Studies of the $t$-$J$ two-leg ladder via series expansions

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Abstract

Series expansions at $T = 0$ are used to study properties of the half-filled $t$-$J$ ladder doped with one or two holes, and at quarter filling. Dispersion curves are obtained for one-hole symmetric and antisymmetric (bonding and antibonding) excitations and for the two-hole bound state. The line in the phase diagram that separates bound and unbound states is determined. For quarter filling we compute the ground state energy and estimate the location of the phase separation line. Comparisons with other numerical and analytical results are presented.

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I. INTRODUCTION

The discovery of materials containing $S = \frac{1}{2}$ ions which form a 2-leg ladder structure \cite{1,2} has stimulated a great deal of theoretical work to understand the unique and surprising features of these systems (for reviews see \cite{3,4}). Early work on magnetic properties confirmed the existence of a spin-gap in the 2-leg ladder with antiferromagnetic (AF) interactions, and hence a qualitative difference between even and odd legged spin ladders. More exotic spin ladders, with frustration, dimerization and other features have been studied more recently. \cite{5–9}.

Even more interesting behaviour may be expected if the system includes charge degrees of freedom. This can be achieved by doping, to create a system of strongly correlated mobile holes, as in the cuprate superconductors. Indeed an understanding of this (arguably simpler) system may yield important consequences for a better understanding of high $T_c$ superconductivity. The simplest model, in this context, is the $t$-$J$ model away from half-filling. Considerable work has been done on the $t$-$J$ model on a 2-leg ladder, through exact diagonalizations \cite{10–16}, the density matrix renormalization group approach \cite{17,18}, and approximate analytic theories \cite{18–21}. A number of broad features have emerged from this work.

The $t$-$J$ ladder is shown in Figure 1. The Hamiltonian is

$$ H = J \sum_{i,a} (S_{i,a} \cdot S_{i+1,a} - \frac{1}{4} n_{i,a} n_{i+1,a}) + J_\perp \sum_i (S_{i,1} \cdot S_{i,2} - \frac{1}{4} n_{i,1} n_{i,2}) $$

$$ -t \sum_{i,a,\sigma} P(c_{i,a,\sigma}^\dagger c_{i+1,a,\sigma}^\dagger + H.c.) P - t_\perp \sum_{i,\sigma} P(c_{i,1,\sigma}^\dagger c_{i,2,\sigma} + H.c.) P $$

(1)

where $i$ runs over rungs, $\sigma$ (=$\uparrow$ or $\downarrow$) and $a$ (=1,2) are spin and leg indices, $c_{i,a,\sigma}^\dagger$ ($c_{i,a,\sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma$ at the $i$th site of the $a$th chain, and $S_{i,a} = \frac{1}{2} c_{i,a,\sigma}^\dagger c_{i,a,\sigma}$ denotes the $S = \frac{1}{2}$ spin operator at the $i$th site of the $a$th chain. $P$ is a projection operator that ensures that doubly occupied states are excluded.

To understand the nature of the ground state and excitations of the system it is helpful to consider the limiting case $J_\perp, t_\perp \gg J, t$ when the states on the rungs of the ladder form an appropriate basis. Many of these features persist even to the isotropic case $J_\perp = J, t_\perp = t$.

At half-filling the charge degrees of freedom are frozen out and the system is equivalent to the Heisenberg spin ladder. The ground state is a gapped spin liquid with each rung in a spin singlet state. Spin excitations originate from exciting one or more of the rungs to triplet states.

Many authors have considered two-hole states. It is energetically favourable for the two holes to form a bond state, on the same rung. The lowest two-hole excitation arises from

$$ 2 \cdot \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{2} $$
a coherent propagation of the two holes along the ladder. This excitation carries charge $2e$ and no spin. There are other, more complex, excitations which are described by Troyer et al. \[11\].

The nature of the system at finite doping is also of considerable interest. Poilblanc et al. \[12\] have conjectured a $T = 0$ phase diagram in the plane of $J/t$ vs electron density $n$. For large $J$ one expects phase separation, where the system separates into hole-free and hole-rich regions. For smaller $J/t$ and at or near half-filling, there is a “C1S0” phase \[22\], with one gapless charge mode and no gapless spin modes. The spin-gap will decrease, as $n$ is decreased from 1, and a transition to a Luttinger liquid phase is predicted. At small $n$ electron-pairing rather than hole-pairing will occur. Müller and Rice \[15\] have extended this phase diagram through the inclusion of a Nagaoka phase at low doping and small $J$, and a “C2S2” phase with gapless charge and spin excitations at larger $J$, between the Nagaoka and spin-gapped phases. Much of this remains somewhat speculative.

