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Exact solutions of two-hole and hole-magnon bound states in a ferromagnet

Y. L. Wang, E. Manousakis, and C. D. Wentworth
Department of Physics and Center for Materials Research and Technology, Florida State University, Tallahassee, Florida 32306
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Exact solutions of the two-hole and hole-magnon bound states have been found in a ferromagnetic system with hole hopping involved. A phenomenological Hamiltonian that contains spin-spin interaction and hole-hopping terms without doubly occupied sites is considered. Two-hole and hole-magnon bound-state conditions, binding energies, and wave functions are shown for one-dimensional and two-dimensional lattices. They illustrate the interplay of charge and spin excitations. The physical picture of bound states is discussed.

I. INTRODUCTION

One interesting aspect of high-T_c superconductors (HTS's) is the possibility that superconductivity in these materials may be primarily of an electronic origin rather than due to the electron-phonon interaction. A common point of departure is to assume that the parent compounds of the HTS's are Mott insulators and can be described, at least in a first approximation, by the s-band Hubbard model in the strong-coupling limit.[1] In this simple picture, the Cu-O planes of the HTS's are modeled by a two-dimensional square lattice with each site representing a CuO_2 unit cell. Electrons can hop between nearest neighbors, and for two electrons on the same site there is strong Coulomb repulsion modeled by the Hubbard U term. In the strong-coupling limit the Coulomb repulsion prevents double occupancy of a lattice site and an effective Hamiltonian can be derived in which there is nearest-neighbor antiferromagnetic exchange and a hole-hopping term (t-J model) (Ref. 2)

$$H=-t\sum_{\langle i,j\rangle\sigma}(1-n_{i,-\sigma})c_{i\sigma}^{\dagger}c_{j\sigma}(1-n_{j-\sigma})-J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j\ , \quad (1)$$

where $J=-4t^2/U<0$. The sums are over all lattice sites i and j and over the two-spin values symbolized by $\sigma=\pm1$. $\mathbf{S}_i$ is the spin operator for an electron at site i, $c_{i\sigma}^{\dagger}$ is the fermion creation operator for site i and spin value σ, and $n_{i\sigma}$ is the fermion occupation number operator. The components of $\mathbf{S}_i$ can be written in terms of fermion operators as

$$S_i^{+}=c_{i1}^{\dagger}c_{i\bar{1}}\ , \quad (2)$$

$$S_i^{-}=c_{i\bar{1}}^{\dagger}c_{i1}\ , \quad (3)$$

$$S_i^{z}=\tfrac{1}{2}(n_{i1}-n_{i\bar{1}})\ . \quad (4)$$

We are considering the case where the electrons are not allowed to double occupy lattice sites and have used the notation $\bar{1}\equiv-1$. In the half-filled band case this model is equivalent to the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model, which from simulation studies[3] and calculations done for the related nonlinear sigma model[4] is known to describe well the antiferromagnetic correlations in La_2CuO_4.[5]

Numerical diagonalization studies of the strong-coupled Hubbard model on small lattices suggest that hole pairing can occur for some range of values of the interaction parameter t/U.[6] More recently analytical and numerical techniques have been employed to study the possibility of such pairing in this model and its possible causes.

It may be interesting to consider the analytic continuation of the t-J model (1) in the positive J plane. We should mention that this model cannot be derived from the strong-coupling Hubbard model and it is not perhaps directly relevant to the HT superconductors. However, the fact that it has a trivial ground state when holes are absent makes its study simple and can illustrate the interplay of charge and spin excitations. Investigations of a ferromagnetic system with hole hopping involved would be of interest, especially since a number of results regarding two-hole and hole-magnon bound states can be obtained exactly.

In this paper we will calculate eigenstates of H given by equation (1), but with $J>0$, exactly for two cases: (1) two holes in a ferromagnetically aligned lattice and (2) one-hole and one-spin deviation in a ferromagnetically aligned lattice. We find that a two-hole bound state always exists for total momentum $\mathbf{K}$ at the Brillouin-zone boundary in both one and two dimensions, but the range of $\mathbf{K}$ values over which the bound state exists depends on the value of J/t. If J/t is greater than a certain critical value then bound states exist over the whole range of $\mathbf{K}$ values, otherwise there exists some region surrounding $\mathbf{K}=0$ for which no bound state exists. For the case of one hole and one magnon in a ferromagnetically ordered lattice, we find that in one dimension a bound state always exists at $\mathbf{K}=0$ for any value of J/t greater than zero while in two dimensions there is a finite range of values, $J_l/t\le J/t\le J_u/t$, for which a bound state can exist.

