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Bound and antibound states of holes in a coupled-chain model

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Abstract. The binding of two holes in a coupled-chain model described by the t–t'–J Hamiltonian is studied. Using the Bethe *Ansatz* analysis, it is shown that two holes form antibound states in a triplet spin state. This result can be extended to the case of more than two holes. The eigenvalue problem when the two holes are in a singlet state is solved exactly and one finds that the two holes can bind for all values of J. In this case, antibound states are found for sufficiently large values of J.

1. Introduction

Recently, much work has been done on strongly correlated systems because of their relevance to high-T_c superconductivity. An appropriate model for studying the effects of strong correlation is the t–J model. The model describes a system of electrons on a lattice with the 'hard-core' constraint that no two electrons can occupy the same site. The electrons can hop from one site to another provided that the second site is empty, i.e. occupied by a hole. The motion of electrons, or equivalently holes, takes place in a background of antiferromagnetically interacting spins. The model describes charge transport, through the motion of holes, in the copper oxide planes of the high-T_c cuprate systems. In the superconducting phase, charge transport occurs through the motion of pairs of holes. Thus, the question of whether two holes can bind in the t–J model is of great interest. There have been several studies [1–9] of the interaction of holes in the t–J model but the results have been far from conclusive. The studies have been mainly based on approximate solutions and exact numerical diagonalization for small systems. The latter studies give evidence for hole binding in certain parameter regimes of the t–J model. Recently, we have proposed a coupled-chain (CC) model described by the t–t'–J Hamiltonian and derived several exact results [10, 11] for the dynamics of a single hole. In this paper, we consider the case of two holes and more than two holes in the CC model. By using the well known Bethe *Ansatz* (BA) technique, we derive the dispersion relations for the antibound states of r holes ($r \geqslant 2$). By using an exact analytical method, we also show that two holes can form a bound state. The same method yields solutions for antibound states of two holes.

The CC model consists of two chains, each described by a t–J model, coupled by t'–J' interactions between them (figure 1). The model is described by the t–J Hamiltonian:

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \mathrm{HC} + \sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j = H_t + H_{t'} + H_J. \tag{1}$$

The constraint that no site can be doubly occupied is implied in the model. The hopping integral t_{ij} has the value t for nearest-neighbour (NN) hopping within a chain and also for diagonal transfer between chains (solid lines in figure 1). The corresponding spin–spin

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interactions J_{ij} are of strength J. The spins have magnitude $\frac{1}{2}$. The hopping integral across vertical links (broken lines) connecting two chains has the strength t'. The corresponding spin–spin interaction strength J_{ij} is assumed to be $2J$ although the exact results derived below hold true also for other interaction strengths. In the following, we assume t and t' to be positive. In the half-filled limit, i.e. in the absence of holes, the t–t'–J Hamiltonian in (1) reduces to H_J. The exact ground state Ψ_g of H_J consists of singlets along the vertical bonds with energy $E_g = -(3J/2)N$, where $2N$ is the number of sites in the system. For $J' > 2J$, the exact ground state is still the same, however, for $J' < 2J$; the state, although an exact eigenstate, may not be the ground state. The exact eigenstates of H_J have a simple structure. In all these eigenstates the spin configuration of each vertical link is any one of four types: a singlet with $S = 0$, $S_z = 0$ or a triplet with $S = 1$ and $S_z = +1, 0$ and -1, respectively. The reason for this simple structure is, as can be easily verified, that the total spin of each vertical link commutes with H_J, i.e. is a conserved quantity. This special property of the CC model makes exact calculations possible.

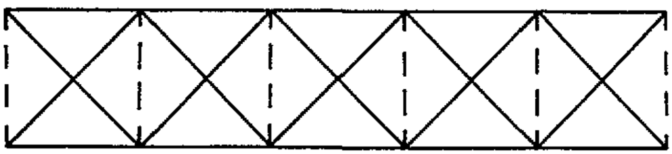

Figure 1. The coupled two-chain model described by the t–t'–J Hamiltonian (1).

