Stability of ferrons in antiferromagnets: The role of zero-point fluctuations

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A free carrier of spin $\frac{1}{2}$, placed in a Heisenberg antiferromagnet, may form a ferron, which is a quasiparticle in which the free carrier is surrounded by a localized region with a net magnetic moment. Type-I ferrons (core not fully saturated) are unstable in lattices with dimensionality $D \geq 2$, although they are stable for $D < 2$, in mean-field theory. With $D = 2$ in mind, we examine the influence of zero-point spin fluctuations on the stability of ferrons, to find they oppose the formation of type-I ferrons, although scaling relations for various contributions to the binding energy are unaffected. We comment on the possible relevance of these results to the high-T_c superconductors; the ground state for a single hole may be a type-II ferron (saturated core), if this picture is applied to these materials.

I. INTRODUCTION

A free carrier (electron or hole) injected into a localized spin magnet will couple to the local moments by means of an exchange interaction. We then have a quasiparticle referred to as a magnetic polaron.

Of particular interest is the case where the host is an antiferromagnet, supposed for the moment to be at the temperature $T = 0$ and described by the Néel ground state. The following mechanism can lead to formation of a self-trapped magnetic polaron. Let the free carrier be localized spatially, and orient its spin to be perpendicular to the two antiparallel sublattices of the host. The free-carrier–local-moment exchange will lead to a canting of the two sublattices in the host, within the wave packet, so one has a local distortion of the antiferromagnet ground state of spin-flop character. This produces a potential well that may trap the free carrier; the resulting entity can also have a substantial magnetic moment. These self-trapped magnetic polarons are referred to as ferrons.

In earlier work,[1,2] we have explored the stability and properties of such ferrons in the perfect crystal, and when the entity is trapped by a donor in an n-type antiferromagnetic semiconductor such as EuTe. It is then referred to as a bound magnetic polaron. We used an adiabatic approximation to describe the wave function of the free carrier in the sea of local moments, whose ground state was taken to be a Néel state distorted by the localized free carrier.

Two types of ferron emerge from the analysis. In the type-II ferron, the free-carrier–local-moment exchange is so strong that the object has a fully saturated ferromagnetic core. The core is unsaturated in the type-I case.

The stability of the type-I ferron realized for modest values of the local-moment–free-carrier exchange depends strongly on the dimensionality of the system. For $D = 1$, the ground state is the self-trapped ferron. For $D = 3$, there is no such self-trapped object, and the free-carrier wave function is always spatially extended. Two dimensions emerge as a marginal dimensionality.

The case of $D = 2$ is of current interest, since one picture of the holes crucial to superconductivity in the high-T_c oxides is extra carriers confined to oxygen sites, which interact with an antiferromagnetically coupled array of local moments localized on the Cu sites. An important question is whether the basic quasiparticle in such a system is a self-trapped magnetic polaron, or spatially delocalized quasiparticle dressed weakly by virtue of the exchange coupling to the local moments.

In the two-dimensional (2D) antiferromagnet, zero-point fluctuations in the spin system contribute importantly to the ground-state energy. These will be influenced locally when one attempts to localize a free carrier added to the system, and thus affect the binding energy of the ferron. The influence of the zero-point fluctuations on the ferron binding energy was not explored in the earlier work cited above. The purpose of this paper is to explore this issue, with particular attention to the case $D = 2$.

Our procedure is to consider a carrier added to an antiferromagnetically coupled lattice of spins S, and evaluate the correction to the ground-state energy the order of $1/S$ in its presence. We can then examine the effect of the ferron on the zero-point fluctuations in its near vicinity, and the influence of this modification on the ground-state energy. We find, of course, only the first term in the expansion of the ground-state energy in inverse powers of S, so its extrapolation to the case $S = \frac{1}{2}$ of interest in the context of high-T_c superconductivity is of questionable virtue, but it does provide us with an indication of the role of zero-point fluctuations. Our conclusion is that it decreases the tendency of the ferron to bind, but in the presence of the zero-point fluctuations, $D = 2$ remains marginal.

