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Single hole doped strongly correlated ladder with a static impurity

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Abstract

We consider a strongly correlated ladder with diagonal hopping and exchange interactions described by a t–J type Hamiltonian. We study the dynamics of a single hole in this model in the presence of a static non-magnetic (or magnetic) impurity. In the case of a non-magnetic (NM) impurity we solve the problem analytically both in the triplet ($S = 1$) and singlet ($S = 0$) sectors. In the triplet sector the hole does not form any bound state with the impurity. However, in the singlet sector the hole forms bound states of different symmetries with increasing J/t values. Binding energies of those impurity–hole bound states are compared with the binding energy of a pair of holes in the absence of any impurity. In the case of magnetic impurity the analytical eigenvalue equations are solved for a large (50×2) lattice. In this case also, with increasing J/t values, impurity–hole bound states of different symmetries are obtained. Binding of the hole with the impurity is favoured for the case of a ferromagnetic (FM) impurity rather than the case of an antiferromagnetic (AFM) impurity. However, the binding energy is found to be maximum for the NM impurity. Comparison of binding energies and various impurity–hole correlation functions indicates a pair-breaking mechanism by the NM impurity.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Since the discovery of high-T_c superconductivity [1] the nature of the order parameter, the symmetry of the bound pair of holes, has been a hotly debated issue [2–10]. It is well known that in the case of conventional superconductors the introduction of magnetic impurities drastically suppresses the transition temperature T_c. Also theoretically it was predicted that magnetic impurities are strong pair breakers for conventional superconductors [11], while non-magnetic (NM) impurities have a pair-breaking effect only for higher orbital momentum states [12, 13] such as the d-wave pairing state. There have been extensive studies on the effect of doping the high-T_c cuprate systems with static magnetic and NM impurities in the last decade [14–17].

Experimental studies have shown that divalent Zn and Ni ions replace the Cu^{2+} ions in the CuO_2 planes and Zn (the NM impurity) is more effective than Ni (the magnetic impurity) in destroying superconductivity. It was suggested by some groups [14, 18, 19] that NM impurities do not simply act as vacancies but induce local magnetic moments in the CuO_2 planes, and the mechanism is still a magnetic pair-breaking mechanism. However, other experimental studies [20] have indicated that the estimated impurity moment-carrier exchange in Zn-doped YBCO is too small to account for the suppression of T_c by a magnetic pair-breaking mechanism satisfactorily. Moreover, the observed difference in behaviour of Zn- and Ni-doped systems could not be properly explained.

In order to explain all these features qualitatively, Poilblanc *et al* initiated numerical studies on a microscopic model, the t–J model. In a series of papers [21–23] they studied the effect of magnetic and NM impurities in very small clusters in two dimensions. Based upon their calculation of local density of states in the presence of an impurity (NM or magnetic), they discovered the existence of successive impurity–hole bound states of d-, s- and p-wave symmetries with increasing J/t values [21, 22]. From the analysis of impurity–hole binding energies and quasiparticle weight of a pair of holes [23] they concluded that an NM impurity has a stronger pair-breaking effect than a magnetic impurity. In this respect we also looked at the effect of magnetic and NM impurities on single hole dynamics in a t–J ladder model introduced by Bose and Gayen [24]. The existence of a bound hole pair and superconducting correlations in a t–J ladder model was first numerically shown by Dagotto *et al* in 1992 [25]. Later, Gayen and Bose [26, 27] proved analytically that the two holes form a bound propagating object in the ground state with a modified d-wave symmetry and the superconducting correlations exist in a t–J ladder model with diagonal interactions.

We divide the paper into the following sections. In section 2 we briefly introduce the model and recapitulate the exact results in the undoped limit as well as for single and two holes doped cases. In section 3 we derive analytical results for single hole dynamics in the presence of a static NM impurity. In section 4 we consider the hole in presence of a static magnetic impurity. In the last section (section 5) we conclude by speculating the implication of a pair-breaking mechanism by NM impurities in our model.

