TWO-HOLE AND HOLE–MAGNON BOUND STATES IN QUANTUM FERROMAGNETS

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Exact solutions of two-hole and hole–magnon bound states are obtained for a phenomenological Hamiltonian involving electrons hopping on a lattice and interacting through ferromagnetic exchange. Conditions for the existence of bound states in this quantum ferromagnet are found for one- and two-dimensional lattices.

The subject of holes moving on a lattice of magnetically interacting particles has received considerable attention recently due to the developing picture of high-T_c superconducting ceramics as strongly correlated electron systems [1] which have significant antiferromagnetic correlations present in both undoped [2] and doped [3] states. A simple theoretical framework for such systems starts from the s-band Hubbard model in the strong-coupling limit where double occupancy of a site is prevented. In this limit one obtains an effective Hamiltonian in which there is nearest-neighbor antiferromagnetic Heisenberg exchange and a hole hopping term ($t-J$ model) [4]. The relevance of this Hamiltonian to $La_{2-x}Sr_xCuO_4$ has been supported by noting that the undoped compound ($x=0$) is an antiferromagnetic insulator with a temperature dependent correlation length which compares favorably with that of the two-dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet [5], equivalent to the effective Hamiltonian in the half-filled band case. Numerical diagonalization of the effective Hamiltonian for finite systems with holes suggests that two-hole bound states can occur [6]. A solution of this problem for large or infinite systems is difficult mainly because there are quantum spin fluctuations in the ground state and also the hole motion creates different types of states. If we consider a model in which the exchange interaction is ferromagnetic then considerable simplification of the problem can be expected. Indeed we show in this Letter that two-hole and hole–magnon bound state solutions can be found exactly. The two-magnon bound state problem for the Heisenberg ferromagnetic exchange model has also been solved exactly, and bound states are found to exist in both one- and two-dimensional lattices [7]. The exact solution of the two-magnon bound state for the antiferromagnetic case has not been found, but the spin-wave approximation shows that two-magnon bound states exist in a one-dimensional lattice but not in a two-dimensional lattice [8]. The ferromagnetic $t-J$ model, however, is not applicable to the copper-oxides which are antiferromagnets; certain concepts regarding the interplay of spin and charge degrees of freedom can be illustrated in this simpler model.

The existence and characteristics of two-hole bound states and the influence of holes on magnetic states can be illustrated clearly by considering the following phenomenological Hamiltonian which has ferromagnetic exchange,

$$H=-\sum_{(i,j)\sigma} t_{ij}(1-n_{i,-\sigma})c^+_{i,\sigma}c_{j,\sigma}(1-n_{j,-\sigma}) - \sum_{(i,j)} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j\,, \quad (1)$$

where $t_{ij}=t$ and $J_{ij}=J>0$ when (i,j) are nearest neighbors and are zero otherwise. The sums are over all lattice sites i and j and over the two spin values symbolized by $\sigma=\pm 1$. $\boldsymbol{S}_i$ is the spin operator for an electron at site i: $c_{i,\sigma}^{+}$ is the fermion creation operator for site i and spin value σ; $n_{i,\sigma}$ is the fermion occupation number operator. The components of $\boldsymbol{S}_i$ can be written in terms of fermion operators: $S_i^{+}=c_{i,1}^{+}c_{i,-1}$, $S_i^{-}=c_{i,-1}^{+}c_{i,1}$ and $S_i^{z}=\frac{1}{2}(n_{i,1}-n_{i,-1})$.

This model is interesting because a number of exact results can be obtained. Furthermore there may be real doped ferromagnets which have mobile holes as postulated here, so that the kinds of states we discuss may possibly be found in real materials. We hope these calculations encourage a search for such materials.

In this paper two situations will be considered: (1) two holes in an otherwise ferromagnetically aligned lattice and (2) one hole and one spin deviation in an otherwise ferromagnetically aligned lattice. One- and two-dimensional lattices will be considered. We will calculate the eigenvalues and eigenstates of H exactly in these two subspaces and address the question of the existence of two-hole and hole–magnon bound states. The solution for three-dimensional lattices can also be obtained using the same method.