The picture which emerges from this work is the following, for $D = 2$. For small values of the free-carrier–local-moment exchange, the quasiparticle wave function is delocalized. As the strength of the exchange is increased, there is a collapse to a highly localized ferron of type-II character. The strength of the exchange

must be the order of the free-carrier bandwidth to initiate the collapse. As the exchange constant increases still further, the type-II ferron evolves continuously into a spatially localized singlet state (when $S=\frac{1}{2}$) physically equivalent to that considered by Zhang and Rice.[3]

II. THE FERRON STATE

We start with the basic Hamiltonian employed in our earlier work,[1,2]

$$H=-\frac{\hbar^2}{2m}\nabla^2+\tfrac{1}{2}\sum_{ij}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j-AV_c\sum_i\mathbf{S}_i\cdot\mathbf{s}\delta(\mathbf{r}-\mathbf{R}_i)$$
$$-\gamma_s H_0 s_z-\gamma_S H_0 S_i^z\ . \tag{2.1}$$

We use an effective-mass approximation for the free carrier, A is the exchange-coupling constant, V_c the volume of the unit cell, and $\mathbf{s}$ the spin of the added carrier. We have an external magnetic field applied perpendicular to the staggered magnetization of the localized spins. The nearest-neighbor exchange constant J_{ij} is positive, so in the ground state we have antiferromagnetic order. As earlier, we assume for the moment that the energy associated with the exchange field $H_E=zJS$ exerted on a given spin by its z neighbors, the free-carrier bandwidth W, and the exchange energy $H_x=AS/2$ are ordered as follows: $H_E\ll H_x\ll W$. Then, as argued earlier, the wave function of the system is well approximated by

$$\Psi=\psi_e(\mathbf{r},\{\mathbf{S}_i\})\Phi(\{\mathbf{S}_i\})\ , \tag{2.2}$$

where $\mathbf{r}$ is the coordinate of the free carrier, and $\{\mathbf{S}_i\}$ denotes the set of quantum numbers required to specify the configurations of the local moments. We have argued earlier that in the parameter regime just outlined, the terms in the free-carrier–local-moment interaction involving $S_i^+s^-$ and $S_i^-s^+$ can be ignored. Consequently, the spin of the free carrier is aligned parallel to the z axis.

In the limit S is large, the array of local moments may be described classically, as assumed in our earlier work.[1,2] For EuTe, the material of primary interest there, $S=\frac{7}{2}$ and this approximation is quite valid. As remarked earlier, we begin with this limit, and examine the quantum corrections to the ferron binding energy of order S^{-1}.

The localized free carrier induces a spatially dependent canting of the local-moment array. It is useful to introduce a coordinate system with axes labeled by (ϵ,ξ,η) at each lattice site. The x axis of the master coordinate system is parallel to the staggered magnetized of the ground state of the antiferromagnet unperturbed by the ferron, the ξ axis of the (ϵ,ξ,η) system at site i is aligned along the direction of the local moment there (with ferron present), and the ϵ,ξ axes lie in the xz plane of the master system. Then we relate the (x,y,z) to the (ϵ,ξ,η) components of $\mathbf{S}_i$ by the relations

$$S_i^x=S_i^\epsilon\cos(\mathbf{Q}\cdot\mathbf{R}_i)\cos(\theta_i)-S_i^\xi\sin(\theta_i)\ , \tag{2.3a}$$

$$S_i^z=S_i^\epsilon\sin\theta_i+S_i^\xi\cos(\mathbf{Q}\cdot\mathbf{R}_i)\cos(\theta_i)\ , \tag{2.3b}$$

$$S_i^y=-S_i^\eta\ , \tag{2.3c}$$

where $\mathbf{Q}$ is the wave vector of the antiferromagnetic structure, i.e., $\mathbf{Q}=(\pi/a_0)(1,1)$ in the case of the 2D square lattice with lattice parameter a_0. The factor $\cos(\mathbf{Q}\cdot\mathbf{R}_i)$ assumes the value ±1 at each site. The angle θ_i describes the orientation of the local moment at site i with respect to the master coordinate system. This is a variational parameter, to be determined below.