2. The model

The ladder model shown in figure 1 consists of two chains joined together by rungs and diagonals. The model is described by the following Hamiltonian:

$$H = -\sum_{\langle i,j\rangle\sigma} t_{ij}\left(C^{\dagger}_{i,\sigma}C_{j,\sigma} + \text{H.c.}\right) + \sum_{\langle i,j\rangle} J_{ij}\vec{S}_i \cdot \vec{S}_j. \tag{1}$$

The hopping integral along the solid (dashed) line is t (t'). The corresponding AFM exchange interaction is J (J'). The spins are of magnitude $\frac{1}{2}$ and a single occupancy constraint is strictly enforced in our model. We use periodic boundary conditions (PBCs). In the undoped limit the ground state consists of singlets along the vertical rungs when $2J = J'$ [24] with ground state energy $E_G = -\frac{3}{4}J'N$. Actually this is the ground state for $J' > 1.401\,484\,038\,97J$ [28]. In this paper we shall consider $J' = 2J$ for simplicity. However, the results are exact for all values of $J' > 1.401\,484\,038\,97J$. When the ladder is doped by a single hole, depending upon the value of J/t the ground state may consist of either the hole bound to an adjacent triplet excitation or the hole can coherently propagate through a sea of singlets [29]. When the ladder is doped with two holes, the ground state consists of a coherently propagating bound state of two holes of modified d-wave symmetry [26].

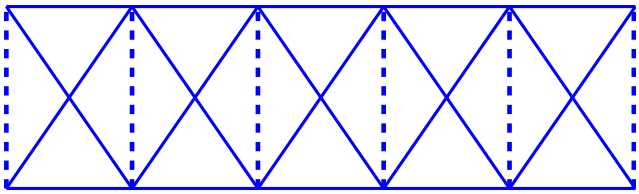

Figure 1. The ladder model with diagonal coupling.

In this context it is important to note that ladder models are not only of theoretical interest but also of experimental relevance [30]. Hiroi *et al* [31] synthesized the family of compounds $Sr_{n-1}Cu_{n+1}O_{2n}$ that can be described well by ladder geometry [32, 33]. Müller and Mikeska [34] discussed the elementary excitations in the compound $KCuCl_3$ which is described by an AFM ladder model with additional diagonal couplings. The compound $LaCuO_{2.5}$, formed by an array of weakly interacting ladders [35], could be doped with holes [36] on replacing La by Sr. Furthermore, the discovery of superconductivity in the doped ladder compound $Sr_{14-x}Ca_xCu_{24}O_{41}$ by Uehara *et al* [37] gave a tremendous impetus to theoretical and experimental research works on ladders.

3. Non-magnetic impurity

The NM impurity is modelled as an inert site located on the first rung of the ladder. PBCs are implied. The ground state consists of singlets along all the rungs except for the first rung, where there is a free spin-$\frac{1}{2}$ along with the impurity. For N rungs the ground state energy will be $E_g = -\frac{3J'}{4}(N-1)$. A single hole can be added in the singlet state by removing the free spin. It can be added to another rung thereby creating another free spin also. The two free spins in the first rung and in the other rung, where a hole had been added, can combine to form either a singlet ($S = 0$) or triplet ($S = 1$) state.

3.1. Triplet ($S = 1$) sector

In the triplet sector we can generate a closed subspace of basis states $\phi(1), \phi(2), \ldots, \phi(N-1)$,

$$\begin{aligned}
\phi(1) &= {}^{*}_{\uparrow}\frac{1}{\sqrt{2}}({}^{\uparrow}_{O}+{}^{O}_{\uparrow})||\cdots \\
\phi(2) &= {}^{*}_{\uparrow}|\frac{1}{\sqrt{2}}({}^{\uparrow}_{O}+{}^{O}_{\uparrow})||\cdots \\
\phi(r) &= {}^{*}_{\uparrow}||\cdots\frac{1}{\sqrt{2}}({}^{\uparrow}_{O}+{}^{O}_{\uparrow})||\cdots
\end{aligned} \tag{2}$$