In this paper we study the $t$-$J$ ladder via the method of series expansions. This approach is complementary to other numerical methods and is able to provide ground state properties, quantum critical points, and excitation spectra to high accuracy. Its other advantage is that one deals, at once, with a large system and hence there are no finite size corrections needed. We have used this approach recently \[23\] in a study of the $t$-$J$ model on the square lattice, and we refer to that paper for details of the method and references to previous works. Early perturbative studies of the $t$-$J$ model \[24\] only considered the lowest order terms. The emphasis of our work is on one- and two-hole states, and we display excitation spectra for these. The method is not well suited to handle finite doping and hence we are not able to add to knowledge of the phase diagram for general $n$. We do however consider the special case of quarter-filling, and obtain an estimate of the boundary of phase-separation in this case. Wherever possible we compare our results with previous work.

This paper is organized as follows. In Sec. II, we consider the system with one and two holes. In Sec. III, we study the system at quarter-filling. The last section is devoted to discussion and conclusions.

II. ONE-HOLE AND TWO-HOLE STATES

The series expansion method is based on a linked cluster formulation of standard Rayleigh-Schrödinger perturbation theory, with the Hamiltonian \((1)\) written in the usual manner as

$$H = H_0 + xV$$  \hspace{1cm} (2)

where $H_0$ is a solved, unperturbed system and $xV$ represents the remaining terms. The most obvious choice is to include all of the rung terms in $H_0$

$$H_0 = J_\perp \sum_i (S_{i,1} \cdot S_{i,2} - \frac{1}{4}n_{i,1}n_{i,2}) - t_\perp \sum_{i,\sigma} P(c_{i,1,\sigma}^\dagger c_{i,2,\sigma} + H.c.)P$$  \hspace{1cm} (3)

and the coupling between rungs as $V$

$$xV = J \sum_{i,a} (S_{i,a} \cdot S_{i+1,a} - \frac{1}{4}n_{i,a}n_{i+1,a}) - t \sum_{i,a,\sigma} P(c_{i,a,\sigma}^\dagger c_{i+1,a,\sigma} + H.c.)P$$  \hspace{1cm} (4)
As discussed above, the eigenstates of \( H_0 \) are direct products constructed from the nine possible rung states, shown in Table I. To compute the perturbation series we fix the values of \( t_\perp/J_\perp \) and \( t/J \) and derive an expansion in powers of \( x \equiv J/J_\perp \) for the quantity of interest. The series is then evaluated (summed) at the desired value of \( J/J_\perp \) by using standard Padé approximants and integrated differential approximants [25]. We set \( J_\perp = 1 \) to define the energy scale. To improve the convergence of the expansion we also try the effect of adding a term to \( H_0 \) and subtracting it from \( V \), for example

\[
H'_0 = (J_\perp + r) \sum_i (S_{i,1} \cdot S_{i,2} - \frac{1}{4} n_{i,1} n_{i,2}) - t_\perp \sum_{i,\sigma} P(c^\dagger_{i,1,\sigma} c_{i,2,\sigma} + H.c.)P
\]

(5)

\[
xV' = xV - r \sum_i (S_{i,1} \cdot S_{i,2} - \frac{1}{4} n_{i,1} n_{i,2})
\]

(6)

and adjusting \( r \) to obtain best convergence. Other types of term could be added and subtracted in this way.

A slightly different formulation takes only the rung spin Hamiltonian as the unperturbed part

\[
H_0 = J_\perp \sum_i (S_{i,1} \cdot S_{i,2} - \frac{1}{4} n_{i,1} n_{i,2})
\]

(7)

with all of the remaining terms, including the rung hopping, included in the perturbation. Both methods have been used, as appropriate.

The series method can be used to compute the ground state energy and other ground state properties such as magnetization, susceptibility, and correlations. In the present study we are mainly interested in the nature of excitations. Rather than calculate the ground state energy we have used the method of Gelfand [26] to compute the excitation energy directly. For the one-hole excitations we start with an initial state with the hole in either the bonding or antibonding state on a particular rung and all other rungs in spin singlet states. The perturbation will then mix this with other states in which the hole moves along the ladder within a fluctuating spin background. For the two-hole case the initial state has both holes on the same rung. During the evolution of the system these holes may separate. Those final states which have the holes together on the same final rung contribute to the two-hole excitation spectrum. The series have been computed to order \( (J/J_\perp)^{12} \) for the one hole case and to order \( (J/J_\perp)^{15} \) for the two-hole case. In special cases we have obtained considerably longer series. In the case of static holes \( (t = 0) \) we have extended the series to order \( (J/J_\perp)^{21} \) for both one- and two-hole cases, while for \( J = 0 \) we have obtained one-hole series to \( (t/J_\perp)^{19} \) and two-hole series to \( (t/J_\perp)^{22} \).