For a given choice of ψ_e in Eq. (2.2), one may derive an effective spin Hamiltonian by taking a partial expectation value by integrating out the free carrier coordinate $\mathbf{r}$. One finds

$$\langle H\rangle=\langle T\rangle+\tfrac{1}{2}\sum_{ij}J_{ij}\{(S_i^\epsilon S_j^\epsilon+S_i^\xi S_j^\xi)[\cos(\mathbf{Q}\cdot\mathbf{R}_i)\cos(\mathbf{Q}\cdot\mathbf{R}_j)\cos\theta_i\cos\theta_j+\sin\theta_i\sin\theta_j]$$
$$+2S_i^\epsilon S_j^\xi[\cos(\mathbf{Q}\cdot\mathbf{R}_j)\cos\theta_j\sin\theta_i-\cos(\mathbf{Q}\cdot\mathbf{R}_i)\cos\theta_i\sin\theta_j]+S_i^\eta S_j^\eta\}$$
$$-\sum_i[\tfrac{1}{2}AV_c|\psi(\mathbf{R}_i)|^2+\gamma_S H_0][S_i^\xi\cos(\mathbf{Q}\cdot\mathbf{R}_i)\cos\theta_i+S_i^\epsilon\sin\theta_i]\ . \tag{2.4}$$

The Zeeman term $\gamma_s H_0 s^z$ has been omitted, since it adds only an overall constant to the energy.

One problem is to find the ground-state energy of the above spin system, perturbed by the spatially nonuniform effective field produced by $|\psi(\mathbf{R}_i)|^2$. As we proceed, we shall assume the ferron has a spatial extent sufficiently large the θ_i varies slowly on the scale of a lattice constant. Thus, when site i and j are nearest neighbors, $\cos(\theta_i)\cos(\theta_j)$ may be replaced by $\cos^2(\theta_i)$.

At $T=0$, the ground-state energy of the system including the influence of zero-point fluctuations may be described by the Holstein-Primakoff transformation. We divide the lattice into the two sublattices A and B. For the A spins, $\cos(\mathbf{Q}\cdot\mathbf{R}_i)=+1$ and for the B spins, $\cos(\mathbf{Q}\cdot\mathbf{R}_i)=-1$. For the A spins,

$$S_i^\epsilon=S-a_i^+a_i\ ,$$
$$S_i^+=(2S)^{1/2}a_i \tag{2.5}$$

and

$$S_i^-=(2S)^{1/2}a_i^+\ ,$$

and a transformation of the same form applies to the B spins, with a_i,a_i^+ replaced by b_i,b_i^+. [The factors of

$\cos(\mathbf{Q}\cdot\mathbf{R}_i)$ incorporated in Eqs. (2.3) mean we write $S_i^{\epsilon}=S-b_i^{+}b_i$ for B spins, rather than $-S+b_i^{+}b_i$.]

With this transformation introduced, the spin Hamiltonian becomes

$$\langle H\rangle=\sum_{m=0}^{4}H_m\ , \tag{2.6}$$

where H_m contains products of m boson operators. For our purposes, we retain only those terms with $m\leq 2$, whose form is

$$H_0=-\frac{zJS^2}{2}\sum_{l_A}\cos(2\theta_{l_A})-S\sum_{l_A}h_{l_A}\sin(\theta_{l_A})$$
$$-\frac{zJS^2}{2}\sum_{l_B}\cos(\theta_{l_B})-S\sum_{l_B}h_{l_B}\sin(\theta_{l_B})\ , \tag{2.7a}$$

$$H_1=\frac{S}{2\sqrt{2}}\sum_{l_A}(zJS\sin2\theta_{l_A}-h_{l_A}\cos\theta_{l_A})(a_{l_A}+a_{l_A}^{+})$$
$$-\frac{S}{2\sqrt{2}}\sum_{l_B}(zJ\sin2\theta_{l_B}-h_{l_B}\cos\theta_{l_B})(a_{l_B}+a_{l_B}^{+})\ , \tag{2.7b}$$