where the argument r implies that the hole is on the $(r+1)$th rung. The vertical solid line along the ith rung stands for a singlet $(\frac{1}{\sqrt{2}}(c_{2i-1\uparrow}c_{2i\downarrow} - c_{2i-1\downarrow}c_{2i\uparrow}))$. A general eigenfunction $\Psi = \sum_{i=1}^{N-1} a_i\phi(i)$ with energy eigenvalue E satisfies the following eigenvalue equations:

$$\begin{aligned}
&\left(\epsilon - \frac{J}{4}\right)a_1 = ta_2 \\
&\epsilon a_2 = t(a_1 + a_3) \\
&\cdots\cdots = \cdots\cdots \\
&\epsilon a_{N-2} = t(a_{N-1} + a_{N-3}) \\
&\left(\epsilon - \frac{J}{4}\right)a_{N-1} = ta_{N-2}
\end{aligned} \tag{3}$$

where $\epsilon = E - \frac{3J'}{4} + t'$. The energy eigenvalue E is measured with respect to the ground state energy E_g. The above eigenvalue equations can be solved analytically with symmetric ($a_n = \cos(k(N/2 - n))$) or antisymmetric ($a_n = \sin(k(N/2 - n))$) eigenfunctions. In the symmetric case the energy eigenvalues are obtained from simultaneous solution of the equations

$$\begin{aligned} \epsilon &= 2t\cos(k) \\ \epsilon - \frac{J}{4} &= t\frac{\cos(k(N/2-2))}{\cos(k(N/2-1))}. \end{aligned} \tag{4}$$

In the antisymmetric case the corresponding equations are

$$\begin{aligned} \epsilon &= 2t\cos(k) \\ \epsilon - \frac{J}{4} &= t\frac{\sin(k(N/2-2))}{\sin(k(N/2-1))}. \end{aligned} \tag{5}$$

In the limit $N \to \infty$ we get a continuum of extended states for real values of k. When $J > 4t$ we can derive antibound state solutions in both cases for imaginary values of k (k replaced by ik). The antibound states are localized states lying above the continuum of extended states with energy eigenvalue $E_{ab} = \frac{3J'}{4} - t' + \frac{J}{4} + \frac{4t^2}{J}$. However, for any positive value of J the hole does not form a bound state with the impurity in the triplet sector.

3.2. Singlet ($S = 0$) sector

The motions of a hole in the presence of an NM impurity was reported by Bose and Gayen [38] earlier. For the sake of convenience we briefly review the salient features here. A basis state ϕ_i will have the hole located in the ith rung. There will be singlets residing on all $N - 2$ rungs except the first and ith rungs. The electronic spins on the first and ith rungs will form a singlet. In the basis state ϕ_1 both the impurity and the hole are on the first rung. A general eigenfunction will have the form $\Psi = \sum_{i=1}^{N} a_i\phi_i$. The exact amplitude equations derived from the time-independent Schrödinger equation with energy eigenvalue E (measured with respect to the ground state energy E_g) are

$$\begin{aligned} &\left(\epsilon + \frac{3J'}{4} - t'\right)a_1 = t\sqrt{2}(a_2 + a_N) \\ &\left(\epsilon + \frac{3J}{4}\right)a_2 = -t\sqrt{2}a_1 + ta_3 \\ &\epsilon a_3 = t(a_2 + a_4) \\ &\cdots\cdots = \cdots\cdots \\ &\epsilon a_{N-1} = t(a_N + a_{N-2}) \\ &\left(\epsilon + \frac{3J}{4}\right)a_N = -t\sqrt{2}a_1 + ta_{N-1} \end{aligned} \tag{6}$$

where $\epsilon = E - \frac{3J'}{4} + t'$. In this problem the eigenfunctions are also symmetric or antisymmetric with respect to reflection about the first rung containing the impurity. In both cases for real values of k one gets extended states. With appropriate choice of complex values of k one can discover bound ($k \to \pi + \mathrm{i}k$) or antibound ($k \to \mathrm{i}k$) states in the symmetric sector. In the case of antisymmetric wavefunction one only discovers bound state solutions. In the $N \to \infty$ limit, we derive the following results.

