Two-hole dynamics in spin ladders

Christoph Jurecka and Wolfram Brenig
Institut für Theoretische Physik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Dedicated to Professor Peter Wölffe on the occasion of his 60th birthday.

(March 22, 2022)

I. INTRODUCTION

Low dimensional quantum-spin systems with local moments arranged in ladder-type geometries have attracted considerable interest in recent years. From a theoretical point of view spin ladders are of interest as a bridging step from one- to two-dimensional systems. From an experimental point of view various spin ladder materials, e.g. SrCu$_2$O$_2$Cl$_2$ or CaV$_2$O$_5$, have been analyzed, allowing to gauge theoretical findings against real systems.

Spin-1/2 two-leg ladders display a quantum disordered ground state with exponentially decaying spin-correlations and a gapful magnetic excitation spectrum. Apart from magnetic excitations the dynamics of charge carriers doped into the quantum disordered ground state is of interest, in particular because of the discovery of superconductivity under pressure in the spin-ladder compound Sr$_{14}$-Ca$_x$Cu$_2$O$_{41}$. The properties of a single hole doped into the spin ladder have been the subject of various numerical $^{15}$ and analytical studies $^{16}$. Moreover, in order to understand two-hole interactions as well as pairing correlations several numerical investigations have been performed focusing on various topics like the formation of bound hole-pairs $^{17,18}$, ground state properties and excitation spectra $^{19,20}$, correlation functions $^{21,22}$ and superconducting fluctuations $^{23}$. Regarding analytical approaches however, only a restricted set of results is available like high order series expansions $^{24}$, mean-field approaches $^{25}$, effective Hamiltonian mappings $^{26}$, perturbative renormalization group analysis $^{27}$, exact solution of a related model $^{28}$ and recurrent variational approach $^{29}$. In particular, the two-hole spectrum remains an interesting issue with many open questions.

In this work we present an analytic theory of the energy spectrum of a two-leg spin ladder doped with two holes. Our approach allows for a direct understanding of the relevant processes. Moreover, while showing results in good agreement with earlier numerical studies $^{28}$, perturbative renormalization group calculations on small systems, our method may equally well be applied to large systems close to the thermodynamic limit.

For the two-leg spin ladder we consider a $t-J$-model with hopping- and exchange-integrals along the rungs and chains of fig. 1, i.e. $t_1$, $J_1$ and $t_2$, $J_2$ respectively. The Hamiltonian reads

$$ H = H_J + H_t $$

$$ H_J = J_1 \sum_n (S_{1,n}S_{2,n} - \frac{1}{4} n_{1,n} n_{2,n}) $$

$$ + J_2 \sum_{i,a} (S_{a,n}S_{a,n+1} - \frac{1}{4} n_{a,n} n_{a,n+1}) $$

$$ H_t = -t_1 \sum_{n,a,\sigma} c_{1,n,a,\sigma}^\dagger \hat{c}_{2,n,a,\sigma} + h.c. $$

$$ -t_2 \sum_{n,a,\sigma} c_{a,n,a,\sigma}^\dagger \hat{c}_{a,n,a+1,\sigma} + h.c. $$

(1)

where $S_{i,n}$ are spin-1/2 operators on site $i$ of rung $n$ and $c_{i,n,\sigma}^{(t)}$ operators for spin $\sigma$ and site $i,n$ projected onto the space of no double occupancy.

The paper is organized as follows. In the next section we briefly restate the bond-operator description of the spin dynamics of the undoped ladder. In section II a mapping of the $t-J$ Hamiltonian in the two-hole sector onto an interacting fermion-boson-model is described. Section III presents a diagrammatic analysis for the energy spectrum. In section IV results are presented and

![FIG. 1. Two-leg $t$-$J$-ladder. $n$ labels the rungs, 1 and 2 denote the sites on the rung.](image-url)
compared to existing numerical data. Finally conclusions will be given.

**II. SPIN DYNAMICS OF THE UNDOPED LADDER**

To describe the spin excitations of the two-leg ladder in the sector of no holes we use the well established bond-operator representation of dimerized spin-1/2 systems. Here we briefly recapitulate this method. The eigenstates of the total spin on a single rung occupied by two electrons are a singlet and three triplets. These can be created by the bosonic bond operators $s_n^\dagger$ and $t_n^\dagger$ with $\alpha = x, y, z$ acting on a vacuum $|0\rangle$ by

$$
\begin{align*}
&\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\rangle_n, \\
&\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)\rangle_n, \\
&\frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)\rangle_n, \\
&\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\rangle_n
\end{align*}
$$