and

$$H_2=\sum_{l_A}(zJS\cos2\theta_{l_A}+h_{l_A}\sin\theta_{l_A})a_{l_A}^{+}a_{l_A}+\sum_{l_B}(zJS\cos2\theta_{l_B}+h_{l_B}\sin\theta_{l_B})b_{l_B}^{+}b_{l_B}$$
$$+\tfrac{1}{2}JS\sum_{l_A}\sum_{\delta}(1+\cos2\theta_{l_A})(a_{l_A}^{+}b_{l_A+\delta}^{+}+a_{l_A}b_{l_A+\delta})+\tfrac{1}{2}JA\sum_{l_A}\sum_{\delta}(\cos2\theta_{l_A}-1)(a_{l_A}b_{l_A+\delta}^{+}a_{l_A}^{+}b_{l_A+\delta})\ . \tag{2.7c}$$

In these expressions,

$$h_l=\gamma_S H_0+\tfrac{1}{2}AV_c|\psi(\mathbf{R}_l)|^2\ .$$

The summations of δ range over the B sites nearest neighbor to l_A.

The ground-state spin configuration is found by requiring that the terms linear in the spin deviation operators vanish [Eq. (2.76)]. These lead to the condition

$$\sin\theta_l=\frac{h_l}{2zJS}\ . \tag{2.8}$$

If we ignore the presence of H_2 and feed this angle back into Eq. (2.7a), we then generate an expression for the energy of the spin system from which the binding energy of the ferron may be extracted, when the presence of $\langle T\rangle$ in Eq. (2.4) is recognized. At this point, we recover a description of the ferron at the temperature $T=0$ identical to that contained in our earlier analyses.

The effect of zero-point fluctuations in the spin system is contained in H_2. These give a contribution to the energy of the spin system smaller than those considered so far by a factor of $1/S$. Upon using the explicit expression for the canting angle given in Eq. (2.8), we split H_2 into two parts,

$$H_2=H_2^{(0)}+H_2^{(p)}\ , \tag{2.9}$$

where

$$H_2^{(0)}=zJS\left[\sum_{l_A}a_{l_A}^{+}a_{l_A}+\sum_{l_B}b_{l_B}^{+}b_{l_B}\right]$$
$$+JS\sum_{l_A,\delta}(a_{l_A}b_{l_A+\delta}+a_{l_A}^{+}b_{l_A+\delta}^{+})$$
$$-JS\sum_{l_A}\sum_{\delta}\sin^2(\theta_\infty)(a_{l_A}^{+}b_{l_A+\delta}^{+}+a_{l_A+\delta}^{+}+\text{H.c.})\ , \tag{2.10a}$$

and

$$H_2^{(p)}=-\frac{AV_c}{8NzJS}\sum_{l_A}\sum_{\delta}|\psi(R_{l_A})|^2[(\gamma_S H_0+\tfrac{1}{2}AV_c|\psi(R_{l_A})|^2]$$
$$\times(a_{l_A}^{+}b_{l_A+\delta}^{+}+a_{l_A}b_{l_A+\delta}^{+}+\text{H.c.})\ . \tag{2.10b}$$

Here θ_∞ is the canting angle in the antiferromagnet far from the ferron, where $|\psi|^2=0$. We have $\sin(\theta_\infty)=\gamma_S H_0/2zJS$.

The terms in Eq. (2.10a) describe the spin excitations in the infinite antiferromagnet, in the absence of the ferron. When this form is diagonalized and its expectation value is taken at $T=0$, we have a description of the zero-point fluctuation contribution to the ground-state energy of the antiferromagnet, which here is a spin-flop state. One proceeds by first transforming to a plane-wave representation,

$$a_{l_A}^{\pm}=\frac{1}{\sqrt{N}}\sum_{\mathbf{k}}e^{\pm i\mathbf{k}\cdot l_A}a_{\mathbf{k}}^{\pm}\ , \tag{2.11}$$

then introducing new boson operators

$$A_{\mathbf{k}}=\frac{1}{\sqrt{q}}(a_{\mathbf{k}}+b_{\mathbf{k}})\ , \tag{2.12a}$$

$$B_{\mathbf{k}}=\frac{1}{\sqrt{2}}(a_{\mathbf{k}}-b_{\mathbf{k}})\ , \tag{2.12b}$$