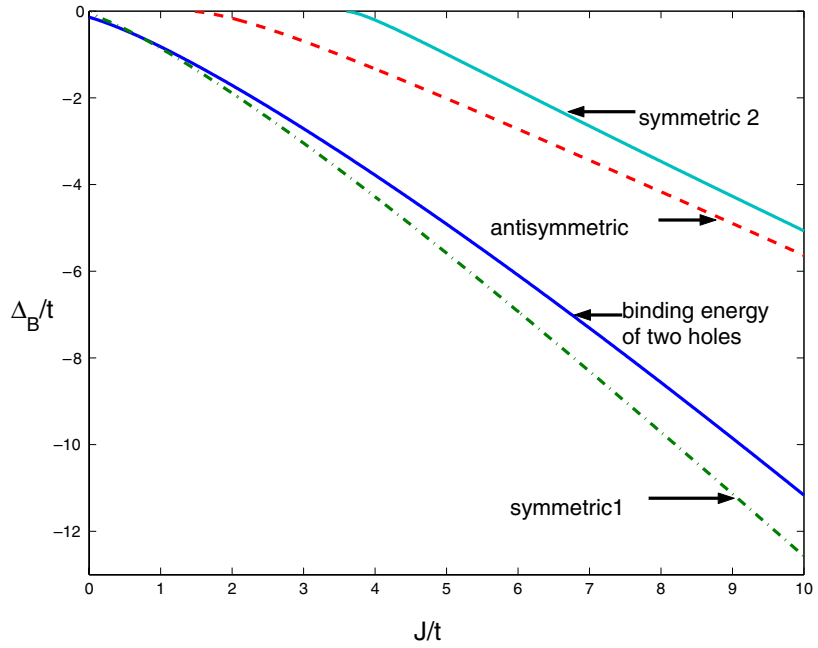

Figure 2. Binding energy Δ_B/t versus J/t for bound states of different symmetries in the case of an NM impurity. The binding energy of a pair of holes is also shown in the figure ($t'/t = 1.0$).

(a) For the symmetric eigenfunctions, (i) for $J < \frac{2}{3}\left[\frac{t'}{2} + 2t - \sqrt{8t^2 + (\frac{t'}{2})^2}\right]$, there can be no bound state solution; (ii) for $J > \frac{2}{3}\left[\frac{t'}{2} - 2t + \sqrt{8t^2 + (\frac{t'}{2})^2}\right]$, we do not find any antibound state; (iii) for $J > \frac{2}{3}\left[\frac{t'}{2} + 2t + \sqrt{8t^2 + (\frac{t'}{2})^2}\right]$, we always find two bound states.

(b) In the case of antisymmetric eigenfunctions, we always get one and only one bound state provided $J > \frac{4tN}{3(N-2)}$. In the $N \to \infty$ limit, the bound state in the antisymmetric sector has energy $E = \frac{3J'}{4} - t' - \frac{3J}{4} - \frac{4t^2}{3J}$.

We use the following quantitative definition of the impurity–hole binding energy introduced by Poilblanc *et al* [21, 23]:

$$\Delta_B(1h, 1i) = (E(1h, 1i) - E(0h, 1i)) - (E(1h, 0i) - E(0h, 0i)). \tag{7}$$

Figure 2 shows the plot of binding energy (Δ_B/t) as a function of exchange interaction (J/t) in different symmetry channels. We also compare the binding energy of a pair of holes computed from the results of Gayen and Bose [26] in the same figure. The binding energy of two holes in the absence of impurity is defined as

$$\Delta_B(2h, 0i) = (E(2h, 0i) - E(0h, 0i)) - 2(E(1h, 0i) - E(0h, 0i)) \tag{8}$$

where $E(nh, 0i)$ is the ground state energy in the presence of n holes and 0 impurity. $E(1h, 1i)$ is the lowest energy in the presence of one hole and one impurity in the particular symmetry channel.