This study forms a complement to the problem of two-magnon states in a ferromagnetically ordered lattice where in one dimension bound states exist over the whole range of two-magnon total momentum, in two dimensions bound states exist for all total momentum values except $K=0$ and in three dimensions bound states exist for some range of K values but not in a finite region surrounding $K=0$ [7]. For the case of two holes in a ferromagnetically ordered lattice we find that a bound state always exists for K at the Brillouin zone boundary in both one and two dimensions, but the range of 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 K values, otherwise there exists some region surrounding $K=0$ 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 $K=0$ for any value of J/t greater than zero while in two dimensions there is a finite range of values, $J_\ell \leqslant J \leqslant J_u$, for which a bound state exists.

The two-hole eigenstates can be labeled by the total momentum $K=k_1+k_2$ of the pair since it is a conserved quantity. The relative momentum $q=(k_1-k_2)/2$ will also be introduced.

We can find coefficients $f_K(q)$ such that the state

$$\Psi_K=\sum_q f_K(q)c_{k_1,1}c_{k_2,1}\,|\mathrm{FM}\rangle \tag{2}$$

is an eigenstate of H where $c_{k,\sigma}$ is the Fourier transform of $c_{i,\sigma}$ to momentum space. The coefficients $f_K(q)$ satisfy the following equation,

$$[E-E_0-t(\tfrac{1}{2}K+q)-t(\tfrac{1}{2}K-q)]g_K(q)$$
$$=-\frac{1}{2N}\sum_{k'}J(k'-q)g_K(k')\,, \tag{3}$$

where $g_K(q)=f_K(q)-f_K(-q)$, $E_0=-NJz/4+Jz/2$, $t(q)=tz\gamma_q$ and $J(q)=Jz\gamma_q$ are Fourier transforms of the hopping and the exchange integrals, z is the number of nearest neighbors, N the number of sites in the system and $\gamma_q=\sum_\delta \exp(-\mathrm{i}q\delta)/z$ where δ is a nearest neighbor of a site.

It is interesting to note that eq. (3) can also be obtained by using a model of bosons instead of fermions except that the coefficient $g_K(q)$ will be symmetric in q instead of antisymmetric.

Eq. (3) must be solved for $g_K(q)$ and E. We note that the state $g_K(q)=C\delta_{q,q'}$ is an eigenstate to order $1/N$. Therefore each value of total momentum K has an associated free two-hole band which extends from the minimum to the maximum value of $\mathscr{E}_K(q)$ defined by

$$\mathscr{E}_K(q)=E_0+t(\tfrac{1}{2}K+q)+t(\tfrac{1}{2}K-q)\,. \tag{4}$$

Other solutions due to interaction of the holes can exist just as in the two-magnon case. We look for bound state solutions, that is solutions with $E-\mathscr{E}_K^{\min}<0$.

Eq. (3) is an integral equation for $g_K(q)$ with separable kernel, therefore it is solved by reduction to a linear algebra problem. We obtain the eigenvalue equations for hypercubic lattices,

$$-1=\frac{J}{N}\sum_q \frac{\sin^2 q_i}{E-\mathscr{E}_K(q)}\,, \tag{5}$$

where $q_i=q_1 ... q_d$, d is the lattice dimension and we have taken the lattice constant as a unit of distance.

For a one-dimensional lattice the bound state energy is

$$E=E_0-\tfrac{1}{2}J[1+(4t\cos\tfrac{1}{2}K)^2/J^2]\,,$$

with the condition $(4t \cos \frac{1}{2}K)^2/J^2 < 1$. A bound state solution always exists at the zone boundary, $K = \pm\pi$. For $J/t < 4$ there will be a minimum value of $|K|$, $|K_{\min}| = 2 \arccos(J/4t)$, required to give a bound state. If $J/t \geq 4$ then a bound state exists across the entire zone.