and their Hermitean adjoints. After these are introduced, a standard Bogolinbov transformation diagonalizes $H_2^{(0)}$:

$$\alpha_{\mathbf{k}}=U_{\mathbf{k}}^{(A)}A_{\mathbf{k}}-V_{\mathbf{k}}^{(A)}B_{\mathbf{k}}\ , \tag{2.13a}$$

$$\beta_{\mathbf{k}}=U_{\mathbf{k}}^{(B)}A_{\mathbf{k}}-V_{\mathbf{k}}^{(B)}B_{\mathbf{k}}\ . \tag{2.13b}$$

One finds

$$H_2^{(0)}=-zNJS+\tfrac{1}{2}\sum_{\mathbf{k}}[\epsilon_1(\mathbf{k})+\epsilon_2(\mathbf{k})]$$
$$+\sum_{\mathbf{k}}[\epsilon_1(\mathbf{k})\alpha_{\mathbf{k}}^{+}\alpha_{\mathbf{k}}+\epsilon_2(\mathbf{k})\beta_{\mathbf{k}}^{+}\beta_{\mathbf{k}}]\ . \tag{2.14}$$

Here

$$\epsilon_1(\mathbf{k})=zJS[(1+\gamma_{\mathbf{k}})(1-\gamma_{\mathbf{k}}\cos 2\theta_\infty)]^{1/2}\ , \tag{2.15a}$$

and

$$\epsilon_2(\mathbf{k})=zJS[(1-\gamma_{\mathbf{k}})(1+\gamma_{\mathbf{k}}\cos 2\theta_\infty)]^{1/2}\ , \tag{2.15b}$$

with $\gamma_{\mathbf{k}}=z^{-1}\sum_{\mathbf{k}}\exp(i\mathbf{k}\cdot\boldsymbol{\delta})$.

In zero external field, the term $-zJNS$ contributed by $H_2^{(0)}$ combines with the term $-zNJS^2$ to give the energy $-zNJS(S+1)$ of N singlet pairs, while the second term in $H_2^{(0)}$ is the zero-point energy of the spin waves. The net effect of $H_2^{(0)}$ is to lower the energy of the spin system below that of the Néel state by quantum effects the order of S^{-1}. In zero external magnetic field, the spin-wave dispersion relations in Eqs. (2.15) reproduce those found for the Heisenberg antiferromagnet.[4,5] Since we have no anisotropy field, an arbitrarily small external field generates the spin-flop configuration in the system.

We can express $H_2^{(p)}$ in terms of the annihilation and creation operators, then take its expectation value at $T=0$ to generate an expression for the change in ground-state energy of the system produced by the ferron. The result of this calculation, which is straightforward but tedious, is the following:

$$\langle H_2^p\rangle_{T=0}=\frac{1}{8zJ}F_0\xi\ , \tag{2.16}$$

where

$$\xi=\frac{zJS}{2NS}\sum_{\mathbf{k}}\left[\gamma_k^2\left[\frac{1}{\epsilon_1(k)}+\frac{1}{\epsilon_2(k)}\right]\cos^2(\theta_\infty)\right.$$
$$+\gamma_{\mathbf{k}}\left[\frac{1+\gamma_k\sin^2(\theta_\infty)}{\epsilon_1(k)}\right.$$
$$\left.\left.-\frac{1-\gamma_k\sin^2\theta_\infty)}{\epsilon_2(k)}\right]\right]\ , \tag{2.17a}$$

and

$$F_0=\sum_l AV_c|\psi(\mathbf{R}_l)|^2[2\gamma_S H_0+\tfrac{1}{2}AV_c|\psi(\mathbf{R}_l)|^2]\ . \tag{2.17b}$$