From figure 2 we find that for any positive value of J/t there is always one bound state in the symmetric (symmetric 1) channel. For $J/t > \frac{4}{3}$ one can find another bound state in the antisymmetric channel. Another bound state is obtained in the symmetric (symmetric 2) channel for all values of $J/t > 3.581\,52$. The co-existence of the bound states in different

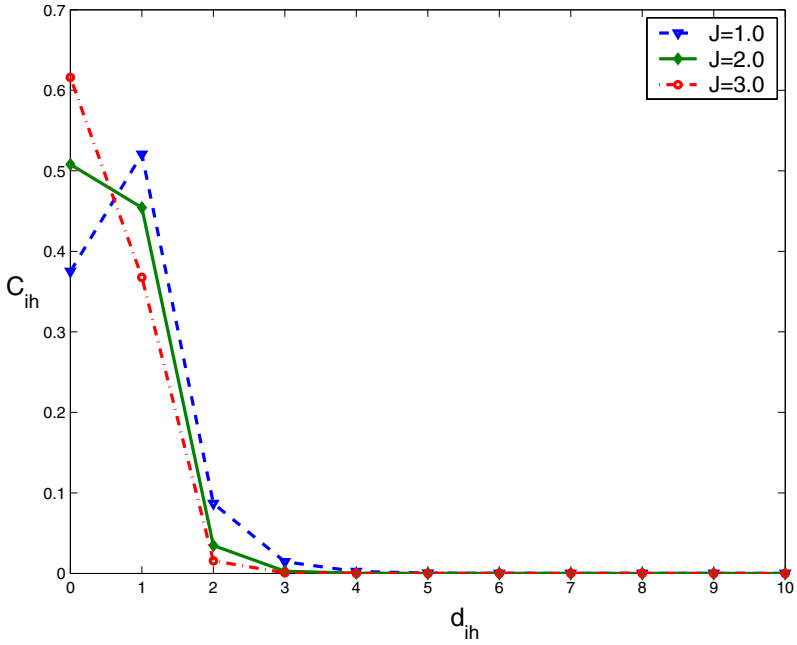

Figure 3. Impurity–hole correlation C_{ih} in the ground state as a function of the distance d_{ih} of the hole from the NM impurity ($t = t' = 1.0$).

symmetry channels is analogous to the appearance of d-, s-, and p-wave bound states in 2D clusters studied by Poilblanc *et al* [21]. However, there is one significant difference in the ladder. The sequence of the bound states appearing in symmetry channels of different parity (even–odd–even) is different from that (even–even–odd) obtained by Poilblanc *et al* [21]. The most significant observation from the graph is that the impurity–hole binding energy in the lowest symmetric sector has magnitude greater than the binding energy of a pair of holes for $J/t > 0.74$. For 2D finite clusters Poilblanc *et al* [21] found the binding energy curve for the pair of holes to be lowest.

In order to have more understanding of the nature of impurity–hole binding we plot (figure 3) the impurity–hole correlation function $C_{ih}(j-1)$ $(= \langle n_i(1)n_h(j)\rangle)$ as a function of the distance d_{ih} between the impurity and the hole in the ground state. When the hole shares the same rung with the impurity, there is no extra cost of energy due to broken singlets along the rungs. If the hole sits one rung away from the impurity, one additional singlet along the rung is broken. But this loss of energy can be compensated by the creation of an extra singlet between the two free spins sitting on the two rungs which are occupied by the impurity and hole also. Moreover, the hole can gain kinetic energy of the amount $-t'$ when it stays one rung away from the impurity. As a result the hole likes to sit one rung away from the impurity in the ground state for smaller values of J (with $t = t' = 1$). However, with increasing J values the probability of the hole sharing the same rung with the impurity increases rapidly.