Substitution of the energy eigenvalue back into the equation for $g_K(q)$ yields

$$g_K(q) = 2 \sin q \{1 + [(4t/J) \cos \tfrac{1}{2}K]^2 + [(8t/J) \cos \tfrac{1}{2}K] \cos q\}^{-1} A_K . \qquad (6)$$

It is interesting to look at the hole positions in a bound state. By projecting Ψ_K onto the state $|r_1, r_2\rangle$ with one hole located at site r_1 and another hole located at site r_2 we obtain

$$\langle r_1, r_2 | \Psi_K \rangle = \mathrm{i} \exp[\tfrac{1}{2}\mathrm{i}K(r_1 + r_2)] \times \frac{1}{N} \sum_q g_K(q) \sin(qr) , \qquad (7)$$

where $r = r_1 - r_2$.

For the largest value of the binding energy, at $K = \pm\pi$, $g_K(q)$ is proportional to $\sin q$. The q-integration in eq. (7) yields a non-zero value only for $r = 1$, therefore the two holes are paired locally. When the binding energy is smaller, such as when $K = 0$, $g_K(q)$ becomes more sharply peaked at values of $q \neq \pi/2$ so that the q-integration can yield significant contributions for larger values of r: the pair becomes a more extended object.

We will now consider a square lattice. Eq. (5) must be solved for $q_i = q_x$ and $q_i = q_y$, so in general we can expect up to two bound states. Fig. 1 shows the bound state energies along the path ΓMXΓ of the Brillouin zone for selected values of the interaction parameter J/t. The band of free two-hole states is also shown. A bound state solution always exists at $K = (\pm\pi, \pm\pi)$, the X point, where $\epsilon = J/2$. If $J/t < 11.008$ then the bound state solutions merge with the band at some finite K_m in the ΓM and ΓX directions. At $J/t = 11.008$ the bound state merges with the band only at the Γ point, and for larger values of J/t a gap always exists between the bound state energies and the bottom of the free two-hole band. The two bound state solutions become degenerate in the ΓX direction where $K_x = K_y$. For this direction the bound state merges with the band at $K_m = 2 \arccos(J\eta/4t)$ with

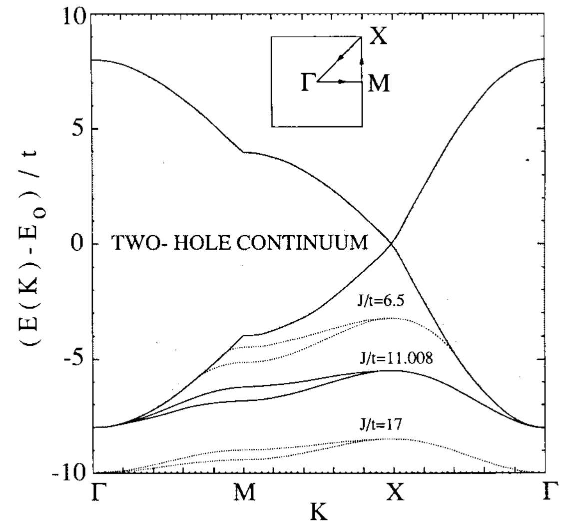

Fig. 1. The two-hole bound state energies $E(K)$ for the square lattice along the path ΓMXΓ. The square shown as an insert represents the Brillouin zone and the high symmetry points are $\Gamma = (0, 0)$, $M = (\pi, 0)$ and $X = (\pi, \pi)$.

$$\eta = \frac{1}{\pi} \int_0^\pi \mathrm{d}q_x \frac{\sin^2 q_x}{[(2 + \cos q_x)^2 - 1]^{1/2}} = 0.36338 . \qquad (8)$$

A simple expression for the bound state energies can be obtained in the MX direction where $K_x = \pi$ and $0 \leq K_y \leq \pi$. One solution is

$$\epsilon = \frac{J}{2} \left[1 + \left(\frac{8t \cos \frac{1}{2}K_y}{J} \right)^2 \right]^{1/2} , \qquad (9)$$

where $\epsilon = E_0 - E$. The other is

$$\epsilon = \frac{J}{2} \left[1 + \left(\frac{4t \cos \frac{1}{2}K_y}{J} \right)^2 \right] . \qquad (10)$$

We note that for $J/t > 11.008$ the ground state of a system with free holes becomes unstable due to the existence of bound states even at $K = 0$. Therefore the free hole wave functions will no longer be a valid starting point for doing perturbation theory.