The present treatment then provides the following expression for the total energy of the system:

$$E_T=\langle T\rangle+H_0+H_2^0+\langle H_2^p\rangle_{T=0}\ , \tag{2.18}$$

where, upon using the relation $\sin(\theta_\infty)=\gamma_S H_0/2zJS$, we find

$$H_0=-\frac{1}{43J}\sum_l(h_l)^2\ . \tag{2.19}$$

When the energy of the infinitely extended lattice is subtracted from that within which the ferron resides, one finds the change in energy of the system upon adding the free carrier is

$$\Delta E_I=\langle T\rangle-\frac{1}{43J}\sum_l[(h_l)^2-(\gamma_S H_0)^2]+\langle H_2^p\rangle_{T=0}\ , \tag{2.20}$$

where the first two terms are those which emerge from our earlier treatment, and the final term is the first quantum correction. If the various terms are gathered together, and we note that the free-carrier wave function is normalized so that

$$V_c\sum_l|\psi(\mathbf{R}_l)|^2=1\ , \tag{2.21}$$

we find

$$\Delta E_I=\langle T\rangle-\frac{AH_0}{4zJ}(1-\xi)-\frac{A^2(1-\xi)V_c}{16zJ}\int d^Dx|\psi_e|^4\ . \tag{2.22}$$

Sums over lattice sites have been converted to an integration, and D is the dimensionality of the lattice.

When ξ is set to zero, this expression reduces to our previous result. The only effect of the zero-point fluctuations is to renormalize the various coefficients in Eq. (2.22) (one has $\xi<1$). For the case where the added particle is in a delocalized state (ψ_e is a plane wave), the last term vanishes, and the second term represents the shift in the band edge upon adding the quasiparticle. This shift is thus renormalized by the factor $(1-\xi)$.

Our previous analysis of the question of whether a localized ferron exists was based on applying the scaling arguments of Emin and Holstein[6] to the energy functional of Eq. (2.22). Indeed, a functional quite equivalent to this, with different physical origin, was explored in their paper. Clearly, inclusion of the influence of zero-point fluctuations on the binding of the ferron does not change the structure of the functional, to first order in $1/S$. It then remains the case that ferrons exist in $D=1$, no binding occurs in $D=3$, and $D=2$ is marginal, so long as we consider a type-I ferron for which the angle θ_l, which emerges from Eq. (2.8), is smaller than $\pi/2$ everywhere. (If, for some sites l near the center of the ferron, $h_l>2zJS$, the angle θ_l saturates at $\pi/2$. This is the type-II ferron, with ferromagnetic core.)

The physical picture of the ferron in two dimensions is then identical to that put forward in our earlier work. In $D=2$, there is no bound state when A is less than a critical value A_c. Here the free carrier is in a plane-wave state, dressed by coupling to the spins. For $A>A_c$, there is a collapse to a "small ferron," a self-trapped free carrier in a state with spatial extent the order of a lattice constant. This is a type-II ferron. Since $\xi>0$, zero-point fluctuations lower the binding energy of this object, and raise A_c by the amount $(1-\xi)^{-1/2}$.

We may estimate A_c through use of a variational wave function in two dimensions of the form

$$\psi_e(p)=\frac{\beta}{(2\pi)^{1/2}}\exp(-\tfrac{1}{2}\beta\rho)\ . \tag{2.23}$$

A short calculation gives the result

$$A_c = \left[\frac{8\pi z J \hbar^2}{m a_0^2 (1-\xi)} \right]^{1/2} , \tag{2.24}$$

where a_0 is the lattice constant. If W is the free-carrier bandwidth ($W \cong \hbar/2ma_0^2$), then we see that

$$A_c = 4\pi^{1/2} (WzJ)^{1/2} .$$

The critical value of A is thus quite substantial.

We conclude with remarks on the possible implications of the results above for the high-T_c superconducting materials.

III. RELEVANCE FOR HIGH-T_c SUPERCONDUCTORS

It is widely believed that the high-T_c superconductivity in the copper oxides arises from holes in the CuO_2 layers.[7] In the $La_{2-x}Sr_xCuO_{4-y}$ family of compounds, for example, electron transport is dominated by holes[8] which predominantly occupy p orbitals on O sites,[9] and interact with the array of spins on the Cu sites.[8] Moreover, in the limit of strong Coulomb repulsion, the Hubbard model can be mapped on to the Heisenberg antiferromagnet.[10] The 2D Heisenberg antiferromagnet thus can be used to describe the Cu spins, if they are indeed localized.