This study forms a complement to the problem of two-magnon states in a ferromagnetically ordered lattice where in one- and two-dimensional lattices bound states exist over the whole range of two-magnon total momentum merging with the continuum at $\mathbf{K}=0$, and in three dimensions bound states exist for some range of $\mathbf{K}$ values but not in a finite region surrounding $\mathbf{K}=0$.[7]

In the next section we will describe how to solve the Schrödinger equation in the two-hole subspace. The equation determining the bound-state eigenenergy as a function of total momentum $\mathbf{K}$ of the two-hole pair will be derived. Section III contains a discussion of the hole-magnon states for one and two-dimensional lattices. Equations determining energy eigenvalues for the bound states are derived and some results are presented.

II. TWO-HOLE BOUND STATES

The atomic representation introduced by Hubbard can be a useful formalism for treating more complicated correlated electron models.[8] We will introduce it here as an illustration of its use in a simple context. Each site can be in one of three states: $|i,1\rangle$ has one up-spin electron at site i, $|i,\bar{1}\rangle$ has one down-spin electron and $|i,0\rangle$ is an empty site. Any single-site operator can be expressed in this representation from the resolution of the identity

$$\hat{1}_i=|i,1\rangle\langle i,1|+|i,0\rangle\langle i,0|+|i,\bar{1}\rangle\langle i,\bar{1}| \ . \tag{5}$$

Define the atomic representation operators U^i_{rs} as

$$U^i_{rs}=|i,r\rangle\langle i,s| \ . \tag{6}$$

These operators satisfy the multiplication rule

$$U^i_{pq}U^i_{rs}=\delta_{qr}U^i_{ps} \tag{7}$$

and the commutation relation

$$[U^i_{pq},U^j_{rs}]_{\mp}=\delta_{ij}(\delta_{qr}U^i_{ps}\mp\delta_{ps}U^i_{rq}) \ , \tag{8}$$

where the upper sign is taken when at least one of the operators has boson character, and the lower sign is taken only if both operators have fermion character. For the model considered here U^i_{10}, $U^i_{\bar{1}0}$, U^i_{01}, and $U^i_{0\bar{1}}$ are the operators encountered with fermionic character. The operators present in H can be expressed in terms of the operators U^i_{rs}

$$S_i^+=U^i_{1\bar{1}} \ , \tag{9}$$

$$S_i^-=U^i_{\bar{1}1} \ , \tag{10}$$

$$S_i^z=\tfrac{1}{2}(U^i_{11}-U^i_{\bar{1}\bar{1}}) \ , \tag{11}$$

$$c^+_{is}(1-n_{i\bar{s}})=U^i_{s0} \ , \tag{12}$$

$$(1-n_{i\bar{s}})c_{is}=U^i_{0s} \ . \tag{13}$$

The Hamiltonian H can be rewritten

$$H=-\sum_{(i,j)s}t_{ij}U^i_{s0}U^j_{0s}-\sum_{(i,j)}J_{ij}[U^i_{1\bar{1}}U^j_{\bar{1}1}+\tfrac{1}{4}(U^i_{11}-U^i_{\bar{1}\bar{1}})(U^j_{11}-U^j_{\bar{1}\bar{1}})] \ . \tag{14}$$

In this section we are interested in eigenstates of H in subspaces with one or two holes introduced on a lattice where each site contains an up spin. Define $\mathcal{F}_1$ and $\mathcal{F}_2$ to be the one-hole and two-hole subspaces. A basis for $\mathcal{F}_1$ is formed from the states

$$|\mathbf{r}_i\rangle=U^i_{01}|F\rangle \ , \tag{15}$$

where $\mathbf{r}_i$ refers to a lattice site and $|F\rangle$ is the state with all sites containing one-spin-up electron. A spanning set for $\mathcal{F}_2$ is formed by

$$|\mathbf{r}_i,\mathbf{r}_j\rangle=U^i_{01}U^j_{01}|F\rangle \ . \tag{16}$$

We will be working with the Fourier transform of these states to momentum space

$$|\mathbf{k}\rangle=\frac{1}{\sqrt{N}}\sum_{\mathbf{r}_1}e^{i\mathbf{k}_1\cdot\mathbf{r}_1}|\mathbf{r}_1\rangle \tag{17}$$

and

$$|\mathbf{k}_1,\mathbf{k}_2\rangle=\frac{1}{N}\sum_{\mathbf{r}_1\mathbf{r}_2}e^{i\mathbf{k}_1\cdot\mathbf{r}_1}e^{i\mathbf{k}_2\cdot\mathbf{r}_2}|\mathbf{r}_1,\mathbf{r}_2\rangle \ . \tag{18}$$

We note that the transverse exchange terms in H have no effect on states in $\mathcal{F}_1$ and $\mathcal{F}_2$ so that they can be dropped for the remainder of this section. The states $|\mathbf{k}\rangle$ are eigenstates of H with energy eigenvalues

$$\varepsilon(\mathbf{k})=-\frac{Jz}{4}(N-2)+tz\gamma_{\mathbf{k}} \ , \tag{19}$$

$$\gamma_{\mathbf{k}}=\frac{1}{z}\sum_{\delta}e^{i\mathbf{k}\cdot\delta} \ , \tag{20}$$

and z is the number of nearest neighbors δ.