4. Magnetic impurity

We assume the static impurity to be a spin-$\frac{1}{2}$ object that interacts with neighbouring spins via exchange interaction J'_m (along the rung) and J_m (along horizontal and diagonal bonds). The

dynamics of the system is governed by $H_{\rm imp}$, which is essentially the Hamiltonian introduced in equation (1) with the fact that the electrons cannot hop on to the impurity site and the spin at the impurity site interacts with the neighbouring spins with different strengths. We assume that the static impurity sits on the first rung. We use PBCs. In the absence of any hole the ground state consists of singlets along all the rungs with energy eigenvalue $-(\frac{3J'}{4}(N-1)+\frac{3J'_m}{4})$ if the impurity exchange interaction is AFM. For FM exchange interaction, all the rungs, except the first one, are singlets. The first rung, where the magnetic impurity is located, has $S=1$ configuration. The corresponding energy eigenvalue is $-(\frac{3J'}{4}(N-1)+\frac{|J'_m|}{4})$. A single hole can be doped in the first rung to create the state

$$\chi = {}^{\uparrow^*}_{O}\,||\cdots. \tag{9}$$

We can diagonalize the Hamiltonian within a closed subspace of basis states denoted by χ, $\phi(1), \phi(2), \ldots, \phi(N-1), \theta(1), \theta(2), \ldots, \theta(N-1), \psi(1), \psi(2), \ldots, \psi(N-1)$. The states are pictorially represented in the following way:

$$\begin{aligned}
\phi(r) &= \left(\frac{1}{\sqrt{2}}\right)^{\uparrow^*}_{\uparrow} ||\cdots({}^{O}_{\downarrow}+{}^{\downarrow}_{O})\cdots|| \\
\theta(r) &= \left(\frac{1}{\sqrt{2}}\right)^{\uparrow^*}_{\downarrow} ||\cdots({}^{O}_{\uparrow}+{}^{\uparrow}_{O})\cdots|| \\
\psi(r) &= \left(\frac{1}{\sqrt{2}}\right)^{\downarrow^*}_{\uparrow} ||\cdots({}^{O}_{\uparrow}+{}^{\uparrow}_{O})\cdots||
\end{aligned} \tag{10}$$

where the argument r implies that the hole is located in the $(r+1)$th rung. A general eigenfunction will have the following form:

$$\Psi = a_0\chi + \sum_{r=1}^{N-1} b_r\phi(r) + \sum_{r=1}^{N-1} c_r\theta(r) + \sum_{r=1}^{N-1} d_r\psi(r). \tag{11}$$

Clearly the total number of basis states will be $mm = 1+3(N-1)$, and we have to diagonalize an $mm \times mm$ Hamiltonian to find the eigenvalues and eigenfunctions. In our numerical calculations we take $J'_m = 2J_m$, in accordance with the interactions ($J' = 2J$) in between the host spins. In this case the eigenfunctions are also found to be symmetric ($b_n = b_{N-n}, c_n = c_{N-n}, d_n = d_{N-n}$) or antisymmetric ($b_n = -b_{N-n}, c_n = -c_{N-n}, d_n = -d_{N-n}$). The lowest energy eigenstate is always obtained in the symmetric sector for both FM and AFM impurities. In figure 4 we compare the binding energy of bound states in different symmetry channels for FM, AFM and NM impurities. The results obtained indicate that the binding of a doped hole with the impurity is favoured in the case of an FM impurity. Binding occurs for a weakly AFM impurity also. However, the binding energy in a particular symmetry channel is maximum if it is an NM impurity. In figure 5 we plot the binding energy in the ground states for FM ($J_m = -0.5$) and AFM ($J_m = 0.5$) impurities and compare them with that in the case of an NM impurity.