The nature of the ground state of the 2D Heisenberg ferromagnet for spin $S = \frac{1}{2}$ is still under discussion.[11,12] For the 1D case, the exact solution is available, and the ground state does not have long-range order.[13] For $D = 2$ and larger spin ($S \geq \frac{3}{2}$), rigorous calculations show that long-range order exists in the ground state,[14] a result compatible with the spin-wave analysis that is the basis of the present work. We also find that in one dimension, the zero-point fluctuations destroy long-range order, because $\epsilon_{1,2}(k) \sim k$ as $k \to 0$. Our calculation is thus compatible with the results obtained more rigorously, though the extrapolation down to $S = \frac{1}{2}$ must be treated with caution. The problem of whether or not long-range order is present for $D = 2$ and $S = \frac{1}{2}$ remains controversial.[15] However, while stoichiometric La_2CuO_4 may be an example of a quantum spin liquid,[16,17] nearly stoichiometric $La_{2-x}CuO_{4-y}$ is antiferromagnetic[18] and becomes superconducting on doping with Sr or Ba.[19]

In such high-T_c superconductors, J estimated from the Néel temperature $T_N \cong 220$ K, is $J \cong 0.025$ eV, while W may be expected to be in the electron volt range. Hence, Eq. (2.24) yields $A_c \sim W$ in numerical magnitude, which is in the range envisioned in earlier work.[20] Thus, if this estimate is correct, the assumption $H_x \ll W$ necessary for the validity of the adiabatic approximation breaks down. Such large values of A mean the $s^- S^+$ terms neglected above enter the analysis importantly. A more appropriate trial wave function for this case has been derived recently by Loh *et al.*[21] Their wave function produces a larger bindings energy for the ferron in the regime $A \sim W$ than does ours; our analysis may then over estimate the value of A_c. It is then quite possible that type-II ferrons are stable in the high-T_c materials, while in conventional antiferromagnetic semiconductors, the values of A realized fall well below those required for the type-II ferron to exist.[2]

Finally, we would like to comment on recent very interesting results obtained by Loh and co-workers[21] in a model that may be viewed as mimicking one-dimensional CuO chains. At least in regard to the description of ferrons, such models are not relevant to the high-T_c materials, because of the very substantial difference in the stability criteria for ferron formation in one and two dimensions. However, the one-dimensional case is interesting in its own right, particularly since the authors of Ref. 21 put forward exact results for rings of six atoms. It is of interest to compare these results with those produced by our picture. This comparison leads to a physical interpretation of a key result which emerges from the numerical work reported by Loh *et al.*[21]

Since we have a one-dimensional problem, the ground state of a single hole in the one-dimensional antiferromagnetic chain is a ferron. For small values of A, we have a type-I ferron, and as A increases, this state evolves into one of type-II character is a continuous manner. In Ref. 7, two holes are placed on the ring, which means we have a large hole concentration, $c_h \sim \frac{1}{3}$. The ferrons thus interact strongly in this circumstance. The nature of this interaction can be appreciated from the schematic drawing in Fig. 1, which shows two ferrons in an antiferromagnetic chain. If the edges of the two ferrons touch or overlap, clearly antiparallel alignment of the hole spins is favored; there is an attractive interaction at large distance, for singlet hole pairs. However, if two localized holes are placed very close together in a single state, the spins in the host are frustrated. This suggests the ferron-ferron interaction should become repulsive at short distances, in the singlet state. We shall see this conclusion is consistent with the results of Ref. 21. (Of course, to model a real material, one would need to take explicit account of Coulomb interactions in this limit.)

