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LETTER TO THE EDITOR

Single-hole dynamics in a coupled-chain model

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**Abstract.** The single-hole dynamics in a coupled-chain model described by the  $t-t'-J$  model is studied. The excitation spectrum is obtained exactly and analytically and shows a structure consisting of bound, antibound and extended states. Based on the exact results obtained, the possibility of a localization-to-delocalization transition for the hole is conjectured.

In high- $T_c$  cuprate superconductors, charge transport in the copper oxide plane occurs through the motion of holes in a background of antiferromagnetically interacting spins. In this context, several studies [1–5] have been carried out on the dynamics of a single hole in a spin background. A single hole, as soon as it starts moving, scrambles the arrangement of spins in the ground state. The calculation of its dynamical properties is a non-trivial many-body problem due to a competition between two processes: the lowering of the kinetic energy of the hole by delocalization and the minimization of the antiferromagnetic exchange interaction energy of the background spins. The issues of interest are whether a coherent propagation of the hole in a Bloch type of state is possible, the effect of spin excitations on the hole dynamics, the nature of the spin configuration in the ground state etc. The model Hamiltonian used for such studies is the well known  $t-J$  model. Recently, we have derived some exact results for single-hole dynamics in a coupled-chain model described by a  $t-t'-J$  Hamiltonian [6]. Some of the conclusions arrived at in our paper were based on numerical solution of the exact eigenvalue equations for finite-sized systems. In this letter, we show that the particular eigenvalue problem can be solved exactly and analytically irrespective of the system size. The results obtained correspond to extended hole states as well as bound and antibound states of the hole with a localized triplet excitation. There is also an indication that a localization-to-delocalization transition occurs for the hole.



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

Our coupled-chain 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

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

The constraint that no site can be doubly occupied is implied in the model. The hopping integral  $t_{ij}$  has value  $t$  for nearest-neighbour hopping within a chain and also for diagonal transfer between chains (solid lines in figure 1). The corresponding spin-spin interactions,  $J_{ij}$ , are of strength  $J$ . The spins have magnitude  $\frac{1}{2}$ . The hopping integral across vertical links (dotted lines) connecting two chains has strength  $t'$ . The corresponding spin-spin interaction strength  $J_{ij}$  is assumed to be  $2J$  though 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  $\Psi_g$  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, though an exact eigenstate, may not be the ground state. We now introduce a single hole into the system. Let  $\Psi(m)$  denote a spin configuration when the single hole is located in the  $m$ th column of the coupled-chain model.

$$\Psi(m) = (1/2)^{1/2} [\Psi_m(p) + \Psi_m(q)]. \quad (2)$$

In  $\Psi_m(p)$  and  $\Psi_m(q)$ , the hole is located in the top and bottom rows, respectively, on the  $m$ th column. The other site in the  $m$ th column is occupied by an up spin. The spin configurations on all the other vertical links are the same as in  $\Psi_g$ , namely, singlets. In our earlier paper we have shown that the wave function

$$\Psi = (1/N)^{1/2} \sum_{m=1}^N e^{ikm} \Psi(m) \quad (3)$$

is an exact eigenfunction of the total  $t-J$  Hamiltonian  $H$  with eigenvalue  $E = 2t \cos(k) - t' - 3J/2(N-1)$ . The periodic boundary condition has been assumed to solve the eigenvalue problem. Let  $\Psi'(m)$  be a single-hole state defined as

$$\Psi'(m) = (1/2)^{1/2} [\Psi_m(q) - \Psi_m(p)]. \quad (4)$$

When  $H$ , in (1) operates on  $\Psi'(m)$ , the hole accompanied by a free spin  $\frac{1}{2}$  moves one lattice constant, leaving behind a triplet excitation. The states generated are  $\kappa(m, m \pm 1)$  given by

$$\kappa(m, m \pm 1) = (1/12)^{1/2} [\kappa_{m,m \pm 1}(p) + \kappa_{m,m \pm 1}(q)]. \quad (5)$$

The first index  $m$  in  $\kappa(m, m + 1)$  denotes the location of the triplet excitation,  $m$  being the column number. The second index in  $\kappa$  denotes the location of the column in which the hole is present. A pictorial representation of the state  $\kappa_{m,m+1}(p)$  is given in figure 2. The dashed line denotes the triplet ( $\alpha\beta + \beta\alpha$ ) where  $\alpha$  and  $\beta$  denote up and down spins respectively. The state  $\kappa_{m,m+1}(q)$  is obtained from  $\kappa_{m,m+1}(p)$  by interchanging the hole and spin positions in the  $m$ th column. The exact eigenvalue equations can be written as

$$H\Psi'(m) = (3J/2 + t')\Psi'(m) - 3^{1/2}t[\kappa(m, m + 1) + \kappa(m, m - 1)] \quad (6a)$$

$$H\kappa(m, m \pm 1) = (5J/2 - t')\kappa(m, m \pm 1) + t\kappa(m, m \pm 2) - 3^{1/2}t\Psi'(m) \quad (6b)$$

$$H\kappa(m, m \pm r) = (7J/2 - t')\kappa(m, m \pm r) + t[\kappa(m, m \pm r \pm 1) + \kappa(m, m \pm r + 1)]. \quad (6c)$$