The two-hole eigenstates can be labeled by the total momentum $\mathbf{K}=\mathbf{k}_1+\mathbf{k}_2$ of the pair since it is a conserved quantity. The relative momentum $\mathbf{q}=\frac{1}{2}(\mathbf{k}_1-\mathbf{k}_2)$ will also be introduced.

We will find that coefficients $f_{\mathbf{k}}(\mathbf{q})$ can be found such that the state $|\Psi_{\mathbf{K}}\rangle$ in $\mathcal{F}_2$ is an eigenstate of H where

$$|\Psi_{\mathbf{K}}\rangle=\sum_{\mathbf{q}}f_K(\mathbf{q})|\mathbf{k}_1,\mathbf{k}_2\rangle \ . \tag{21}$$

Projecting the time-independent Schrödinger equation with the bra $\langle\{\mathbf{K}/2+\mathbf{q}'\},\{\mathbf{K}/2-\mathbf{q}'\}|$ we obtain

$$\begin{aligned}E[f_{\mathbf{K}}(\mathbf{q})-f_{\mathbf{K}}(-\mathbf{q})]&=\left[E_0+t\left(\frac{\mathbf{K}}{2}+\mathbf{q}\right)+t\left(\frac{\mathbf{K}}{2}-\mathbf{q}\right)\right][f_{\mathbf{K}}(\mathbf{q})-f_{\mathbf{K}}(-\mathbf{q})]\\&\quad-\frac{1}{2N}\sum_{\mathbf{q}'}J(\mathbf{q}')[f_{\mathbf{K}}(\mathbf{q}+\mathbf{q}')-f_{\mathbf{K}}(-\mathbf{q}+\mathbf{q}')] \ ,\end{aligned} \tag{22}$$

where $E_0=-(Jz/4)N+Jz$, $J(\mathbf{q})=Jz\gamma_q$ and $t(\mathbf{q})=tz\gamma_{\mathbf{q}}$. Since we are interested in lattices with an inversion symmetry, $\gamma_{\mathbf{q}}$ has the property $\gamma_{-\mathbf{q}}=\gamma_{\mathbf{q}}$. Therefore

$$\sum_{\mathbf{q}'}J(\mathbf{q}')f_{\mathbf{K}}(-\mathbf{q}+\mathbf{q}')=\sum_{\mathbf{q}'}J(\mathbf{q}')f_{\mathbf{K}}(-\mathbf{q}-\mathbf{q}') \ , \tag{23}$$

since the sum is over the entire Brillouin zone. With $\mathbf{k}'$ defined by $\mathbf{k}'=\mathbf{q}+\mathbf{q}'$, equation (22) can be written as

$$\left[E-E_0-t\left[\frac{\mathbf{K}}{2}+\mathbf{q}\right]-t\left[\frac{\mathbf{K}}{2}-\mathbf{q}\right]\right]g_{\mathbf{K}}(\mathbf{q})=-\frac{1}{2N}\sum_{\mathbf{k}'}J(\mathbf{k}'-\mathbf{q})g_{\mathbf{K}}(\mathbf{k}')\ , \tag{24}$$

where

$$g_{\mathbf{K}}(\mathbf{q})=f_{\mathbf{K}}(\mathbf{q})-f_{\mathbf{K}}(-\mathbf{q})\ . \tag{25}$$

Equation (24) must be solved for $g_{\mathbf{K}}(\mathbf{q})$ and E. We note that the free-hole states

$$|\Psi_{\mathbf{K}}\rangle=C|\mathbf{k}_1,\mathbf{k}_2\rangle \tag{26}$$

are eigenstates to order $1/N$ with energy

$$\mathscr{E}_{\mathbf{K}}(\mathbf{q})=E_0+t\left[\frac{\mathbf{K}}{2}+\mathbf{q}\right]+t\left[\frac{\mathbf{K}}{2}-\mathbf{q}\right]\ . \tag{27}$$

Therefore each value of total momentum $\mathbf{K}$ has an associated band of solutions that extends from the minimum to the maximum value of $\mathscr{E}_{\mathbf{K}}(\mathbf{q})$. Coherence between the free-hole states caused by the interaction can produce bound-state solutions with $E-\mathscr{E}_{\mathbf{K}}^{\min}<0$.