The moving holes should also affect magnetic states of the system. We will explore here the possibility that a hole and a magnon form a bound state. The Hamiltonian H will be diagonalized in a subspace with one hole and one spin deviation placed on a lattice with all up spins.

An eigenstate

$$\phi_K = \sum_q f_K(q) c_{k_1,1} S_{k_2}^- |\mathrm{FM}\rangle \qquad (11)$$

of H can be constructed in this subspace. We obtain the eigenvalue equation

$$[E-E_0-t(\tfrac{1}{2}K+q')+J(\tfrac{1}{2}K-q')]f_K(q)$$
$$=\frac{1}{N}\sum_q [t(q+q')-J(q-q')+J(\tfrac{1}{2}K-q')$$
$$-t(\tfrac{1}{2}K+q')]f_K(q)\,, \qquad (12)$$

where $E_0=-NJz/4+3Jz/2$. Eq. (12) yields a band of states for each K with E ranging from the minimum to the maximum value of $\mathscr{E}_K(q)$ where

$$\mathscr{E}_K(q)=E_0+t(\tfrac{1}{2}K+q)-J(\tfrac{1}{2}K-q)\,. \qquad (13)$$

The general gap equation for d dimensions is more complicated than in the two-hole case and will be discussed in detail in a future publication. Here the bound state energy will be presented for selected values of K. For the one-dimensional lattice at $K=0$ we obtain $\epsilon=a^2[1+(b/a)^2]/2b$ for all $J>0$ where $a=2(t-J)$ and $b=2(t+J)$. This indicates a bound state with a maximum binding energy at $J=t$. The solution merges with the bottom of the band at $K=\pm\pi$ so that a bound state exists across the entire zone.

For the square lattice at $K=0$ the bound state energy is a solution of the equation

$$1-\frac{b}{2\pi}\int_{-\pi}^{\pi} \mathrm{d}q_x \frac{\sin^2 q_x}{[(\epsilon+a\cos q_x)^2-c^2]^{1/2}}=0\,, \qquad (14)$$

where $c=a$. Eq. (14) gives solutions only for a finite interval of J/t: $0.466942 \leqslant J/t \leqslant 2.14159$. This is in marked contrast to the one-dimensional case. Fig. 2 shows ϵ as a function of J/t for $K=0$ and compares the solution with the bottom of the free hole-magnon band.

At $K_x=K_y=\pi$ the bound state solution merges with the bottom of the band. The energy for $K_x=\pi$ and $K_y=0$ is a solution of eq. (14) with $c=b$. A bound state can be obtained for $0.710952 \leqslant J/t \leqslant 1.40656$. Fig. 2 also shows the bound state energy for this case.

The ferromagnetic model considered here illustrates some concepts in a simple way: the existence of two-hole bound states for particular values of total pair momentum depends on the exchange being large enough; the pairs can be locally bound in position space; the existence of mobile holes can affect the magnetic excitations. Other properties such as Bose condensation of pairs for finite concentration of holes and the existence of bound states involving more than two holes would be interesting to investigate in this simple model.

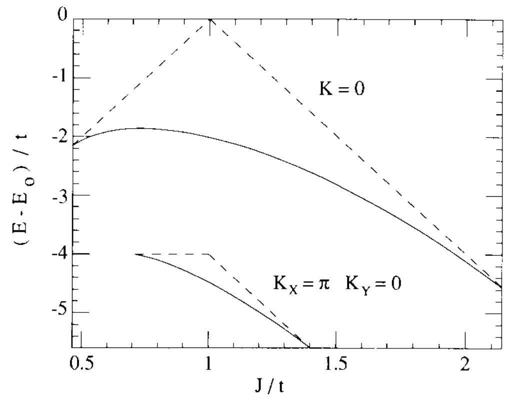

Fig. 2. The hole–magnon bound state energy as a function of J/t. Square lattice case. The top part is for $K=(0,0)$, and the bottom part is for $K=(\pi,0)$. The dashed lines are the bottom of the free hole–magnon band.

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