In the earlier paper, a numerical solution of equations (6a-c) was given for finite-sized systems and only the lowest-energy state was discussed. We now show that the eigenvalue spectrum described by the eigenvalue equations can be derived exactly and analytically for any value of  $N$ . The spectrum consists of both bound and extended states. An eigenfunction has the form

$$\Psi_1 = a_0 \Psi'(m) + \sum_{n=1}^{N-1} a_n \kappa(m, m+n). \quad (7)$$

The eigenfunction is either symmetric or antisymmetric with respect to reflection about the  $m$ th column in which the triplet excitation is located. For an asymmetric state, considering  $N$  to be even, both the coefficients  $a_0$  and  $a_{n/2}$  are zero.

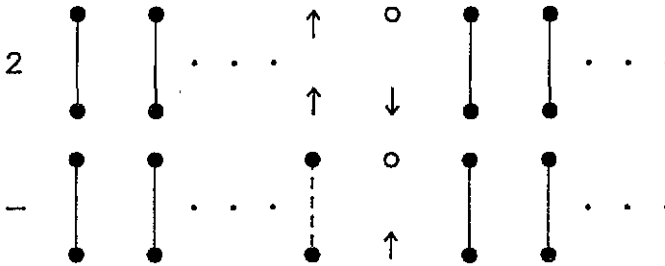


Figure 2. A pictorial representation of the wave function  $\kappa_{m,m+1}(p)$  defined in (5). The solid lines denote singlets and the dashed line denotes the triplet ( $\alpha\beta + \beta\alpha$ ) with  $S^z = 0$  located in the  $m$ th column. The empty circle denotes the hole located in the  $(m+1)$ th column and the vertical arrow represents a free spin  $\frac{1}{2}$ .

We first consider the Nagaoka limit  $J = 0$ . In this case the eigenvalue equations (6a-c) are similar to those for a single hopping electron in a 1D chain of atoms with the atom number 'zero' being an impurity atom. The other atoms are located at positions 1, 2, 3, ... and  $-1, -2, -3, \dots$ . The electron can hop from one atom to its nearest neighbours with amplitude  $t$ . The site energy of the impurity atom is different from that of the other atoms. The problem has been extensively discussed in the *Feynman Lectures*, vol III [7] and provides physical insight for our eigenvalue problem. In our case, the localized triplet excitation is the 'impurity' atom, the hole accompanied by a free spin- $\frac{1}{2}$  constitutes the propagating object and the singlets along the vertical links are the 'other atoms' of the lattice. In terms of the coefficients  $a_0, a_n$  (the coefficients  $a_{N-1}, a_{N-2}, \dots, a_{N-(N/2-1)}$  are redesignated as  $a_{-1}, a_{-2}, \dots, a_{-(N/2-1)}$  with  $a_{-N/2} = a_{N/2}$ ) the eigenvalue equations (6a-c) reduce to the equations

$$\begin{aligned} E a_2 &= (7J/2 - t') a_2 + t [a_3 + a_1] \\ E a_1 &= (5J/2 - t') a_1 - 3^{1/2} t a_0 + t a_2 \\ E a_0 &= (3J/2 + t') a_0 - 3^{1/2} t [a_1 + a_{-1}] \\ E a_{-1} &= (5J/2 - t') a_{-1} - 3^{1/2} t a_0 + t a_{-2} \\ E a_{-2} &= (7J/2 - t') a_{-2} + t [a_{-1} + a_{-3}]. \end{aligned} \quad (8)$$

For  $J = 0$  we illustrate the 'impurity atom' analogy by deriving the eigenfunctions and eigenvalues for the antisymmetric case. The triplet excitation located at the zeroth position acts as a scatterer, so an incident wave coming from, say, the left may be scattered backwards. We can choose the following forms for the coefficients  $a_n$ :

$$\begin{aligned} a_n(\text{for } n < 0) &= e^{ikx_n} + \beta e^{-ikx_n} \\ a_n(\text{for } n > 0) &= \gamma e^{ikx_n}. \end{aligned} \quad (9)$$

The wave is incident from the left and  $\beta$ ,  $\gamma$  are the respective amplitudes with which the wave is scattered backwards or is transmitted in the forward direction. The equations involving the coefficients  $a_n$  with  $n \leq -1$  and  $n \geq 1$  are all satisfied by (9) with the condition that  $k$  is related to  $E$  by (the lattice spacing is assumed to be unity)

$$E = -t' + 2t \cos(k). \quad (10)$$

By using the formulae for  $a_{-1}$  and  $a_{+1}$  from (9), the three middle equations in (8) allow us to solve for  $a_0$  and also for the two coefficients  $\beta$  and  $\gamma$ . One finds that

$$-3^{1/2}a_0 = 1 + \beta = \gamma.$$

For antisymmetric eigenfunctions,  $a_0 = 0$ , so  $\beta = -1$ , i.e.,  $\gamma = 0$ . Thus the 'impurity atom' gives rise to perfect backward scattering and hence zero transmission. The coefficient  $a_n$  is given by

$$a_n \sim \sin(kx_n)(x_n = n).$$

For antisymmetric solution  $a_{N/2} = 0$ , i.e.,  $k = 2m\pi/N$  where  $m$  is an integer. The energy is given by (10). The 'impurity' analogy can further be extended to the case of symmetric solutions as well as bound states. We, however, consider the general case  $J \neq 0$  when we have impurities at sites 0, 1 and  $-1$ . It is more convenient now to solve the eigenvalue problem directly. In the following, we quote the final results for the eigenfunctions and eigenvalues. As mentioned before, the eigenfunctions are either symmetric or antisymmetric.