To find the bound-state solutions Eq. (24) is written

$$g_{\mathbf{K}}(\mathbf{q})=-\frac{J}{2N}\sum_{\mathbf{k}',\boldsymbol{\delta}}\exp(-i\mathbf{q}\cdot\boldsymbol{\delta})\exp(i\mathbf{k}'\cdot\boldsymbol{\delta})\frac{g_{\mathbf{K}}(\mathbf{k}')}{E-\mathscr{E}_{\mathbf{K}}(\mathbf{q})}\ . \tag{28}$$

This equation can be solved in the following way. First we take

$$G_{\mathbf{K}}(\boldsymbol{\delta})=\frac{1}{N}\sum_{\mathbf{k}}\exp(i\mathbf{k}'\cdot\boldsymbol{\delta})g_{\mathbf{K}}\mathbf{k}')\ . \tag{29}$$

Then we have

$$G_{\mathbf{K}}(\boldsymbol{\delta}_i)=\sum_{\boldsymbol{\delta}}C_{\boldsymbol{\delta}_i,\boldsymbol{\delta}}G_{\mathbf{K}}(\boldsymbol{\delta})\ , \tag{30}$$

where

$$C_{\boldsymbol{\delta}_i,\boldsymbol{\delta}}=-\frac{J}{2N}\sum_{\mathbf{q}}\frac{\exp[i\mathbf{q}\cdot(\boldsymbol{\delta}_i-\boldsymbol{\delta})]}{E-\mathscr{E}_{\mathbf{K}}(\mathbf{q})}\ . \tag{31}$$

To find the bound-state energies the matrix equation

$$|\hat{\mathbf{1}}-C|=0 \tag{32}$$

needs to be solved. In fact this equation can be simplified by considering the symmetry of the lattice. For a hypercubic d-dimensional lattice the solutions of Eq. (32) become

$$-1=\frac{J}{N}\sum_{\mathbf{q}}\frac{\sin^2(q_i)}{E-\mathscr{E}_{\mathbf{K}}(\mathbf{q})} \tag{33}$$

with $q_i=q_1,\ldots,q_d$ and taking the lattice constant as a unit of distance. Thus for a chain and a two-dimensional square lattice the bound-state energies can be found by solving Eq. (33).

Some features of two-hole bound states in a square lattice will be described. Figure 1 shows the two-hole bound-state energies along selected paths in the first Brillouin zone for selected values of J/t. For $J/t\geq 11.008$ there exists a bound state for all values for total momentum. This indicates an instability in the ground state of the free-hole system. Two distinct solutions exist along the paths ΓM and MX, whereas the two solutions are degenerate along ΓX due to the symmetry $K_x=K_y$. For $4\leq J/t\leq 11.008$ the bound-state solutions merge with the bottom of the two-hole continuum along the ΓM and ΓX paths at $\mathbf{K}_m$. Figure 2 shows the $\mathbf{K}_m$ for which this merging occurs along these paths. $\mathbf{K}_m$ is obtained by substituting the energy of the bottom of the continuum for a particular value of $\mathbf{K}$ into Eq. (33) and calculating J/t. For example along ΓX we obtain

$$K_{mx}=K_{my}=2\arccos(J\eta/4t)\ , \tag{34}$$

$$\eta=\frac{1}{\pi}\int_0^{\pi}dq_x\frac{\sin^2 q_x}{[(2+\cos q_x)^2-1]^{1/2}}=0.363\,380\,23\ . \tag{35}$$

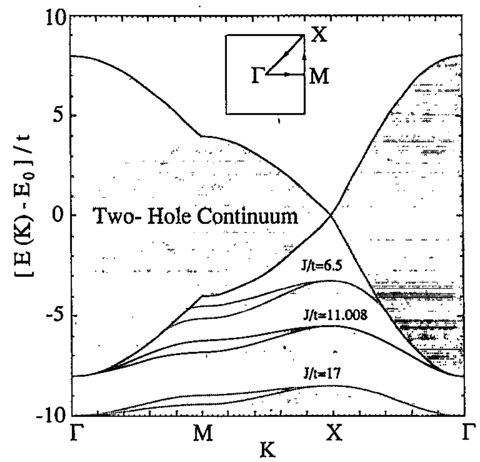

FIG. 1. The two-hole bound-state energies for the square lattice at selected values of J/t. The Brillouin zone is shown at the top of the figure, and the high-symmetry points are $\Gamma=[0,0]$, $M=[\pi,0]$ and $X=[\pi,\pi]$.

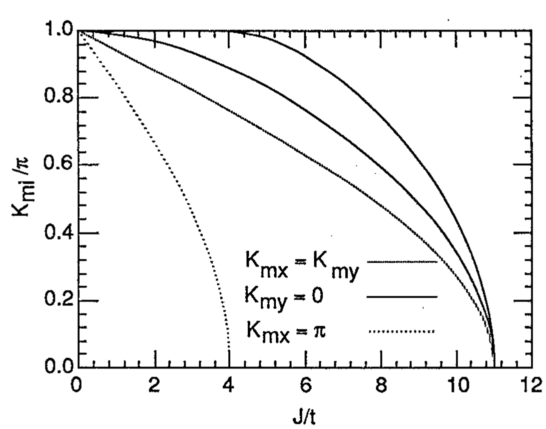

FIG. 2. The two-hole total momentum at which the bound-state energy merges with the bottom of the free-hole continuum as a function of J/t.