2. Bound and antibound states of holes

We now consider the case of two holes in the CC model. The holes are introduced in the ground state of the model in two different vertical links so that the dimers along these links are broken. The two free spins from the broken dimers combine to make the total spin of the system either $S = 1$, i.e. a triplet, or $S = 0$, i.e. a singlet. We first consider the case $S = 1$ and $S_z = +1$. The states $S = 1$, $S_z = 0, -1$ are degenerate with the $S_z = +1$ state. Let the holes by located in the vertical links numbered m_1 and m_2 respectively, where $m_1 < m_2$. The eigenfunction Ψ of the t–t'–J Hamiltonian is given by

$$\Psi = \sum_{m_1<m_2} a(m_1, m_2)\Psi(m_1, m_2) \qquad (2)$$

where the basis function $\Psi(m_1, m_2)$ is given by

$$\Psi(m_1, m_2) = \tfrac{1}{2}\Big[\cdots \underset{m_1-1}{\Big|} \begin{pmatrix}\uparrow & + & \circ \\ \circ & {}_{m_1} & \uparrow\end{pmatrix} \underset{m_1+1}{\Big|} \cdots \Big| \begin{pmatrix}\uparrow & + & \circ \\ \circ & {}_{m_2} & \uparrow\end{pmatrix} \Big| \cdots\Big]. \qquad (3)$$

The solid vertical lines represent singlets, the arrows stand for up-spins and the open circles denote holes. We have to solve the eigenvalue problem $H\Psi = E\Psi$, where E is the energy eigenvalue of the system. A hole can hop either to a NN site in the vertical and horizontal directions or to NN diagonal positions. The fermionic nature of the background spins is taken into account during the hopping of the hole. In general, when a hole hops, it scrambles up the spin arrangement in its neighbourhood and the eigenvalue problem becomes difficult to solve. In the present case, when $H_t + H_{t'}$ in equation (1) operates on the state $\Psi(m_1 m_2)$ in equation (3), there is a neat cancellation of terms in which spin configurations other than those in equation (3) occur in the vicinity of the hole. As a result, the hole simply translates to a NN position with the spin background unchanged. The eigenvalue equation when $m_2 \neq m_1 + 1$, i.e. when the holes do not occupy NN links, is given by

$$Ea(m_1, m_2) = (-2t' + 3J)a(m_1, m_2) + t[a(m_1 - 1, m_2) + a(m_1 + 1, m_2) + a(m_1, m_2 - 1) + a(m_1, m_2 + 1)]. \tag{4}$$

The energy E has been measured with respect to the ground-state energy in the undoped state. The amplitude $a(m_1, m_2)$ is given by the BA [12]

$$a(m_1, m_2) = \exp[\mathrm{i}(k_1 m_1 + k_2 m_2 + \Phi/2)] + \exp[\mathrm{i}(k_2 m_1 + k_1 m_2 - \Phi/2)]. \tag{5}$$

The wavevectors of the two holes are denoted by k_1 and k_2 and Φ is analogous to a 'phase shift'. Since the two holes cannot occupy a single site, the holes in general should be treated as spinless fermions. In 1D the holes can also be treated as hard-core bosons. The statistics of the holes are irrelevant in this case since a pair of them cannot be interchanged owing to the constraint of no double occupancy at every site. In dimensions greater than 1, different statistics will give rise to different results [13]. In the present case, although the model has a strip geometry with the possibility of exchange of holes, the model basically reduces to a 1D problem as will be clear after the derivation of equation (7). Thus the choice of statistics does not matter. We have treated the holes as bosons (see equations (3) and (5)) in the present problem. The hard-core constraint is built into the model. One can verify that on assigning fermionic statistics to the holes (antisymmetrize $a(m_1, m_2)$ in equation (5) rather than symmetrize) the final results do not change. The eigenvalue equation (4) is satisfied by the *Ansatz* (5) with the eigenvalue

$$E = (-t' + 3J/2 + 2t\cos k_1) + (-t' + 3J/2 + 2t\cos k_2). \tag{6}$$

The eigenvalue equation when the holes occupy NN links, i.e. $m_2 = m_1 + 1$, is

$$Ea(m_1, m_1 + 1) = (-2t' + 13J/4)a(m_1, m_1 + 1) + t[a(m_1 - 1, m_1 + 1) + a(m_1, m_1 + 2)]. \tag{7}$$