where the first (second) entry in the kets refers to site (2) of the rung $n$ of Fig. 1. On each site we have $[s, s^\dagger] = 1$, $[s^{(1)}, s^{(1)}] = 0$, and $[t_\alpha, t_\beta] = \delta_{\alpha\beta}$. The bosonic Hilbert space has to be restricted to either one singlet or one triplet per site by the constraint

$$
s_n^\dagger s_n + t_{\alpha,n}^\dagger t_{\alpha,n} = 1. \quad (3)
$$

Expressing the spin part $H_J$ of the Hamiltonian (1) by the bond operators yields an interaction of singlets and triplets with two-particle interactions mediated by the inter-rung coupling $J_2$. At $J_2 = 0$ these interactions vanish leaving a sum of purely local rung Hamiltonians, which lead to a product ground-state of singlets localized on the rungs and a set of $3^N$-fold degenerate triplets. For finite $J_2$ the inter-rung interactions can be treated approximately by a linearized Holstein-Primakoff (LHP) approach (3). The LHP method retains spin-rotational invariance and reduces $H_J$ to a set of three degenerate massive magnons

$$
H_J = \sum_k \omega_k \gamma_{\alpha,k} \gamma_{\alpha,k}^\dagger + \text{const}. \quad (4)
$$

with

$$
\begin{align*}
t_{\alpha,k}^\dagger &= u_k \gamma_{\alpha,k}^\dagger + v_k \gamma_{\alpha,-k}, \\
\omega_k &= J_1 \sqrt{1 + 2\epsilon_k}, \\
\epsilon_k &= \frac{J_2}{J_1} \cos k, \\
u[v]_k^2 &= \frac{1}{2} \left( \frac{J_1(1 + \epsilon_k)}{\omega_k} + [-1] \right)
\end{align*}
$$

where $\gamma_{\alpha,k}$ is a bond-operator representation in the sector of no holes we use the well established bond-operator representation of dimerized spin-1/2 systems. Here we briefly recapitulate this method. The eigenstates of the total spin on a single rung occupied by two electrons are a singlet and three triplets. These can be created by the bosonic bond operators $s_n^\dagger$ and $t_n^\dagger$ with $\alpha = x, y, z$ acting on a vacuum $|0\rangle$ by

$$
\begin{align*}
&\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)\rangle_n, \\
&\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)\rangle_n, \\
&\frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)\rangle_n, \\
&\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)\rangle_n
\end{align*}
$$

where the first (second) entry in the kets refers to site (2) of the rung $n$ of Fig. 1. On each site we have $[s, s^\dagger] = 1$, $[s^{(1)}, s^{(1)}] = 0$, and $[t_\alpha, t_\beta] = \delta_{\alpha\beta}$. The bosonic Hilbert space has to be restricted to either one singlet or one triplet per site by the constraint

$$
s_n^\dagger s_n + t_{\alpha,n}^\dagger t_{\alpha,n} = 1. \quad (3)
$$

Expressing the spin part $H_J$ of the Hamiltonian (1) by the bond operators yields an interaction of singlets and triplets with two-particle interactions mediated by the inter-rung coupling $J_2$. At $J_2 = 0$ these interactions vanish leaving a sum of purely local rung Hamiltonians, which lead to a product ground-state of singlets localized on the rungs and a set of $3^N$-fold degenerate triplets. For finite $J_2$ the inter-rung interactions can be treated approximately by a linearized Holstein-Primakoff (LHP) approach (3). The LHP method retains spin-rotational invariance and reduces $H_J$ to a set of three degenerate massive magnons

$$
H_J = \sum_k \omega_k \gamma_{\alpha,k} \gamma_{\alpha,k}^\dagger + \text{const}. \quad (4)
$$

with

$$
\begin{align*}
t_{\alpha,k}^\dagger &= u_k \gamma_{\alpha,k}^\dagger + v_k \gamma_{\alpha,-k}, \\
\omega_k &= J_1 \sqrt{1 + 2\epsilon_k}, \\
\epsilon_k &= \frac{J_2}{J_1} \cos k, \\
u[v]_k^2 &= \frac{1}{2} \left( \frac{J_1(1 + \epsilon_k)}{\omega_k} + [-1] \right)
\end{align*}
$$

The $'[]'$-bracketed sign on the rhs. in (8) refers to the quantity $v$ on the lhs.. The spin-gap $\Delta = \min\{\omega_k\}$ resides at $k = \pi$ with $\Delta = \sqrt{J_1^2 - 2J_1J_2}$. Note that because of (3) the ground state $|D\rangle$, which is defined by $\gamma_{\alpha,k}|D\rangle = 0$, contains quantum-fluctuations beyond the pure singlet product-state. To lead ordering the dispersion $\omega_k$ is identical to perturbative expansions. Beyond the LHP approach triplet interactions and more elaborate consideration of the constraint (3) lead to a renormalization of $\omega_k$ and the formation of multi-magnon bound states (13), (14). However, for $J_2 \ll J_1$ these renormalizations can be neglected.

