there is considerable freedom that can be exercised in their choice. For example, the long-distance behavior $w(\mathbf{x})\sim|\mathbf{x}|^{-d}$, can be modified by replacing $w(\mathbf{x})$ (in 1D) by

$$w(x)=\int_{-\infty}^{\infty}\frac{dq}{2\pi}e^{iqx}w_q \ ,$$

where w_q is an infinitely differentiable function of q which is constant for $-Q<q<Q$. Such a weight function $w(x)$ decreases at large distances faster than any negative power of $|x|$.

The Schrödinger equation (A2) for the carrier wave function in a classical spin configuration involves the product of the wave function with $\mathbf{S}_n=\boldsymbol{\mu}_n\pm\boldsymbol{\omega}_n$, where we assume that $\boldsymbol{\mu}$ and $\boldsymbol{\omega}$ are smooth and vary slowly in space. It is not difficult to show that the continuum approximation to products such as $\boldsymbol{\mu}_n f_n$, where f is also smooth and slow, is given—again to better than power law accuracy—by the product $\boldsymbol{\mu}(x)f(x)$. In other words, the equations of motion for smooth, slow quantities are given directly by the lattice equations expressed in terms of smooth, slow quantities.

Finally we show that a formula similar to (B1) can be used to make a continuation of the spin operators in an antiferromagnet; and that this continuation preserves the matrix elements of spin operators and matrix elements of their commutation relations taken between smoothly varying antiferromagnetic spin states.

First we assume that the matrix elements of A- and B-site spins are smooth, slow functions so that we can interpolate them by

$$\mathbf{S}^A(x)=\sum_m w[\tfrac{1}{2}(x-2m)]\mathbf{S}_{2m} \ ,$$

$$\mathbf{S}^B(x)=\sum_m w[\tfrac{1}{2}(x-2m-1)]\mathbf{S}_{2m+1} \ .$$

Then the operators $\mathbf{S}^A$ and $\mathbf{S}^B$ commute, as they are constructed from variables from different sublattices, while

$$\int dy\, f(y)[S_a^A(x),S_b^A(y)]$$
$$=ie_{abc}\sum_m\left[\int dy\, f(y)w(\tfrac{1}{2}y-m)\right]w(\tfrac{1}{2}x-m)S_{c,2m} \ .$$

If the test function $f(y)$ is smooth and slow we have

$$\int dy\, f(y)w(\tfrac{1}{2}y-m)\approx 2f(2m), \quad L\to\infty \ ,$$

so that

$$\int dy\, f(y)[S_a^A(x),S_b^A(y)]\approx ie_{abc}\sum_m 2f(2m)\times w(\tfrac{1}{2}x-m)S_{c,2m}$$
$$\approx 2ie_{abc}f(x)S_c^A(x), \quad L\to\infty \tag{B3}$$

for the spin states of interest, or

$$[S_a^A(x),S_b^A(y)]\approx 2ie_{abc}S_c^A(x)\delta(x-y) \ . \tag{B4}$$

There is a corresponding commutation relation for the operators $\mathbf{S}^B$.

We are now in a position to define the operators $\boldsymbol{\mu}(x)$ and $\boldsymbol{\omega}(x)$ by

$$\mathbf{S}^A(x)=S[\boldsymbol{\mu}(x)+\boldsymbol{\omega}(x)] \ ,$$

$$\mathbf{S}^B(x)=S[\boldsymbol{\mu}(x)-\boldsymbol{\omega}(x)] \ .$$

Using the commutation relations for $\mathbf{S}^A$ and $\mathbf{S}^B$ we find

$$[\mu_a(x),\mu_b(y)]\approx[\omega_a(x),\omega_b(y)]\approx ie_{abc}\mu_c(x)\delta(x-y)/S \tag{B5a}$$

and

$$[\mu_a(x),\omega_b(y)]\approx ie_{abc}\omega_c(x)\delta(x-y)/S \ . \tag{B5b}$$

The commutation relation for $\boldsymbol{\mu}(x)$ shows that it can be interpreted as the density of spin or magnetization. The relations (B5) should be interpreted in the same sense as (B4): when multiplied by a smooth, slowly varying test function, the matrix elements taken between smooth, slowly varying antiferromagnetic states will be given by (B3) to within quantities that vanish faster than any inverse power of the lengthscale L.

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