The series are available on request. For the interest of the reader we give some of the low order terms for both one and two-hole series in Appendix A. As usual with series methods the convergence is judged by consistency of different Padé (or integrated differential) approximants. In the present case convergence worsens for increasing \( J/J_\perp \) and \( t/J_\perp \). Error estimates are shown in the figures displaying our results.

Figure 2 shows the excitation spectra for one-hole symmetric and antisymmetric states for \( J/J_\perp = 0, 0.5, 1.0 \) and various \( t/J_\perp \). To avoid excessive data we have set \( t = t_\perp \) throughout. The quantities graphed are the gaps \( \Delta E^{1S}/J_\perp, \Delta E^{1A}/J_\perp \), where for instance
\[ \Delta E^{1S} = E^{1S} - E_0 \]

and \( E_0 \) is the energy of the half-filled ground state. We draw attention to the following features.

- The series yield smooth dispersion curves throughout the 1-d Brillouin zone. There is consistency between different approximants and we believe the error is small. The only exception is for some of the antisymmetric states where the figure shows larger error bars.

- For fixed \( J/J_\perp \) the energies decrease with increasing \( t \). The kinetic energy gain, proportional to \( t \), exceeds the loss in potential energy from breaking antiferromagnetic bonds. The bandwidth also increases with increasing \( t \), as expected. The gap vanishes or goes negative when \( t/J_\perp \) gets large, i.e. the 1-hole state lies lower in energy than the half-filled ground state.

- The main effect of increasing \( J \) is in the position of the minimum. For the symmetric states this is at \( k = \pi \) for small \( J \), and moves to a value near \( k = 2\pi/3 \) for \( J \) greater than a critical value around \( J/J_\perp \approx 0.6 \), almost independent of \( t \).

- The antisymmetric state shows greater sensitivity to the value of \( J \), with a qualitative change in the one-hole dispersion curve between \( J = 0 \) and 0.5.

These dispersion curves are in broad qualitative agreement with those obtained by other methods [11,21], but with significant quantitative differences. In Figure 3 we reproduce our results for the one-hole symmetric state spectrum for \( J/J_\perp = 1 \), and compare with the diagonalizations of Troyer et al. [11], and an approximate analytic result of Sushkov [21]. The dispersion curve obtained from exact diagonalization has a very similar shape to our one, but lies at somewhat lower energies. The difference may be due to finite size effects in the diagonalization results. The analytic calculation, on the other hand, lies at high energies and appears to overestimate the dispersion. The discrepancy is greatest at \( k = 0 \). Note that ref. [21] does not include the \(-n_in_j/4\) terms in the \( t-J \) Hamiltonian and hence a constant 0.75 must be added.

We now turn to the two-hole excitations. Figure 4 shows the excitation spectra, again for \( J/J_\perp = 0, 0.5, 1.0 \) and for various values of \( t/J_\perp \). The quantity graphed is again the 2-hole gap

\[ \Delta E^{2h} = E^{2h} - E_0 \]

where \( E^{2h} \) is the energy of the lowest-lying singlet 2-hole state. The following features are apparent

- The minimum now occurs at \( k = 0 \) for all \( t, J \).

- The curves are quite flat for small \( t/J_\perp \), as expected, and develop greater dispersion and more structure as \( t \) increases. The matrix element for two holes to hop from one rung to the next is of order \( t^2 \).
The energy at \( k = \pi \) depends only weakly on \( t \). For the special case \( J = 0 \) the energy at \( k = \pi \) is in fact completely independent of \( t \). It is possible to prove this result quite simply by looking at matrix elements of two-hole hopping processes. We do not have a simple physical explanation.

The two-hole gap vanishes or goes negative for small \( k_x \) when \( t/J_\perp \) gets large.