We assume the presence of repulsion at short distances. Then as the hole (and thus the ferron) concentration is increased, there must be a first-order "insulator-metal" Mott transition, at the hole concentration $c_h \sim r_F/a_0$, with r_F the linear size of the isolated ferron. In conventional magnetic insulators, such insulator-metal transitions are realized experimentally in a given material (i.e., one has W, J, and A fixed) by changing the carrier concentration c_h.[22,23] The calculations presented by Loh *et al.*,[21] carried out at fixed hole concentration instead with model parameters varied, produce a first-order

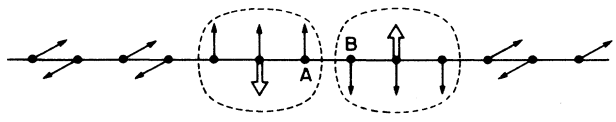

FIG. 1. A schematic illustration of two type-II ferrons on the one-dimensional antiferromagnetic chain. The double arrow refers to the spin polarization of the localized hole, while the single arrows describe the orientations of the spins in the host matrix. If A and B are neighboring spins, the exchange energy JS is gained if the hole spins are antiparallel. But if the ferrons merge with hole spins antiparallel, the core spins are frustrated, leading to a repulsive interaction at short range.

phase transition whose physical character is not discussed in detail in their paper. We argue they realize the insulator-metal transition just described. Indeed, if we use the parameters where the first-order phase transition occurs in the calculations presented in Ref. 21, the Mott criterion cited above places the critical hole concentration near $c_h \sim \frac{1}{3}$.[24]

As a function of the coupling strength A between the hole and the localized spins, our picture is the following. The insulator-metal transition occurs at $A = A^*$. For $A < A^*$, the ferron size r_F exceeds the separation between the holes, the cores thus overlap strongly, and frustration inhibits ferron-ferron binding. We thus realize a metallic state, of course, with each hole a quasiparticle dressed by coupling to the local moments. For $A > A^*$, the ferrons are "small," and the attractive couplings illustrated schematically in Fig. 1 lead to spin singlet ferron pairs. The ring breaks into weakly communicating parts.

The authors of Ref. 21 deduced from their results that the interaction between holes is repulsive; our conclusion is the opposite, so long as the cores do not overlap. We see in their results, as A is increased, the onset of real space pairing as soon as r_F is small enough for the ferron pair to fit on the six membered ring. At this point, we have a singlet pair from two ferrons, each formed with three spins each, each hole localized within its ferron, i.e., at opposite sides of the ring. This position of the holes is consistent with the hole correlation function calculation (the function g_{ij}) reported by Loh *et al.* In the limit of strong coupling, $A \to \infty$, their Eq. (III.4) gives $r = -\pi/4$ for the mixing angle which enters the variational wave function of Ref. 21. This leads to an isolated ferron binding energy $3A/4 = AS(S+1)/2$, where $S = s = \frac{1}{2}$. This state may be identified with the spin singlet discussed by Zhang and Rice.[23]

If we extend the above picture to two dimensions, the ground-state phase diagram is more complex. As we have seen, for $A < A_c$, a single hole does not form a ferron (self-trapped magnetic polaron). Instead, we have a quasiparticle of plane-wave character. For $A > A_c$, the single quasiparticle collapses to a small ferron. These may bind into real-space singlets at small hole concentration, then unbind to form an itinerant gas of spin-$\frac{1}{2}$ ferrons for $A > A^*$. If the ferron extends to nearest neighbors of the central spin, we would expect the critical hole concentration to be the order of z^{-1}. It would be intriguing to explore this question analytically, or within numerical calculations similar to those report in Ref. 21. Either approach appears formidable.

IV. CONCLUDING REMARKS

We have investigated the ground state of holes in an antiferromagnetic medium, with emphasis on the case of dimensionality $D < 3$. For $D = 1$, our picture agrees with that based on exact numerical calculations,[21] though our view of the underlying physics differs from that put forward earlier. In $D = 1$, the ground state of a single hole is always a ferron, which evolves continuously from type-I to type-II character as A increases. We have a spin singlet when $A \to \infty$. We argue that the attractive coupling between two ferrons is not specific to one dimension, as has been suggested by other authors in the context of high-T_c superconductivity.[8,25–27] However, in the case $D = 2$, the exchange constant A must exceed A_c for a single hole to form a ferron. Upon further increase of A, at least in theory one may achieve real-space pairing of the ferrons.

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energy with respect to N_l gives $N_l \sim 3$. This corresponds to $r_F = 3a$, and the Mott criterion mentioned in the text gives $C_h \sim \frac{1}{3}$ for the critical hole concentration.

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