The states $\Psi(m_1, m_2)$ form a closed subspace of states in which the Hamiltonian operates so that Ψ given by equation (2) is an eigenfunction. When H_t operates on the state $\Psi(m_1, m_1 + 1)$, there is an exact cancellation of terms in which two holes occupy the same vertical link. This makes the application of the BA formalism possible; the two-chain problem basically reduces to a 1D problem. The subspace of states defining the present eigenvalue problem ($S = 1$, $S_z = +1$) does not contain the state in which two holes occupy the same vertical link. This state has to occur as an intermediate state in the physical exchange of two holes, but the absence of the state in the subspace of states rules out the possibility of exchange of holes as in the case of 1D. By comparing equations (4) and (7), one finds that the exchange interaction energy increases when the holes occupy NN links. This unfavourable energy increase is due to the triplet configuration of the free spins. Equation (7) is also satisfied by the BA (equation (5)) provided that

$$-(J/4)a(m_1, m_1 + 1) + t[a(m_1 + 1, m_1 + 1) + a(m_1, m_1)] = 0 \tag{8}$$

from which, using the BA form for the amplitudes, one derives the condition

$$\cot\left(\frac{\Phi}{2}\right) = \frac{\sin(k_1/2 - k_2/2)}{(2/\alpha)\cos(k_1/2 + k_2/2) - \cos(k_1/2 - k_2/2)} \tag{9}$$

where $\alpha = J/4t$. Further, the periodic boundary condition gives $a(m_1, m_2) = a(m_2, m_1 + N)$ so that

$$\begin{aligned} &Nk_1 - \Phi = 2\Pi\lambda_1 \\ &Nk_2 + \Phi = 2\Pi\lambda_2 \\ &\lambda_1, \lambda_2 = 0, 1, 2, \ldots, N-1. \end{aligned} \tag{10}$$

The sum $k = k_1 + k_2$ is a constant of motion by translational symmetry. For real k_1, k_2 and $\Phi(-\Pi \leqslant \Phi \leqslant \Pi)$ and with the choice $(\lambda_2 - \lambda_1) \geqslant 2$, as in Bethe's solution [14], one gets ${}^{N-1}C_2$ solutions with the eigenvalues given by equation (6). This gives rise to a continuum of scattering states. The rest of the $N - 1$ solutions are obtained by assigning complex values to k_1 and k_2 (the total number of solutions including both real and complex values of k_1 and k_2 is ${}^{N}C_2$). Let

$$k_1 = u + \mathrm{i}v \qquad k_2 = u - \mathrm{i}v. \tag{11}$$

Then, from equation (9)

$$\cot\left(\frac{\Phi}{2}\right) = \frac{\mathrm{i}\sinh v}{(2/\alpha)\cos u - \cosh v}. \tag{12}$$

Now, from equation (10),

$$N(k_1 - k_2) = 2N\mathrm{i}v = 2\Pi(\lambda_1 - \lambda_2) + 2\Phi. \tag{13}$$

Put $\Phi = \Psi + \mathrm{i}\kappa$ so that

$$\Psi = \Pi(\lambda_2 - \lambda_1) \qquad \kappa = Nv. \tag{14}$$

When v is non-zero, κ is very large for large N, so that $\cot(\Phi/2) \simeq -\mathrm{i}$. Then, from equation (12), one derives the condition

$$\exp(-v) = (2/\alpha)\cos u. \tag{15}$$

From equation (6), using equations (11) and (15), we get

$$\begin{aligned} &E_b(2) = (-2t' + 3J) + (4t/\alpha)\cos^2 u + \alpha t \\ &k = 2u(\text{modulo } 2\Pi). \end{aligned} \tag{16}$$

For real values of k_1 and k_2, equation (6) gives the energy of a continuum of scattering states. The energy $E_b(2)$ lies above the upper boundary of the energy continuum and hence corresponds to an antibound state of two holes.