The two-hole binding energy can be computed from our excitation energies by

\[
E_b = \Delta E^{2h} - 2\Delta E^{1h} = E^{2h} - 2E^{1h} + E_0
\]

where \( \Delta E^{1h} \) is the lowest 1-hole energy, which is the symmetric one in our case. Negative \( E_b \) corresponds to binding of the two holes. Figure 5 shows \( E_b \) versus \( t/J_\perp \) for various values of \( J/J_\perp \). For \( t = 0 \) all the curves converge to the vicinity of \(-1\), which is the exact (trivial) binding energy for \( J = 0 \). For larger \( J \) this value increases slightly (to approximately \(-0.87\) for large \( J \)), but this is below the resolution of this figure. For small \( J \) the binding energy decreases in magnitude for increasing \( t \), and the two holes no longer bind beyond a critical \( t_c \), which is itself an increasing function of \( J \). For larger \( J \) binding seems to occur for any \( t \). Our results are numerically consistent with those of Hayward et al. [14] and Troyer et al. [11]. For the isotropic case \( J = J_\perp \), the two hole state is bound for all values of \( t \).

III. THE QUARTER-FILLED CASE

We have obtained a number of results for the case of quarter filling, i.e., where there is one electron (or hole) per rung. This value of electron density lies within the Luttinger liquid (C1S1) phase in the conjectured phase diagram [12], but rather near and parallel to the line separating this phase from the spin-gapped phase. There has been recent interest in this case as a model for \( \text{NaV}_2\text{O}_5 \) [27–29].

To develop the perturbation expansions for quarter-filling we start from an unperturbed state which is a direct product of alternating spin-up and spin-down rung bonding states. In the absence of \( V \) this is but one of \( 2^{N/2} \) degenerate states, because the spin-up and spin-down rung bonding states have the same energy. To remove this degeneracy, we have considered the effect of the perturbation \( V \) on a system of two rungs, and have included the diagonal terms in the unperturbed Hamiltonian. This splits the degeneracy and favours a Néel type ordering along the ladder. To improve the convergence of the expansion we also try the effect of adding the following term \( \Delta H \) to \( H_0 \) and subtracting it from the perturbation \( V \),

\[
\Delta H = r' \sum_i (-1)^i S^z_{\text{tot}}(i) [1 - |S^z_{\text{tot}}(i)|]
\]

where \( i \) runs over rungs, and \( S^z_{\text{tot}}(i) \) is the total spin in \( z \)-direction for rung \( i \). We adjust the coefficient \( r' \) to obtain best convergence. The series have been computed to order \( x^{13} \) for the ground state energy.

In Figure 6 we present results for the ground state energy as a function of \( J/J_\perp \) (taking, as usual, \( t_\perp = t \)). Also shown is the curve for the half-filled ground state energy (divided by a factor of 2). The crossing points provides an estimate of the locus of the phase separation...
line, where it becomes energetically favourable for the electrons to cluster together. These results are plotted and discussed in the following section.

An interesting limiting case is where $t_{\perp} \gg t, J, J_{\perp}$. In this limit there is a mapping to a single $S = \frac{1}{2}$ antiferromagnetic Heisenberg chain with $J_{\text{eff}} = J/2$. This mapping arises from replacing the rungs with effective $S = \frac{1}{2}$ spins, and can be established by a detailed investigation of matrix elements. The corresponding effective Hamiltonian for this mapping is

$$H_{\text{eff}} = -t_{\perp}N/2 + J_{\text{eff}} \sum_i (S_i \cdot S_{i+1} - 1/4)$$  \hspace{1cm} (12)

In Figure 7 we show the ground-state energy per spin versus $J/t_{\perp}$ for two choices of $(t, J_{\perp})$, together with the energy per site of the corresponding chain

$$E_0/N = -t_{\perp}/2 - J \ln 2/4$$  \hspace{1cm} (13)

The agreement is exact near $J = 0$ and quite good even up to $J/t_{\perp} = 1$ provided $t$ and $J_{\perp}$ are small.

IV. DISCUSSION AND CONCLUSIONS

We have carried out the first comprehensive series study of the $t$-$J$ ladder system, which is applicable to real materials as well as being of theoretical interest in its own right. We have considered the system near half-filling (one and two holes) and for exactly quarter filling. Our results provide a comparison for other numerical and analytical studies of the $t$-$J$ ladder, especially exact diagonalizations for small systems which have been extensively used.