In the symmetric case

$$\begin{aligned} a_n &= \cos(k(N/2 - n)) \\ a_{-n} &= \cos(k(-N/2 + n)) = a_n. \end{aligned} \quad (11)$$

The eigenvalues  $\varepsilon (= E - 7J/2 + t')$  are obtained by simultaneously solving the equations

$$\varepsilon + J = 6t^2 / [\varepsilon + 2(J - t')] + t \cos(k(N/2 - 2)) / \cos(k(N/2 - 1)) \quad (12a)$$

and

$$\varepsilon = 2t \cos(k). \quad (12b)$$

One can easily verify that  $a_n$  given by (11) satisfies the eigenvalue equations for  $n \geq 2$  with eigenvalue given by (12b). The other eigenvalue condition (12a) is obtained from the eigenvalue equations for  $a_0$  and  $a_1$  with  $a_1$  and  $a_{-1}$  given by (11). The antibound state eigenfunctions and eigenvalues are obtained from (11) and (12) by making  $k$  imaginary.

The energy of the antibound state is greater than the highest energy of the extended states. The bound state eigenfunctions and eigenvalues are described by equations of types (11) and (12) with  $k$  made imaginary along with a real phase shift of  $\pi$ . The energy of the bound states is lower than the lowest energy of the extended states.

In the antisymmetric case

$$a_n = \sin(k(N/2 - n)). \quad (13)$$

The eigenvalues are obtained by simultaneously solving the equations

$$\varepsilon + J = t \sin(k(N/2 - 2)) / \sin(k(N/2 - 1)) \quad (14a)$$

$$\varepsilon = 2t \cos(k). \quad (14b)$$

There is no antibound state. The bound state eigenfunctions and eigenvalues are obtained from (13) and (14) by making the same changes as in the symmetric case. The total number of bound and antibound states is at most three. For values of  $J$  large compared to  $t$  and  $t'$ , all three states are bound states. In all parameter regimes a bound state always exists.

For small  $J/t$ , the bound state energy is lower than not only the extended state energies corresponding to the eigenvalue problem defined by (6a-c) but also the lowest energy of the band of coherent propagating states described by (3). For example, for  $J = 0$  and  $t' = t$ , the bound state has an energy  $-3.13959$  for  $N = 22$ . In this limit, the lowest energy corresponding to  $\Psi$  in (3) is  $-3$ . The lowest energy for a ferromagnetic arrangement of spins is also  $-3$ . We have not been able to find any extended state with energy lower than  $-3$ . The lowest possible theoretical bound, obtained from the spectrum of a single electron in an empty lattice, is  $-5$  but, due to the frustrated topology of the coupled-chain model, the lowest energy is expected to be above the theoretical bound. Since the bound state describes a localized wave function of the hole and appears to be the lowest-energy state for small  $J/t$  ( $0 \leq J/t < 0.05$ ), the ground state of the hole in this parameter regime is localized. For  $J/t > 0.05$ , there is a localization-to-delocalization transition when the extended state  $\Psi$  has lower energy. The localization of the hole in our case is caused by spin fluctuation (the triplet excitation). This has been exactly demonstrated in our model and suggests the possible mechanism of hole localization that occurs in cuprate superconductors for small dopant concentrations. The localization of the hole has also been shown to take place in the string picture developed by Shraiman and Siggia [8] for the conventional  $t - J$  model. A hole is introduced into a perfect Néel background of spins, which is the ground state of the Ising model. In this case, the hole distorts the spin background when it moves, creating a 'string' of overturned spins. At least for small  $J_z$ , it is possible to write an effective Hamiltonian for the hole that describes a non-relativistic particle in a linear confining potential. The eigenfunctions are Airy functions and are localized. If quantum fluctuations are included, the strings may be erased, giving rise to coherent quasiparticle propagation, and the autolocalization of the hole breaks down. In the case of our model, the effect of quantum fluctuations has been calculated exactly and one always finds the existence of a bound state. The existence of antibound states has also been exactly shown. Such states possibly give rise to the 'midgap' states of which the existence has been conjectured [9] for cuprate superconductors.

To sum up, for our coupled-chain model it is possible to treat the effects of strong correlation and quantum fluctuations, both key ingredients in the hole dynamics of cuprate systems, exactly. The exact analytical results for the excitation spectrum show interesting structure consisting of bound, antibound and extended states. The possibility of a

localization-to-delocalization transition has been conjectured. The problem of more than one hole in our coupled-chain model will be discussed elsewhere.

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