Note that two solutions exist for all values of K along MX for this range of J/t values. For $J/t<4$ only one solution exists along ΓM. Along MX one solution merges with the bottom of the continuum at

$$K_{my}=2\arccos(J/4t)\ . \tag{36}$$

The other solution along MX exists for all values of K_y as long as $J/t>0$.

It is interesting to look at the hole positions in position space to see whether the bound state is localized or not. By projecting $\Psi_{\mathbf{K}}$ onto the state $|\mathbf{r}_1,\mathbf{r}_2\rangle$ with one hole located at site $\mathbf{r}_1$ and another hole located at site $\mathbf{r}_2$ we obtain

$$\langle \mathbf{r}_1,\mathbf{r}_2|\Psi_{\mathbf{K}}\rangle = ie^{i\mathbf{K}\cdot\mathbf{R}}\frac{1}{N}\sum_q g_{\mathbf{K}}(\mathbf{q})\sin(\mathbf{q}\cdot\mathbf{r})\ , \tag{37}$$

where

$$\mathbf{r}=\mathbf{r}_1-\mathbf{r}_2=n_x\hat{\mathbf{x}}+n_y\hat{\mathbf{y}},\quad \mathbf{R}=\frac{\mathbf{r}_1+\mathbf{r}_2}{2} \tag{38}$$

and $n_x,n_y=\{0,\pm1,\pm2,\dots\}$ (the lattice constant is taken to be one).

This two-hole wave function can be calculated analytically. Consider the one-dimensional case first. The solution of Eq. (33) is

$$\varepsilon=\frac{J}{2}\left[1+\left[\frac{4t}{J}\cos K/2\right]^2\right] \tag{39}$$

with the condition $(4t\cos K/2)^2/J^2<1$ where $\varepsilon=E_0-E$. Substitution of the energy eigenvalue back into the equation for $g_K(q)$ yields

$$g_K(q)=\frac{2\sin q}{1+\left[\frac{4t}{J}\cos\frac{K}{2}\right]^2+\frac{8t}{J}\cos\frac{K}{2}\cos q}A_K\ , \tag{40}$$

where A_K is a normalization factor.

To obtain the wave function we must calculate the integral

$$\mathcal{S}_n(\alpha)=\frac{1}{\pi}\int_0^{\pi}dq\frac{\sin(q)\sin(qn)}{\alpha+\cos(q)} \tag{41}$$

for $n=\{\pm1,\pm2,\pm3,\dots\}$. We obtain

$$\mathcal{S}_n(\alpha)=\frac{1}{\pi}\int dq\frac{\cos(n-1)q}{\alpha+\cos q}-\frac{1}{\pi}\int dq\frac{\cos(nq)\cos q}{\alpha+\cos q}$$
$$=\alpha C_n(\alpha)+C_{n-1}(\alpha)\ , \tag{42}$$

where

$$C_n(\alpha)=\frac{1}{\pi}\int_0^{\pi}dq\frac{\cos(qn)}{\alpha+\cos q}\ . \tag{43}$$

A recursion formula for C_n can be derived by using the appropriate recursion formula for $\cos(qn)$:

$$C_n(\alpha)=-2\alpha C_{n-1}(\alpha)-C_{n-2}(\alpha)\ . \tag{44}$$

This is a homogeneous linear difference equation with initial conditions

$$C_0(\alpha)=\frac{1}{(\alpha^2-1)^{1/2}} \tag{45}$$

and

$$C_1(\alpha)=1-\alpha C_0(\alpha)\ . \tag{46}$$

It can be solved by the choice $C_n(\alpha)=cb_\alpha^n$. We obtain

$$C_n(\alpha)=\frac{1}{(\alpha^2-1)^{1/2}}[-\alpha+(\alpha^2-1)^{1/2}]^n\ . \tag{47}$$

Summarizing the results for one dimension gives

$$\langle r_1r_2|\psi_K\rangle=\mathcal{N}_Ke^{i(K/2)(r_1+r_2)}[(\alpha_K^2-1)^{1/2}-\alpha_K]^{|r_1-r_2|} \tag{48}$$

with $r_1\neq r_2$ and

$$\alpha_k=\frac{1+\left[\frac{4}{J}\cos\frac{K}{2}\right]^2}{\frac{8}{J}\cos\frac{K}{2}} \tag{49}$$

and $\mathcal{N}_K$ is a normalization factor.