We now point out that equation (9) for the phase shift is identical with that for an anisotropic Heisenberg Hamiltonian [15] with $2/\alpha$ playing the role of the anisotropy parameter Δ. An extensive literature exists [13, 15, 16] on the eigenvalue problem corresponding to $\Delta \geqslant 1$, $\Delta \leqslant -1$ and $-1 < \Delta < 1$ for both real and complex values of the momentum wavevectors and for the number of elementary excitations equal to 2 or more. Some of the results of the Heisenberg model are expected to be true for the t–t'–J model also. We give just one example to illustrate this. For $\alpha = 2$, i.e. $J = 8t$, the situation for r holes is described by the same kind of equations as in the case of r magnons in an isotropic, $S = \frac{1}{2}$, 1D ferromagnet.

Let us consider r holes. Let the holes be located in the vertical links numbered $m_1, m_2, \ldots, m_r$, respectively. The eigenfunction Ψ is now a linear combination of the ${}^N C_r$ functions $\Psi(m_1, \ldots, m_r)$:

$$\Psi = \sum_{\{m\}} a(m_1, m_2, \ldots, m_r)\Psi(m_1, m_2, \ldots, m_r). \tag{17}$$

Each of the numbers $m_1, \ldots, m_r$ runs over the possible values 1 to N subject to the condition $m_1 < m_2 < \ldots < m_r$. This gives ${}^N C_r$ states. The general BA for the r-hole state can be written as

$$a(m_1, m_2, \ldots, m_r) = \sum_P \exp\left[i\left(\sum_{l=1} k_{Pl} m_l + \tfrac{1}{2}\sum_{l<n}^{1,r} \phi_{Pl,Pn}\right)\right]. \tag{18}$$

P is any permutation of r numbers $1, 2, \ldots, r$. Pl is the number obtained by operating P on l. Equation (5) is a special case of equation (18) for $r = 2$. The same analysis as in the case of two holes can be applied. The energy eigenvalue of Ψ is given by

$$E(r) = \sum_{i=1}^{r}\left(-t' + \frac{3J}{2} + 2t\cos k_i\right). \tag{19}$$

The k_i-values are determined as before by applying the periodic boundary condition which leads to the r equations

$$Nk_i = 2\Pi\lambda_i + \sum_i \phi_{ij}. \tag{20}$$

The λ_i are r integers and the ϕ_{ij} are the phase shifts. These are determined by equations identical with equation (9), one such equation for each pair of indices. These equations are $r(r-1)/2$ in number since $\phi_{ij} = -\phi_{ji}$. Together with equation (20), there are $r(r+1)/2$ equations for as many unknowns. We shall not consider the various solutions in detail but consider a particular type of solution in which r holes move together as a block occupying r NN vertical links. Again, as in the case of $r = 2$, the possibility that two holes occupy the same vertical link does not occur. The wavevectors k_i for the case considered are complex. One assumes that $r \ll N$ and only the phases $\phi_{12}, \phi_{23}, \ldots, \phi_{r-1,r}$ are large [14, 17]. Without any loss of generality we may put $\phi_{l-1,l} > 0$. Then, from equation (20)

$$\begin{aligned}
&\operatorname{Im}\phi_{12} = N\operatorname{Im}k_1 = Nx_1\\
&\operatorname{Im}(\phi_{23} - \phi_{12}) = N\operatorname{Im}k_2 = Nx_2\\
&\vdots\\
&-\operatorname{Im}(\phi_{r-1,r}) = N\operatorname{Im}f_r = Nx_r.
\end{aligned} \tag{21}$$

Note that $\sum_{i=1}^{r} \geqslant 0$ for all r. For $\alpha = 2$, i.e. $J = 8t$, equation (9) for a phase shift reduces to

$$2\cot(\phi_{ln}/2) = \cot(k_l/2) - \cot(k_n/2). \tag{22}$$

Making use of equation (21), we get, to an accuracy of $\exp(-N)$,

$$2\cot(\phi_{ln}/2) \simeq -2\mathrm{i}. \tag{23}$$

Thus

$$\begin{aligned} -2\mathrm{i} &= \cot(k_1/2) - \cot(k_2/2) \\ -2\mathrm{i} &= \cot(k_2/2) - \cot(k_3/2) \end{aligned} \tag{24}$$