Both one-hole and two-hole states propagate as quasi-particles with well defined excitation energies, and our estimates of these are, we believe, the most accurate available. They are in qualitative agreement with exact diagonalization results but the latter are for small systems and may have substantial finite size correction terms. We have obtained precise numerical estimates for the two-hole binding energy.

a) Half-filling

Figure 8 shows the resulting “phase diagram” for the half-filled case. From Figure 5 we can estimate the critical line at which the 2-hole binding energy vanishes, shown as line (A) in Figure 8. Below the line two holes bind, above the line they are unbound. Also shown are the lines where the 1-hole gap vanishes (B), and the 2-hole gap vanishes (C).

The binding of two holes is a necessary requirement for phase separation, where holes clump together to form separate hole-rich and hole-poor regions; but it is not sufficient. The usual criterion for the phase separation boundary is taken to be \[^{11,13}\] the point where the inverse compressibility vanishes:

$$\frac{1}{\eta^2 \kappa} = \frac{1}{2L} [E(N + 2) - 2E(N) + E(N - 2)]$$  \hspace{1cm} (14)

where $N$ is the number of electrons (or holes). In other words, phase separation occurs when the energy surface becomes locally convex with respect to the addition or subtraction of
hole pairs; whereas the binding energy (10) measures the convexity with respect to addition of single holes. We are unable to compute the quantity (14). Tsunetsugu et al. [11] and Hayward et al. [13] use criterion (14) to find the phase separation boundary at line (D) in Figure 8, very much lower than the 2-hole binding boundary (A).

This model is also believed [12,11] to exhibit a “C1S0” phase above the phase separation boundary with gapped spin excitations but gapless charge excitations. Troyer et al. [11] discuss how the bound hole pairs form a gapless band of charge fluctuations, and how the dispersion relation for the pair becomes linear near $k = 0$. The most naive criterion for the boundary of the C1S0 phase would be the vanishing of the two-hole gap, line (C) in Figure 8. That would imply the possibility of a narrow intermediate region between lines (C) and (D), corresponding to a “C0S0” phase where phase separation has not yet occurred. Other authors [29] define the “charge gap”

$$\Delta_c = \frac{1}{2}[E_0(N_\uparrow + 1, N_\downarrow) - 2E_0(N_\uparrow, N_\downarrow) + E_0(N_\uparrow - 1, N_\downarrow)]$$  \hspace{1cm} (15)$$

which cannot be computed with our current techniques of series expansions.

b) Quarter-filling

From Figure 6, we can estimate the boundary at which

$$E_0(n = \frac{1}{2}) = E_0(n = 1)/2$$  \hspace{1cm} (16)$$

where $n$ is the number of electrons per site ($n = 1$ for half-filling, $n = 1/2$ for quarter-filling). This is a sufficient but not necessary criterion for phase separation, implying a ‘global’ convexity of the energy surface, so that the system could save energy by separating completely into a hole-empty and hole-full region. Estimates based on this criterion are given by the dotted line in Fig. 9. Estimates based on the inverse compressibility [11] are shown by the open points in Figure 9: they lie a little above our estimates, but quite close to it, and are hardly distinguishable within present accuracy limits.

We have noted on a mapping (exact at the limit $t, J, J_\perp \ll t_\perp$) from the quarter-filled $t$-$J$ ladder to an $S = \frac{1}{2}$ antiferromagnetic Heisenberg spin chain. This idea can be generalized to other systems, such as the dimerized $t$-$J$ chain or dimerized $t$-$J$ model on a square lattice, and we will report on this in future work.

Note added in proofs: After submission we learnt of recent work of Bose and Gayen [30] in which they obtain exact results for 1 and 2-hole states in a $t$-$J$ ladder with additional diagonal interactions. The physics of two systems appears similar.

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APPENDIX A:

If we take the term in Eq. (7) as the unperturbed Hamiltonian, and all the remaining terms as the perturbation, we can get a double series for the excitation energies. The series up to order $t^j J^i$ $(i + j \leq 4)$ for the excitation spectra of the one-hole symmetric state $\Delta E^{1S}$ is (with $J_\perp = 1$ and $t_\perp = t$)

$$\Delta E^{1S} = 1 + (J/2 - t) + (3J^2/8 - 3t^2/2) + (3J^3/16 + 3tJ^2/4 - 9t^2J/4 + 3t^3)$$
$$+ (-3J^4/32 + 3tJ^3/4 - 69t^2J^2/32 + 9t^3J - 105t^4/16)$$
$$+ (t - 3tJ/2 - 9tJ^2/8 + 3t^2J - 9t^3/4 + 9tJ^3/32 + 9t^2J^2/2 - 15t^3J/2 + 9t^4) \cos(k_x)$$
$$+ (15t^2J^2/16 + 3t^3J/2 - 3t^4/2) \cos(2k_x) + \cdots$$