In figure 6 we plot the impurity–hole correlation function (C_{ih}) for different types of impurities. We notice that the impurity–hole correlation is maximum when the hole is just one rung away from the impurity. This is expected from figure 3 for the present choice of parameters ($J = t = t'$). When the hole is one rung away from the impurity, all other parameters remaining the same, the magnitude of the correlation function is maximum for an AFM impurity and minimum for an FM impurity. Actually for an AFM impurity all three basis states $\phi(1)$, $\theta(1)$ and $\psi(1)$ (all of them have the hole occupying the first rung) contribute to a large extent to the correlation function. For an FM impurity there is little contribution form

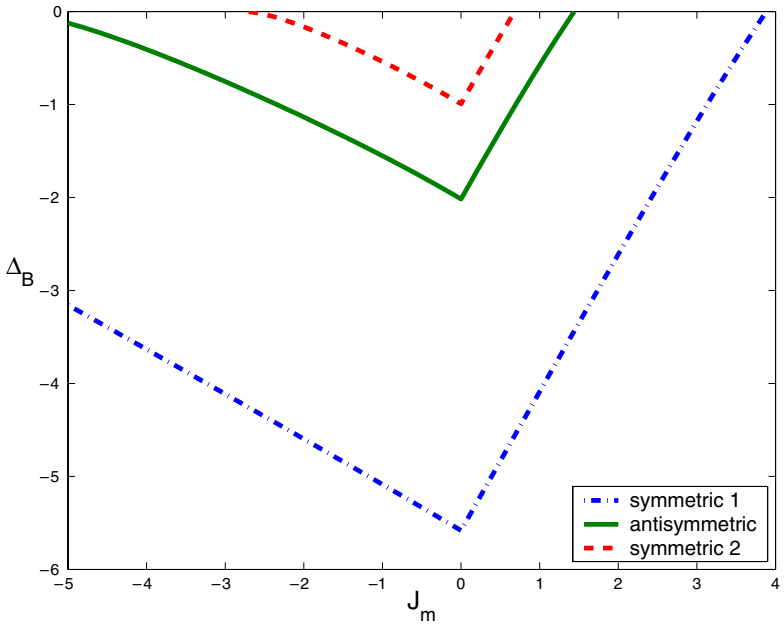

Figure 4. Binding energy of bound states of different symmetries as a function of impurity exchange coupling J_m ($J = 5.0$, $t = t' = 1.0$, $N = 50$).

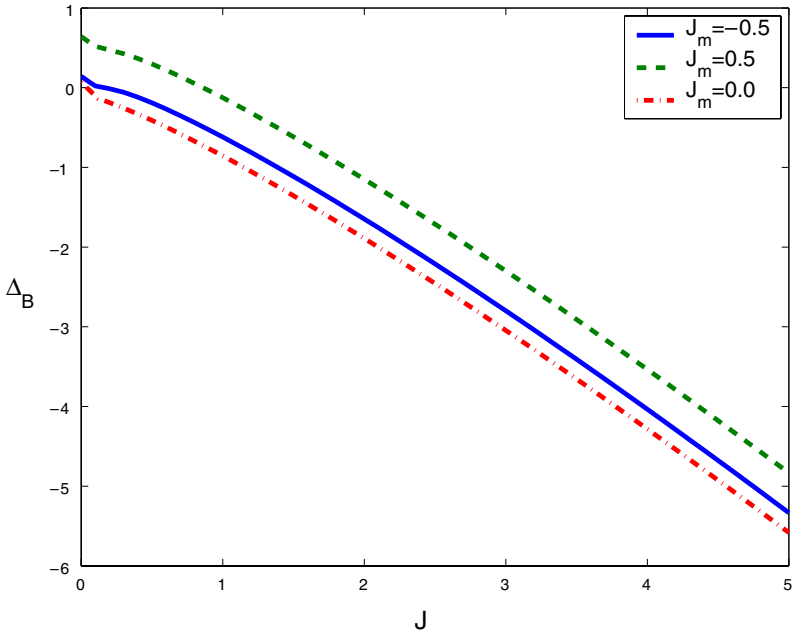

Figure 5. Binding anergy of the ground state as a function of J/t for FM ($J_m = -0.5$), AFM ($J_m = 0.5$) and NM ($J_m = 0.0$) impurities ($t = t' = 1.0$, $N = 50$).

the basis state $\psi(1)$ due to unfavourable configuration (two of the three bonds are frustrated). However, if the hole and impurity are on the same rung, the correlation function has largest value for an NM impurity and smallest value for an AFM impurity.