etc. Hence,

$$\cot(k_l/2) = 2\mathrm{i} + \cot(k_{l-1}/2). \tag{25}$$

The solution is

$$\cot(k_l/2) = 2\mathrm{i}l + C. \tag{26}$$

To determine C, consider the total momentum K of the r-hole system

$$K = \sum_{i=1}^{r} k_i = \frac{2\Pi}{N} \sum_{i=1}^{r} \lambda_i. \tag{27}$$

The wavefunction Ψ is multiplied by $\exp(\mathrm{i}k)$ under a shift $m_i \to m_i + 1$ and the energy levels are characterized by K; we obtain

$$C = \frac{2ri - \mathrm{i}[\exp(\mathrm{i}k) - 1]}{\exp(\mathrm{i}k) - 1}$$

$$\exp(\mathrm{i}k_l) = \frac{r + l[\exp(\mathrm{i}k) - 1]}{r + (l-1)[\exp(\mathrm{i}k) - 1]}.$$

The energy eigenvalue is obtained from equation (19) as

$$E_b(r) = r(2t - t' + 3J/2) - (2t/r)(1 - \cos K). \tag{28}$$

This energy is greater than the energy eigenvalues corresponding to the continuum of scattering states for real k_i obtained from equation (19). The eigenstate is thus an antibound state of r holes. The dispersion relation of the r-magnon bound state in the case of the isotropic $S = \frac{1}{2}$, 1D ferromagnet is

$$\varepsilon^{(r)} = \frac{1}{r}(1 - \cos K). \tag{29}$$

The similarity of the dispersion relations (28) and (29) is a result of the fact that the BA equations for the phase shifts are identical in both the cases.

We next consider the case when the free spins from the broken dimers (after the introduction of two holes in the ground state) form a singlet with total spin $S = 0$. In this case, the reduction of the strip problem to a 1D situation is not possible as the subspace of states now includes the state in which two holes occupy the same vertical link, leading to the possibility of exchange of holes. Now the holes are treated as spinless fermions in contrast with the previous case where the statistics do not matter. Define the wavefunctions

$$\phi(m_1, m_2) = \frac{1}{2\sqrt{2}}\Big[\Big|\cdots\Big|\begin{pmatrix}\uparrow & \circ\\ \circ & \uparrow\end{pmatrix}_{m_1}^{+}\Big|\cdots\begin{pmatrix}\downarrow & \circ\\ \circ & \downarrow\end{pmatrix}_{m_2}^{+}\Big|\cdots\Big|$$
$$-\Big|\cdots\Big|\begin{pmatrix}\downarrow & \circ\\ \circ & \downarrow\end{pmatrix}^{+}\Big|\cdots\begin{pmatrix}\uparrow & \circ\\ \circ & \uparrow\end{pmatrix}^{+}\Big|\cdots\Big|\Big]$$

and

$$\phi(m, m) = \Big|\Big|\cdots \underset{m}{\overset{\circ}{\circ}} \cdots\Big|\Big|.$$

Define also the Fourier transforms

$$\phi(m, m+r) = \frac{1}{N^{1/2}}\sum_k \exp\left[ik\left(m+\frac{r}{2}\right)\right]\phi_k(r) \qquad \text{for } 0 \leqslant r \leqslant \frac{N}{2} - 1$$

and

$$\phi\left(m, m+\frac{N}{2}\right) = \left(\frac{2}{N}\right)^{1/2}\sum_k \exp\left[ik\left(m+\frac{N}{2}\right)\right]\phi_k\left(\frac{N}{2}\right). \tag{30}$$

The two holes are separated by a distance r. From the periodic boundary condition and for $r \neq N/2$, the allowed values of k are $k = 2\Pi\lambda/N$, with $\lambda = 0, 1, 2, \ldots, N-1$. For $r = N/2$, the allowed values of k are odd multiples of $2\Pi/N$. An eigenfunction in the momentum space is given by

$$\psi_e^k = \sum_{r=0}^{N/2-1} a_k(r)\phi_k(r) \tag{31}$$

where k is an even multiple of $2\Pi/N$. When k is an odd multiple of $2\Pi/N$, the eigenfunction is ψ_o^k and the sum in equation (31) runs from 0 to $N/2$. The exact eigenvalue equations for the amplitudes are as follows.