In two-dimensions there are two bound-state solutions. For the solution corresponding to $q_i=q_x$ in Eq. (33) we obtain

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi_{\mathbf{K}}\rangle_1=\mathcal{N}_{\mathbf{K}}e^{i\mathbf{K}/2\cdot(\mathbf{r}_1+\mathbf{r}_2)}I_n^x(\alpha_{\mathbf{K}})\ , \tag{50}$$

where

$$I_n^x(\alpha_{\mathbf{K}})=\frac{1}{\pi}\int_0^{\pi}dq_y\mathcal{S}_{n_x}(\alpha_{\mathbf{K}},q_y)\cos(q_yn_y)\ , \tag{51}$$

$$\mathcal{S}_{n_x}(\alpha_{\mathbf{K}},q_y)=\alpha_{\mathbf{K}}(q_y)C_{n_x}(\alpha_{\mathbf{K}}(q_y))+C_{n_x-1}(\alpha_{\mathbf{K}}(q_y))\ , \tag{52}$$

$$\alpha_{\mathbf{K}}(q_y)=\frac{\varepsilon+4\cos(K_y/2)\cos q_y}{4\cos(K_x/2)}, \tag{53}$$

and $C_{n_x}(\alpha_{\mathbf{K}}(q_y))$ is given by Eq. (47). For the other solution a similar result is obtained

$$\langle \mathbf{r}_1\mathbf{r}_2|\psi_{\mathbf{K}}\rangle_2=\mathcal{N}_{\mathbf{K}}e^{i\mathbf{K}/2\cdot(\mathbf{r}_1+\mathbf{r}_2)}I_n^y(\alpha_{\mathbf{K}})\ , \tag{54}$$

where $I_n^y(\alpha_{\mathbf{K}})$ is defined from Eqs. (51) and (52) with n_x,q_y replaced by n_y,q_x.

The two-hole wave functions take especially simple forms for $\mathbf{K}=[\pi,0]$. We find that

$$I_n^x=c_1\left\{\frac{J}{8t}-\left[1+\left[\frac{J}{8t}\right]^2\right]^{1/2}\right\}^{|n_y|}(\delta_{n_x,1}+\delta_{n_x,-1}) \tag{55}$$

and

$$I_n^y=c_2(-4t/J)^{|n_y|}\delta_{n_x,0}\ , \tag{56}$$

where $n_y\neq0$ and c_1 and c_2 are constants involving J/t. The first solution has one hole at the origin and the other hole on a line parallel to the y axis but displaced by one lattice spacing in either the plus or the minus x direction. The second solution has a hole at the origin and the second hole along the y axis. Both solutions are very lo-

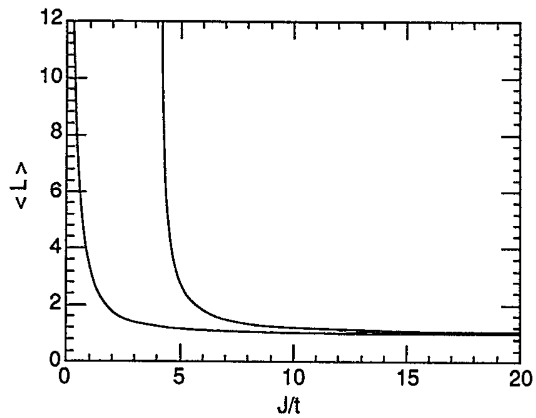

FIG. 3. The average distance between two bound holes for the special point $\mathbf{K}=[\pi,0]$.

calized in the x direction with the amount of y localization depending on J/t. The average hole separation can be calculated from

$$\langle l \rangle = \frac{\sum_n l_n (I_n^i)^2}{\sum_n (I_n^i)^2} , \tag{57}$$

where $i=\{x,y\}$ and

$$l_n=(1+n_y^2)^{1/2} \text{ for } i=x , \qquad l_n=n_y \text{ for } i=y . \tag{58}$$

Figure 3 shows $\langle l \rangle$ as a function of J/t for the two cases. It is apparent that both solutions show the hole remaining tightly bound until the binding energy is very small compared to J/t. This occurs at $J/t=0$ for the first case and $J/t=4$ for the second case.

III. HOLE-MAGNON BOUND STATES

In the last section we explored how the ferromagnetic background can affect holes moving in the lattice. The moving holes should also affect the magnetic states of the system. We will explore here the possibility that a hole and a magnon interact to form a bound states. The Hamiltonian H will be diagonalized in a subspace $\mathcal{F}_{11}$ with one-hole and one-spin deviation placed on a lattice with all up spins. A spanning set for $\mathcal{F}_{11}$ is formed from the states

$$|\mathbf{r}_i,\mathbf{r}_j\rangle = U_{01}^i U_{\bar{1}1}^j |F\rangle \tag{59}$$