**III. TWO-HOLE HAMILTONIAN**

In the two hole sector a mapping of the Hamiltonian (1) onto a rung basis requires for operators which describe singly occupied as well as empty rungs in addition to the singlet and triplet operators (2) of the undoped spin system. We label a rung occupied by a single-hole by introducing an additional pseudo-fermion (holon). I.e. instead of the rung being in one of the states given by (2) it can also be in the states

$$
a_{j,n,\sigma}^\dagger |0\rangle_n = |j\sigma\rangle_n, \quad (9)
$$

where the l.h.s. denotes the vacuum, i.e. $|0\rangle$, with a single rung at site $n$ in a one-hole state of spin $\sigma$ with $j = 1, 2$ referring to the two positions available for the hole on the bond. Moreover two holes on the same rung are created by an additional boson

$$
b_n^\dagger |0\rangle_n = |00\rangle_n, \quad (10)
$$

where now the l.h.s. refers to the vacuum $|0\rangle$ with one hole-pair at site $n$. Both, the single-hole operators $a_{j,i,\sigma}$ and the hole-pair operators $b_n$ are required to obey the standard fermionic and bosonic operator algebras.

In the two-hole sector each rung necessarily is in one of the states (2), (3) or (10). As a consequence an extended hard-core constraint (3) has to be fulfilled

$$
s_n^\dagger s_n + t_{\alpha,n}^\dagger t_{\alpha,n} + \sum_{j=1,2} a_{j,n,\sigma}^\dagger a_{j,n,\sigma} + b_n^\dagger b_n = 1 \quad (11)
$$

with a summation over repeated spin-indices implied.

Creation of a physical hole in the (half-filled) ground state $|D\rangle$ of the spin-system is described by (2)

$$
\hat{c}_{j,n,\sigma} = \frac{p_j}{\sqrt{2}} (a_{j,n,\sigma}^\dagger p_j^\dagger s_n + t_{z,n} + \gamma_{\sigma,x,n}^\dagger (\pi_{x,n} + it_{y,n}) + b_n^\dagger a_{j,n,\sigma} \quad (12)
$$

where $p_j = (+(-), \gamma = 2(1)$ for $j = 1(2)$ and $p_\tau = (+(-), \gamma = \pm \tau \dagger$ for $\sigma = \dagger (-)$. In terms of (12) the creation of a physical hole can be interpreted as the removal of a spin-rung followed by the creation of a single-hole state or the
removal of a single-hole state followed by the creation of a hole-pair state. The particular linear combination of the \(a_{j,n}^\dagger\) operators on the r.h.s. ensures that the total spin is \(S = 1/2\) and \(S_z = \pm 1/2\). Using the constraint (13) and the bosonic (fermionic) commutation relations for the \(b_n (a_{j,n})\) it is straightforward to show, that the r.h.s. of (12) indeed satisfies the usual Hubbard-operator algebra. The pseudo-particle representation of the spin operators reads

\[
S_{j,n}^\sigma = \frac{1}{2} (p_j s_{j,n}^\dagger t_{j,n} + p_j t_{j,n}^\dagger s_{j,n} - i \sum_{\gamma} \epsilon_{\beta,\gamma} t_{j,n}^\dagger t_{\gamma,j}) + \frac{1}{2} \sum_{\sigma,\sigma'} a_{j,n,\sigma}^\dagger \tau_{\sigma\sigma'} a_{j,n,\sigma'}. \tag{13}
\]

where \(\tau_{\sigma\sigma'}\) are Pauli-matrices.

Inserting (12) and (13) into Hamiltonian (10) various processes are found: First, single-hole processes like (i) intra-rung hopping, (ii) inter-rung hopping, and (iii) exchange scattering of the pseudo-fermions. Second, two-hole processes result like the (iv) decay of a hole-pair on a rung and a singlet (triplet) into two separated pseudo-fermions. Second, two-hole processes are found: First, single-hole processes like (i) hard-core constraint (3) on the average, i.e. by setting \(s_n = s_h = |s_n| = s\) with

\[
s^2 = 1 - \sum_\alpha (t_{\alpha,n}^\dagger t_{\alpha,n}) = 1 - \frac{3}{N} \sum_q a_{q}^2. \tag{17}
\]

In principle this equation can be used to determine the LHP magnon-dispersion selfconsistently which however we will refrain from here.