(i) When k is an odd multiple of $2\Pi/N$,

$$Ea_k(0) = \tfrac{3}{2}Ja_k(0) - 2Ta_k(1) \tag{32a}$$

$$Ea_k(1) = -2Ta_k(0) + (-2t' + \tfrac{9}{4}J)a_k(1) + Ta_k(2) \tag{32b}$$

$$Ea_k(2) = (-2t' + 3J)a_k(2) + T[a_k(1) + a_k(3)]$$

$$\vdots \tag{32c}$$

$$Ea_k(N/2-1) = (-2t' + 3J)a_k(N/2-1) + T[a_k(N/2-2) + \sqrt{2}a_k(N/2)]$$

$$Ea_k(N/2) = (-2t' + 3J)a_k(N/2) + T\sqrt{2}a_k(N/2-1)$$

where $T = 2t\cos(k/2)$. It is clear from the eigenvalue equations that the exchange energy is the smallest when the holes occupy the same link and smaller when the holes occupy NN vertical links than when they are farther apart. This is in contrast with the situation when the holes are in a triplet spin state. Thus the singlet spin state is favourable for the formation of hole bound states. Equations (32) have the solutions

$$a_k(n) = \begin{cases} \cos[q(N/2-n)] \\ (1/\sqrt{2})\cos[q(N/2-n)] \end{cases} \quad \text{for} \quad \begin{cases} 1 \leqslant n < N/2 \\ n = N/2 \end{cases} \tag{33}$$

where q is the relative momentum wavevector ($0 \leqslant q \leqslant \Pi$). Defining $\epsilon = E - 3J + 2t'$, and from equation (32c) one derives the condition

$$\epsilon = 2T\cos q. \tag{34}$$

From equations (32a) and (32b), one gets

$$\epsilon + \frac{3J}{4} = \frac{4T^2}{\epsilon + \frac{3}{2}J - 2t'} + \frac{T\cos[q(N/2-2)]}{\cos[q(N/2-1)]}. \tag{35}$$

The eigenvalues ϵ are obtained from the simultaneous solution of equations (34) and (35). For real values of q, the energies correspond to free hole states. Energies for bound and antibound states are obtained by making q complex. When T is positive, making the changes $q \to \mathrm{i}q$ and $q \to \Pi + \mathrm{i}q$, one gets the energies for antibound and bound states, respectively. When T is negative, the reverse is true. The bound-state energies for different values of q are lower than the lowest of energies for real values of q. The antibound-state energies lie higher than the highest of energies for real values of q.

(ii) When k is an even multiple of $2\Pi/N$, the same eigenvalue equations as in equations (32) hold true except that $a_k(N/2) = 0$. The amplitudes now have the form

$$a_k(n) = \sin[q(N/2-n)] \qquad \text{for } 1 \leqslant n \leqslant N/2 - 1. \tag{36}$$

The energy eigenvalues are obtained by simultaneously solving the equations

$$\epsilon = 2T\cos q$$

and

$$\epsilon + \frac{3J}{4} = \frac{4T^2}{\epsilon + 3J/2 - 2t'} + \frac{T\sin[q(N/2-2)]}{\sin[q(N/2-1)]}. \tag{37}$$

The energies for real values of q correspond to free hole states. The energies for bound and antibound states are obtained by making q complex in the same manner as in the case when k is an odd multiple of $2\Pi/N$. For both cases, antibound states do not exist for very small values of J. On the other hand, bound states exist for all values of J including $J = 0$. The greater the value of J, the smaller is the spread of the bound-state wavefunction. Recently, Tsunetsugu *et al* [18] have considered doped t–J ladders (the t–J ladder is similar to our CC model but with the frustrating diagonal interaction and the hopping terms missing). They have carried out exact diagonalization studies of finite-sized ladders using the Lanczos method. They find evidence of the binding of two holes in the ground state.

To conclude, we have derived some exact results for the doped CC model. The effects of strong correlation and quantum fluctuation have been taken into account in an exact manner. The results derived show that two holes can bind in a singlet spin state but not in a triplet spin state. In the triplet spin state, r holes ($r \geqslant 2$) can form antibound states. We have not been able to extend our exact analysis for bound states to the case of more than two holes.

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