An eigenstate $\phi_{\mathbf{K}}$ of H can be constructed in the subspace $\mathcal{F}_{11}$

$$|\phi_{\mathbf{K}}\rangle = \sum_{\mathbf{q}} f_{\mathbf{K}}(\mathbf{q})|\mathbf{k}_1,\mathbf{k}_2\rangle . \tag{60}$$

We can obtain the eigenvalue equation for H:

$$\left[E-E_0-t\left[\frac{\mathbf{K}}{2}+\mathbf{q}\right]+J\left[\frac{\mathbf{K}}{2}-\mathbf{q}\right]\right]f_{\mathbf{K}}(\mathbf{q})=\frac{1}{N}\sum_{\mathbf{q}'}\left[t(\mathbf{q}'+\mathbf{q})-J\left[\mathbf{q}'-\mathbf{q}\right]+J\left[\frac{\mathbf{K}}{2}-\mathbf{q}\right]-t\left[\frac{\mathbf{K}}{2}+\mathbf{q}\right]\right]f_{\mathbf{K}}(\mathbf{q}') , \tag{61}$$

where

$$E_0=-\frac{NJz}{4}+\tfrac{3}{2}Jz . \tag{62}$$

Similar to the two-hole case, Eq. (61) yields a band of free-hole-magnon states for each $\mathbf{K}$ with E ranging from the minimum to the maximum value of $\mathcal{E}_{\mathbf{K}}(\mathbf{q})$ where

$$\mathcal{E}_{\mathbf{K}}(\mathbf{q})=E_0+t\left[\frac{\mathbf{K}}{2}+\mathbf{q}\right]-J\left[\frac{\mathbf{K}}{2}-\mathbf{q}\right] . \tag{63}$$

To obtain the hole-magnon bound-state solutions for two-dimensional square lattices we must solve the determinant equation

$$|\hat{\mathbf{1}}-C|=0 \tag{64}$$

with C given by

$$\begin{bmatrix} a\alpha_{2000} & -b\alpha_{1100} & a\alpha_{1010} & -b\alpha_{1001} & c_1 \\ a\alpha_{1100} & -b\alpha_{0200} & a\alpha_{0110} & -b\alpha_{0101} & c_2 \\ a\alpha_{1010} & -b\alpha_{0110} & a\alpha_{0020} & -b\alpha_{0011} & c_3 \\ a\alpha_{1001} & -b\alpha_{0101} & a\alpha_{0011} & -b\alpha_{0002} & c_4 \\ a\alpha_{1000} & -b\alpha_{0100} & a\alpha_{0110} & -b\alpha_{0001} & c_5 \end{bmatrix} . \tag{65}$$

We have used the definitions

$$\alpha_{ijkl}=\frac{1}{N}\sum_{\mathbf{q}}\frac{(\cos q_x)^i(\sin q_x)^j(\cos q_y)^k(\sin q_y)^l}{E-\mathcal{E}_{\mathbf{K}}(\mathbf{q})} ; \tag{66}$$

$$c_r=-a\cos(K_x/2)\alpha_{r1}+b\sin(K_x/2)\alpha_{r2} , \quad -a\cos(K_y/2)\alpha_{r3}+b\sin(K_y/2)\alpha_{r4} , \tag{67}$$

where α_{ri}, $i=1,2,3,4$, are the integrals α_{ijkl} involved in the first four entries of the rth row in $\mathbf{C}$. Also, $a=2(t-J)$ and $b=2(t+J)$.

The largest binding energy occurs at $\mathbf{K}=[0,0]$ and solutions only exist for $0.466\,942\le J/t\le 2.141\,593$. At $\mathbf{K}=[\pi,0]$ a bound state can also exist, but it occurs for a smaller J/t interval: $0.710\,952\le J/t\le 1.406\,565$. At $\mathbf{K}=[\pi,\pi]$ the bound state is always coincident with the bottom of the hole-magnon continuum. The energy is the lowest at $\mathbf{K}=[\pi,\pi]$.

It is worthwhile to compare the two-hole bound-state situation with this hole-magnon bound state in the square lattice. A two-hole bound state always exists for any $J/t>0$, but the hole-magnon bound states exist only for a restricted range of J/t values. This result is physically reasonable since when t is small compared to J the hole remains fairly localized: It is harder for it to hop through the lattice at least compared to the ease with which a magnon propagates. Binding of this slowly moving hole with the quickly moving magnon becomes problematic. When t is large compared to J the hole propagates easily compared to the magnon so that again binding becomes problematic.

The largest binding energy occurs for $J/t=1$. We will present calculations of the energy along the high-symmetry path $\Gamma MX\Gamma$ of the first Brillouin zone for this case. Since $a=0$ there is considerable simplification in the equations.