After Fourier transforming (12) and inserting the Bogoliubov representation (3) we get

\[
H = H_1 + H_S + H_T + H_b \tag{18}
\]

\[
H_S = \sum_{k,q} S_{kq} b_k^\dagger b_k \tag{19}
\]

\[
H_T = \sum_{k,q,q'} T_{kqq'} b_{k-q}^\dagger b_{k+q}^\dagger \tag{20}
\]

\[
H_b = -J_1 \sum_b b_k^\dagger b_k \tag{21}
\]

For the sake of completeness \(H_1\) is listed in appendix A. The remaining processes (v) and (vi) are contained in \(H_b\), while \(H_T\) represents process (iv) of the the final Hamiltonian which reads

\[
H = H_1 + H_T + H_f \tag{22}
\]

\[
H_f = \frac{t_2}{\sqrt{2}} \sum_{j,n,\sigma} p_{\sigma} b_{j+1,n,\sigma} a_{j,n,\sigma} a_{j,n+1,\sigma} + |n + 1| + h.c. - \frac{t_2}{\sqrt{2}} \sum_{j,n,\sigma} b_{j+1,n,\sigma}^\dagger \tau_{\sigma,\sigma} a_{j,n,\sigma}^\dagger a_{j,n+1,\sigma} + (p_{\sigma} t_{j,n} - i t_{j,n}^\dagger) a_{j,n,\sigma}^\dagger a_{j,n+1,\sigma} + |n + 1| + h.c. \tag{23}
\]

\[
H_b = -J_1 \sum_k b_k^\dagger b_k + J_2 \sum_{k,j} (\mathbf{S}_{k,j,n}^\dagger \mathbf{S}_{k,j,n+1,\sigma} - \frac{1}{4} a_{j,n,\sigma}^\dagger a_{j,n+1,\sigma}), \tag{24}
\]

\[
\mathbf{S}_{k,j,n} = \frac{1}{2} \sum_{\sigma_1,\sigma_2} a_{j,n,\sigma_1}^\dagger a_{j,n,\sigma_2} a_{j,n,\sigma_1} a_{j,n,\sigma_2}^\dagger, \quad n_{n,j}^\dagger = (a_{j,n,\sigma}^\dagger a_{j,n,\sigma}), \quad a_{j,n,\sigma}^\dagger = 1 \text{ to lowest order.}
\]

Regarding the charge dynamics we improve upon this by requiring that the condensate density of the singlet is determined by satisfying the hard-core constraint (3) on the average, i.e. by setting \(s_n = s_h = |s_n| = s\) with

\[
U = U_0 \sum_{n,\sigma\sigma'} b_{j,n,\sigma}^\dagger b_{j,n,\sigma'}^\dagger a_{j,n,\sigma} a_{j,n,\sigma'}, \tag{25}
\]

with \(U_0 \to \infty\). A similar hard-core potential, however to study the two-triplet sector has been used in refs. 14.
IV. TWO-HOLE SPECTRUM

The primary goal of this work is to evaluate the momentum dependent energy spectrum of a two-hole state on the ladder. The physical single-hole excitations are composite objects, c.f. (12), their deviations from the pseudo fermions are small for \( J_2 \ll J_1 \), i.e., for a small triplet density induced by quantum fluctuations (see also ref. 24). Therefore, as a first step towards our goal we approximate the two-hole energy spectrum by that of two pseudo-fermions based on the limit of strong intra-rung exchange. This leaves (i) a two-particle problem to be solved, with however (ii) strongly renormalized one-particle excitations. On the bare two-particle level (i) can be achieved exactly by summing the T-matrix incorporating the interactions \( H_S, H_T \) and \( U \). For an approximate account of (ii), we will sum the T-matrix using renormalized one-particle pseudo-fermion Green’s functions

\[
G_{\kappa\sigma}(k, t) = \langle 0 | \sum_{\kappa'} \{ a_{\kappa',\kappa\sigma}(t) a_{\kappa',\kappa\sigma}^\dagger \} | D \rangle. \tag{26}
\]

The main source of renormalization for a single pseudo-fermion is known to be multi-triplet emission which can be accounted for by a selfconsistent resummation of all noncrossing n-loop graphs to the self energy (25). This is equivalent to the selfconsistent-Born-approximation (SCBA) which has been employed for the one- and two-dimensional t-J-models (26). On the ladder the SCBA leaves a finite quasi-particle residue to the pseudo-fermion propagator, which is a consequence of the spin gap. Yet, the spectra acquire a substantial incoherent part as well as renormalization of the quasi-particle dispersion (for details see ref. 24).