(A1)

The series for the one-hole antisymmetric state is related to that for the symmetric case by

$$\Delta E^{1A}(t, J, k_x) = \Delta E^{1S}(-t, J, \pi - k_x)$$

(A2)

The two-hole excitation energy $\Delta E^{2h}$ is

$$\Delta E^{2h} = 1 + J + 3J^2/4 - 4t^2 + 3J^3/4 - 3J^2/32 + 3t^2J^2/2 + t^4/2$$
$$+ (-4t^2 + 3t^2J^2/4 + 6t^4) \cos(k_x) + \cdots$$

(A3)
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FIGURES

FIG. 1. Structure and parameters of the $t$-$J$ ladder.

FIG. 2. Excitation spectra for one-hole symmetric and antisymmetric states for $J/J_\perp = 0,0.5,1.0$ and various $t/J_\perp$. In each case the dispersionless energy for $t = 0$ is also shown.

FIG. 3. Comparison of our results (points connected by dashed line) for the one-hole symmetric spectrum with exact diagonalizations (Troyer et al. [11], solid curve) and an approximate analytic theory (Sushkov [21], dotted curves).

FIG. 4. Excitation spectra for two-hole states for $J/J_\perp = 0,0.5,1.0$ and various $t/J_\perp$. In each case the dispersionless energy for $t = 0$ is also shown.

FIG. 5. Binding energy of two holes vs $t/J_\perp$. The $J = 0$ case shows estimates for different integrated differential approximants, which begin to spread out for $t/J_\perp \gtrsim 1$. The points where $E_b = 0$ give the two-hole binding line shown in Fig. 3. Also shown are the results of Hayward et al. [14] for the isotropic case $J/J_\perp = 1$ (the big full points connected by the dot-long dash line).

FIG. 6. Ground state energy per site for quarter-filling versus $J/J_\perp$ for various $t/J_\perp$. The solid line is the ground state energy for the phase separated state. The crossing points yield the phase separation line shown in Fig. 3.

FIG. 7. Comparison of the ground state energy per site for quarter-filling for the case of $t = 0$ (note that the results are independent of $J_\perp$ for a small value of $J_\perp$) and the case of $J_\perp = t = J$ with the results of an approximate mapping to a Heisenberg spin chain (solid line).

FIG. 8. Phases and critical lines for the $t$-$J$ ladder at half-filling, in the plane of $t/J_\perp$ versus $J/J_\perp$ (see text). Two holes do not bind in the region marked NB.

FIG. 9. Phase separation boundary at quarter-filling in the $t/J_\perp$ versus $J/J_\perp$ plane. The region marked PS is where phase separation occurs. The open points mark the boundary value found by Hayward and Poiblanc [11] for periodic (PBC) and open (OPC) boundary conditions on 8-rung finite chains.


TABLE I. The nine rung states and their energies.

| No. | Eigenstate | Eigenvalue | Name |
|-----|------------|------------|------|
| 1   | $\frac{1}{\sqrt{2}}(|↑↓⟩−|↓↑⟩)$ | $-J_\perp$ | singlet |
| 2   | $|↓↓⟩$ | 0 | triplet ($S^z_{\text{tot}} = -1$) |
| 3   | $\frac{1}{\sqrt{2}}(|↑↓⟩+|↓↑⟩)$ | 0 | triplet ($S^z_{\text{tot}} = 0$) |
| 4   | $|↑↑⟩$ | 0 | triplet ($S^z_{\text{tot}} = 1$) |
| 5   | $|00⟩$ | 0 | hole-pair singlet |
| 6   | $\frac{1}{\sqrt{2}}(|0↓⟩+|↓0⟩)$ | $-t_\perp$ | electron-hole bonding ($S^z_{\text{tot}} = -\frac{1}{2}$) |
| 7   | $\frac{1}{\sqrt{2}}(|0↑⟩+|↑0⟩)$ | $-t_\perp$ | electron-hole bonding ($S^z_{\text{tot}} = \frac{1}{2}$) |
| 8   | $\frac{1}{\sqrt{2}}(|0↓⟩−|↓0⟩)$ | $t_\perp$ | electron-hole antibonding ($S^z_{\text{tot}} = -\frac{1}{2}$) |
| 9   | $\frac{1}{\sqrt{2}}(|0↑⟩−|↑0⟩)$ | $t_\perp$ | electron-hole antibonding ($S^z_{\text{tot}} = \frac{1}{2}$) |