For $K_y=0$, along ΓM two separable equations for E can be derived. The first is

$$1+4\alpha_{0002}=0 \tag{68}$$

and gives a finite binding energy at $\mathbf{K}=[0,0]$ and at $\mathbf{K}=[\pi,0]$. The other equation is

$$1-4\sin(K_x/2)\alpha_{0100}+4\alpha_{0200}=0 \tag{69}$$

and gives a solution that merges with the continuum at $\mathbf{K}=[\pi,0]$. One bound state exists along MX. Along the path ΓX the two solutions are degenerate. Figure 4 shows the $\mathbf{K}$ dependence of the bound-state energies along the three paths considered. It is interesting to note that for all $\mathbf{K}$ values [except at $\mathbf{K}=(\pi,\pi)$] the bound state of a hole with a flipped spin lies below the state in which the hole moves with the same momentum in a ferromagnetically polarized environment.

The wave functions of hole-magnon bound states can be found with the same procedure as for the two-hole bound states. For the case of $J=t$ and total momentum $\mathbf{K}=0$ the wave function has the simple form

$$|\psi_{\mathbf{K}=0}\rangle=\frac{1}{4N}\sum_r\{|\mathbf{r},\mathbf{r}+\hat{\mathbf{x}}\rangle-|\mathbf{r},\mathbf{r}-\hat{\mathbf{x}}\rangle+|\mathbf{r},\mathbf{r}+\hat{\mathbf{y}}\rangle-|\mathbf{r},\mathbf{r}-\hat{\mathbf{y}}\rangle\}\ , \tag{70}$$

where

$$|\mathbf{r},\mathbf{r}'\rangle=U_{01}(\mathbf{r})U_{\bar{1}1}(\mathbf{r}')|F\rangle\ . \tag{71}$$

It is obvious that the bound state has the hole and flipped spin localized next to each other.

In the case of $\mathbf{K}=[\pi,0]$, i.e., at the zone boundary point M, the hole-magnon bound-state wave function becomes

$$|\psi_{K_x=\pi,K_y=0}\rangle=C\sum_{\mathbf{R},n_x,n_y=\pm1}e^{i\mathbf{K}\cdot\mathbf{R}}(-1)^{(n_x+n_y)/2}\times\left[\frac{\sqrt{5}-1}{2}\right]^{|n_x|}\left|\mathbf{R}+\frac{\mathbf{r}}{2},\mathbf{R}-\frac{\mathbf{r}}{2}\right\rangle\ . \tag{72}$$

It has a form similar to the wave function for one of the two-hole bound states at point M. The average distance between the hole and flipped spin is 1.52 in the units of the lattice constant.

IV. CONCLUSION

We have studied the interplay of charge and spin excitations in a quantum ferromagnet model. Exact solutions of two-hole and hole-magnon bound states, resembling the two-magnon bound states of a ferromagnet,[8] can be obtained for a general lattice.

In this paper we have shown the conditions for obtaining two-hole and hole-magnon bound-states, binding energies and wave functions for one- and two-dimensional lattices. The physical picture of bound states can be illustrated by using their wave functions. For example, by studying the two-hole wave function in real space we find that pairing is predominantly nearest neighbor except in a very narrow region of J/t close to the critical value. We have also found that if the effective spin-spin interaction J is sufficiently strong compared with the hole hopping integral t, the ground state of the system is not just ferromagnetically aligned spins with free-hole hopping; the energy of the system with the two-hole bound state is lower.

The other multihole bound states have to be studied to determine the ground state with finite density of holes. The kind of ground state that this system has depends on the competition between the energy gain due to bound holes breaking fewer exchange bonds than separate holes and the kinetic energy gain which separates holes have from being more mobile. We expect that as J/t is increased from zero the system goes through a regime where the two-hole bound state is lowest in energy, then a regime is obtained where the three-hole bound state is lowest, and so on until finally a phase separation occurs. The two-hole bound states investigated here will be relevant in that window of J/t where they are the true ground state. Finally, we note that the bound states should influence the low-temperature thermodynamics of such systems.

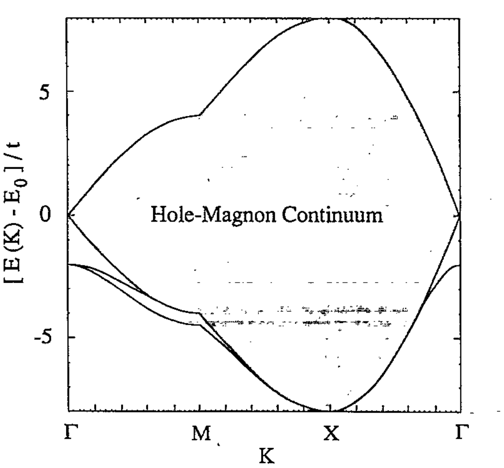

FIG. 4. The hole-magnon bound-state energies for the square lattice at $J/t=1$. The path in the first Brillouin zone is the same as shown in Fig. 1.

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