To evaluate the T-matrix we note that the two-leg ladder is symmetric with respect to reflections at a plane perpendicular to the rungs (25). This leaves the corresponding parity a good quantum number. The (anti)bonding single-hole states \( a_{\uparrow\pi\mu\sigma}^\dagger | D \rangle \) are of even(odd) parity, the hole-pair state \( b_{\pi\mu\pi\sigma} | D \rangle \) is of even parity, and the triplet \( t_{\pi\pi\mu\pi\sigma}^\dagger | D \rangle \) is of odd parity. Apart from parity the two-hole states can be classified additionally according to their total spin, with four subspaces, i.e., \( S = 0 \) even, \( S = 0 \) odd, \( S = 1 \) even, and \( S = 1 \) odd arising. Two pseudo-fermion scattering induced by Hamiltonian \( (19, 23) \) occurs only in the the \( S = 0 \) even channel (via \( H_S \)) and in the \( S = 1 \) odd channel (via \( H_T \)). Therefore we will focus on these channels in the following.

A. \( S = 0 \) even channel

To calculate the even parity \( S = 0 \) energy spectrum we start from the hole-pair Green’s function

\[
G_b(k, t) = -i\Theta(t)\langle D | [b_k(t)b_k^\dagger] | D \rangle, \tag{27}
\]

where the bare hole-pair propagator is set by \( H_b \) of (22).

![FIG. 2. T-matrix hole-pair Green’s function \( G_b(k, \omega) \).](image)
in the $S = 0$ even and the $S = 1$ odd subspace, the two-pseudo-fermion continua are degenerate with respect to total spin. For even parity states only diagonal elements of $U_{\mu\nu}$ enter the calculation, odd parity states imply off-diagonal elements.

**B. $S = 1$ odd channel**

The odd parity part of the spectrum is extracted from the triplet-hole pair Green's function

$$G_{bt}(k,\omega) = -i\Theta(t)\sum_q g_{kq}^2 \langle D| b_{k-q}\gamma_{z,q}\gamma_z^+ b_{k-q}|D\rangle$$

(32)

where $\gamma_{z,q}$ is the Bogoliubov-transform \cite{1} of the triplet and the choice of the $z$ triplet is arbitrary due to spin rotational invariance. The form factor $g_{kq} = (2/N)^{1/2}u_q\cos(\frac{\pi k}{N} - q)$ has been introduced for computational convenience: the matrix elements of $H_T$ which enter the T-matrix resummation are of the form $u_q u'_q T_{kq'q''} = 2\sqrt{2}g_{kq}g_{kq'}$ where, due to the limit $J_1 \gg J_2$, we have neglected contributions $\propto v_q$. Thus $g_{kq}$ reduces the number of distinct two-particle reducible element to the T-matrix summation. This form factor changes the weight but not the position of the T-matrix eigenvalues.

The hole-pair-triplet Green’s function is coupled to two pseudo-fermion scattering states via $H_T$. With respect to the interactions $H_T$ and $U$ the T-matrix evaluation, fig. 3, proceeds analogous to that in $S = 0$ even subspace. Note however, that to the zeroth order in the pseudo-fermion scattering states the hole-pair-triplet Green’s function $G_{bt}^0(k,\omega)$

$$G_{bt}^0(k,\omega) = -\frac{1}{\pi} \sum_q g_{kq}^2 \int d\omega' (\text{Im} D(q,\omega')) \times$$

$$\sum_q g_{kq}^2 G_b(k - q,\omega - \omega')$$

(33)

contains interaction effects already, since $G_b(k,\omega)$ is the interacting hole-pair Green’s function \cite{29} of Fig. 2. $D(q,\omega) = 1/(\omega - \omega_q)$ is the triplet Green’s function obtained from \cite{1}. The full T-matrix reads

$$G_{bt}(k,\omega) = (0 G_{bt}^0(k,\omega) (1_2 - M'(k,\omega))^{-1} (0 1)$$

(34)

with the $2 \times 2$ matrix

$$M'_{11} = \frac{U_0}{N} \sum_q I_{0\pi}(k,q,\omega)$$

$$M'_{12} = 2\sqrt{\frac{2}{N}} G_{bt}^0(k,\omega) \sum_q g_{kq} I_{0\pi}(k,q,\omega)$$