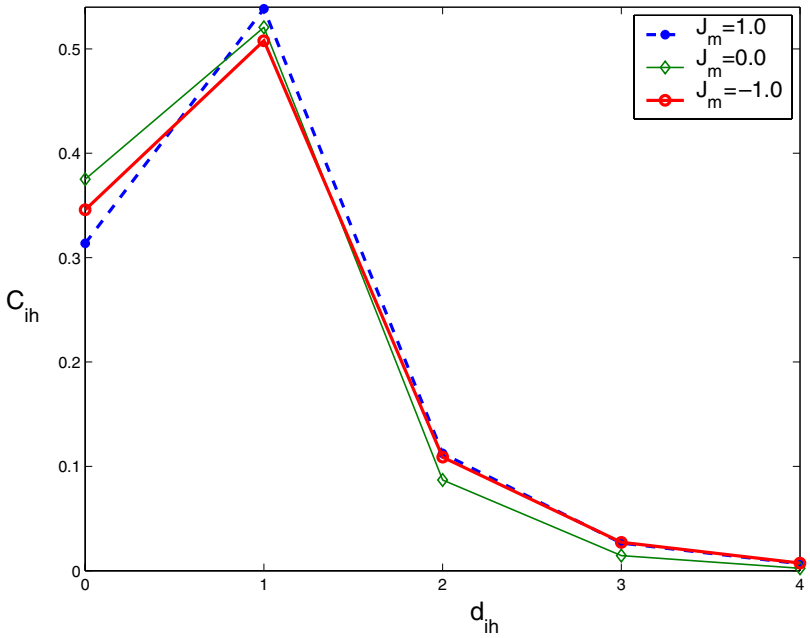

Figure 6. Impurity–hole correlation C_{ih} in the ground state as a function of the distance d_{ih} of the hole from the impurity (FM, AFM and NM) ($J = t = t' = 1.0$, $N = 50$).

5. Conclusions

In this paper we have solved analytically the many-body problem of a single hole in presence of an NM impurity and infinite number of electrons for a ladder of infinite length. A continuum of scattering states and antibound states are obtained in the triplet sector. In the singlet sector, in addition to the states found in the triplet sector, bound states of the hole with the impurity are also found. As the ratio J/t is increased from zero, successive bound states in the symmetric, antisymmetric and symmetric channel appear. For large values of J/t all the three bound states co-exist. As pointed out by Poilblanc *et al* [21], this is a characteristic feature of strong correlation. Our analytical calculations for the ladder model can qualitatively confirm the numerical results for small 2D clusters by Poilblanc *et al* [21, 22]. However, contrary to the observation by Poilblanc *et al*, we find that the binding energy curve for the impurity–hole bound state (in the symmetric sector) is lower than that of a bound pair of holes in almost the whole of the parameter space, and this definitely indicates a strong pair-breaking effect [39] by an NM impurity in the t–J ladder model. In the case of a single hole in the presence of a magnetic impurity, the eigenvalue problem is solved numerically for a finite-sized ladder. Since the number of basis states increases as N we can solve a large size ladder with relative ease. Again, the results obtained are in qualitative agreement with those obtained by Poilblanc *et al* [22] for 2D finite clusters. Impurity–hole binding is more favourable in the case of an FM impurity than in the case of an AFM impurity. With increase in the strength of the AFM interaction of the impurity with surrounding electronic spins, the magnitude of binding energy rapidly decreases to zero. Comparison of the results between magnetic and NM impurities indicates that NM impurities should act as stronger pair-breaking agents in strongly correlated systems than magnetic impurities.

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