$$M'_{22} = 4\pi^2 G_{bt}^0(k,\omega) \sum_q g_{kq}^2 I_{0\pi}(k,q,\omega).$$

V. RESULTS AND DISCUSSION

The energy spectrum in the even (odd) parity sector of the two-hole spectrum results from an evaluation of the hole-pair-(triplet) Green’s functions $G_{b(t)}(k,\omega)$ and a subsequent determination of the regions of nonvanishing spectral density $A_{b(t)}(k,\omega) = -\pi M_{b(t)}(k,\omega)/\pi$, an example of which is depicted in Fig. 4 for $k = 0$ at $J_1/t_1 = 3$, $J_2/t_1 = 0.3$, $t_1 = t_2 = 1$, and $N = 32$. In evaluating $G_{b(t)}$, both the $\omega$ integrations and $k$ summations are performed numerically for small, but finite $\eta$ and $U_0/t_1 = 10^6$. We have checked that beyond the latter value the spectrum is insensitive to any further increase of $U_0$. Moreover, and except for later comparison to results of exact diagonalization we use a system size of $N = 32$ rungs for the remainder of this work. We
have checked that for larger system sizes the spectrum remains almost unchanged suggesting that our results are sufficiently close to the thermodynamic limit.

Figure 3(b) shows the dispersion of the even (odd) parity low energy two-hole excitations of a spin ladder with $J_2/t_1 = 3$, $J_1/t_1 = 0.3$ and $t_2 = t_1$. The state of lowest energy is a two-hole bound state with $S = 0$ and even parity, which is split off from the continuum. The binding effect is due to two holes residing on the same rung and thereby maximizing the number of singlets.

The overall ground state of the ladder is this $S = 0$ even bound-state at $k = 0$. The charge excitations of lowest energy are intra-band excitations in the $S = 0$ even bound state and therefore gapless, while the lowest spin excitations are inter-band excitations between the ground state and the $S = 1$ even continuum and therefore gapful. Thus a Luther-Emery [30] rather than a Luttinger-liquid [31] applies to the present case. This ground state is consistent with that found by Lanczos diagonalization, density matrix renormalization group (DMRG) [32], and high order series expansion [33].

In the odd parity spectrum of fig. 3(b) an $S = 1$ bound state is observed which is consistent with results from exact diagonalization [34,35]. In the T-matrix this state arises as a collective excitation due to local mixing of the hole-pair-triplet state with two pseudo-fermions. For very strong coupling $J_1 \gg J_2, t_1, t_2$ an additional anti-bound state arises, which however merges with the continuum already at intermediate couplings, because the continuum is strongly spread due to the incoherent part of the single-hole spectra.

To emphasize the difference between the bound states in the $S = 0$ and $S = 1$ sector, we show the binding energy $E_B \equiv \min(E_{\text{cont}}) - \min(E_{\text{bs}})$ as a function of $J_1$ for a constant ratio $J_2/J_1 = 0.1$ in fig. 6 where $\min(E_{\text{cont(bs)}})$ denotes the minimum energy of the continuum (bound state). For large $J_1$ a linear behavior of the $S = 0$ binding energy is found in contrast to a constant binding energy for the $S = 1$ state. This difference reflects the different binding mechanisms: the energy gain of the $S = 0$ bound state is due to the additional singlet which accompanies this state. In this case the energy gain is $\propto J_1$. In the $S = 1$ sector, and regarding $J_1$ only, the local hole-pair-triplet state is energetically equivalent to a two pseudo-fermion scattering state. Therefore binding in this channel is mainly due to kinetic delocalization of the hole-pair-triplet into two pseudo-fermions on the neighboring sites. We note, that only for a finite range of parameters $J_1/t_1 \gtrsim 1$ the bound states exist over the entire Brillouin zone. This is shown in the inset of fig. 6 which depicts the maximum values of $k$ for which the bound states can be separated from the continuum.

Returning to fig. 3(a) and (b) it is evident, that in the even parity sector the high energy states form two continua, degenerate in $S = 0$ and $S = 1$. The lower one of these, i.e. between $E \approx -4t_1$ and $E \approx -t_1$, is due to two pseudo-fermion scattering states formed out of the bonding orbitals, while the higher ones are due to either the incoherent parts of the bonding spectra or to two pseudo-fermion scattering states both in antibonding orbitals. Note that in fig. 6 we have cut off the spectrum at high energies with additional continua existing above the cut off.

The lower bound of the $S = 1$ odd continuum in fig. 6(b) shows two local minima at $k = 0$ and $k = \pi$. This structure is due to the two types of excitations which contribute to the continuum. (i) scattering states of a triplet and the hole-pair on a rung, i.e. the hole-pair-triplet bubble in fig. 3 of the diagrammatic theory.
and (ii) the continuum of two pseudo-fermions, i.e. the pseudo-fermion bubble in fig. 3. The latter is degenerate with the \( S = 0 \) odd excitations and its minimum of energy is at \( k = \pi \), while the former one has no counterpart with \( S = 0 \) and has its minimum at \( k = 0 \). This excitation has a dispersion of its lower edge which is reminiscent of that of the single triplet on the undoped ladder. For the parameters chosen in Fig. (5) both minima of the continua are nearly degenerate whereas in general it depends on the particular choice of \( t_1, t_2, J_1, J_2 \), which minimum is at the lowest energy.

Next a comparison of our diagrammatic results with exact diagonalization data is performed. To this end, in fig. 7 a two-hole spectrum reproduced from the work of Troyer et al. [6] is depicted together with our results from a T-matrix evaluation. In order to perform the comparison identical parameters, and in particular identical systems sizes have been chosen. Thick lines in this figure represent the diagrammatic, thin lines the numerical result. Obviously the agreement is very good. We emphasize that this kind of agreement is promoted by the limit of strong rung coupling \( J_2 / J_1 \gg 1 \) which pertains to fig. 7. We do not expect similar agreement for \( J_2 / J_1 \to 1 \).

To conclude this section we discuss the spin-gap of the doped ladder. From the spectrum of fig. 7 it is obvious that various \( S = 1 \) states are found in the doped ladder: (i) the even parity continuum, (ii) the odd parity bound state, and (iii) the odd parity continuum consisting (a) of triplet-hole-pair scattering states with a minimum at \( k = \pi \) and (b) of two pseudo-fermion scattering states with minimum at \( k = 0 \). All of these excitations are gapped, with the actual spin gap set by the lowest energy \( S = 1 \) excitation. Fig. 8 shows the excitation energies for all of the different \( S = 1 \) states for \( J_1/t_1 = 3 \) and \( t_1 = t_2 \) as a function of \( J_2 \). The spin gap of the undoped ladder is also displayed for comparison. For nearly the entire range of \( J_2 \) in fig. 8 the even parity continuum (i) defines the spin gap. The gap-size is set by the energy difference to the \( S = 0 \) bound state at \( k = 0 \). The continuum (i) has no counterpart in the undoped ladder. Thus we find that the spin gap evolves discontinuously upon doping in this parameter regime. The excitations at higher energies are the bound state (ii) and the continuum (iii) for \( J_2/t_1 < 0.9 \), while the bound states merge with the continuum at this particular value of \( J_2 \). For \( J_2 > 0.3 \) the lower edge of the odd parity continuum is set by the triplet-hole-pair scattering state, i.e. (iii a). As noted above this edge of the continuum has a dispersion similar to that of the triplet excitation on the undoped ladder and therefore leads to a spin gap also comparable to that of the undoped ladder. For \( J_2/t_1 < 0.3 \) the lowest odd parity continuum state is the two pseudo-fermion state, i.e. (iii b), which explains the deviation from the spin gap of the undoped ladder. Finally at \( J_2/t_1 \approx 1.2 \) a level crossing occurs and the hole-pair-triplet continuum, i.e. (iii b), becomes the lowest \( S = 1 \) excitation. Only in this parameter regime the spin gap evolves continuously upon doping.

Unfortunately the LHP approximation considerably underestimates the spin-gap of the triplet excitation for \( J_2 \to J_1 \) compared to numerically exact results [4]. Therefore the results for the spin-gap in Fig. 8 are qualitative only as \( J_2 \) increases. Nevertheless the level crossing cited above has been found also in numerical diagonalization [6]; however at a parameter range not accessible to our diagrammatic approach. Introducing a diagonal next-neighbor hopping \( t' \) between site 1(2) of rung \( n \) and site 2(1) of rung \( n+1 \) it has been shown in numerical studies that the spin gap can be tuned continuously from being set by the triplet of the undoped ladder via the hole-pair-triplet bound-state to the even parity continuum. Finally, very recently, it was found that a strongly negative
t' changes the nature of the ground state from the S = 0 bound state to that of the S = 0 even continuum \( \frac{1}{2} \), thus from a Luther-Emery liquid to a scenario with gapless charge and spin excitations.

VI. CONCLUSIONS

In conclusion we have analyzed the excitations in spin ladders doped with two holes. Applying a mapping of the generalized t-J model onto a coupled boson-fermion model the impact of both, scattering by the spin background and hole-hole interactions on the two hole spectrum has been analyzed in detail. We find the ground state to be a two-hole bound state, whereas excitations consist of various continuum states with S = 0, 1 and even or odd parity. Additionally, depending on the particular choice of parameter, S = 1 odd parity bound and antibound states are found. The binding energy of the bound states and the spin gap of the system have been analyzed. Our results compare well with numerical studies of finite systems. Yet, our method allows for a study of system sizes close to the thermodynamic limit.

ACKNOWLEDGMENTS

This research was supported in part by the Deutsche Forschungsgemeinschaft under Grant No. BR 1084/1-1 and BR 1084/1-2.

APPENDIX A:

In this appendix, and for the sake of completeness we list the Hamiltonian \( H_1 \) of (14), i.e. of the single-hole sector

\[
H_1 = -t_1 \sum_{n,\sigma} a_{1,n,\sigma}^\dagger a_{2,n,\sigma} + h.c.
\]

\[
+ \frac{t_2}{2} \sum_{j,n,\sigma} a_{j,n,\sigma}^\dagger a_{j,n-1,\sigma} + h.c.
\]

\[
+ t_2 s \sum_{j,n} t_j^\dagger (-1)^{j-1} \left( S_{n-1,n}^{ij} + S_{n+1,n}^{ij} \right) + h.c.
\]

\[
+ \frac{J_3}{2} s \sum_{j,n} t_j^\dagger (-1)^{j-1} \left( S_{n-1,n-1}^{ij} + S_{n+1,n+1}^{ij} \right) + h.c.
\]

\[
+ \frac{t_2}{2} \sum_{j,n,\sigma} t_{j,n}^\dagger a_{j,n,\sigma}^\dagger a_{j,n-1,\sigma} + h.c.
\]

\[
- t_2 \sum_{j,n} \left( t_n^\dagger \times t_{n+1} \right) \left( S_{n+1,n}^{ij} + S_{n-1,n}^{ij} \right) + h.c.
\]

\[
- \frac{J_2}{2} \sum_{j,n} \left( t_n^\dagger \times t_n \right) \left( S_{n+1,n+1}^{ij} + S_{n-1,n-1}^{ij} \right).
\]

where \( t_n^\dagger = (t_{x,n}^\dagger, t_{y,n}^\dagger, t_{z,n}^\dagger) \). This Hamiltonian includes (i) intra-rung hopping, (ii) inter-dimer hopping and (iii) exchange scattering. Interdimer hopping can be either spin-diagonal or accompanied by spin-flip scattering. This includes (ii,a) singlet-singlet and (ii,b) singlet-triplet and (ii,c) triplet-triplet transitions of the spin background upon hole doping. For further details see Ref. [1].

1 For reviews see: E. Dagotto and T. M. Rice, Science 271, 618 (1996); M. Takano, Physica C 263, 468 (1996); S. Maekawa, Science 273, 1515 (1996); T. M. Rice, Z. Phys. B 103, 165 (1997); H. Tsunetsugu, Physica B 237-238, 108 (1997). E. Dagotto, cond-mat/9908257. Rep. Prog. Phys. 62, 1525 (1999).

2 Z. Hiroi, M. Azuma, M. Takano and Y. Bando, J. Solid State Chem. 95, 230 (1991); M. Azuma, Z. Hiroi, M. Takano, K. Ishida and Y. Kitaoka, Phys. Rev. Lett. 73, 3463 (1994).

3 H. Iwase, M. Isobe, Y. Ueda and H. Yasuoka, J. Phys. Soc. Jpn. 65 2397 (1996).

4 M. Uehara, T. Nagata, J. Akimitsu, H. Takahashi, N. Mori, and K. Kinoshita, J. Phys. Soc. Jpn. 65, 2764 (1996).

5 E.M. McCarron, M.A. Subramanian, J.C. Calabrese, und R.L. Harlow, Mater. Res. Bul. 23, 1355 (1988)

6 H. Tsunetsugu, M. Troyer, T. M. Rice, Phys. Rev. B 49, 16078 (1994).

7 H. Tsunetsugu, M. Troyer, and T. M. Rice, Phys. Rev. B 51, 16456 (1995).

8 M. Troyer, H. Tsunetsugu, T. M. Rice, Phys. Rev. B 53, 251 (1996).

9 S. Haas and E. Dagotto, Phys. Rev. B 54, 3718 (1996).

10 S. R. White, D. J. Scalapino, Phys. Rev. B 55, 6504 (1997).

11 M. Brunner, S. Capponi, F. F. Assaad, A. Muramatsu, Phys. Rev. B 63, 180511(R) (2001).

12 R. Eder, Phys. Rev. B 57, 12832 (1998).

13 O. P. Sushkov, Phys. Rev. B 60, 3289 (1999).

14 C. Jurecka, W. Breitig, Phys. Rev. B 63, 094409 (2001).

15 R. E. Dagotto, J. Riera, D. Scalapino, Phys. Rev. B 45, 5744 (1992).

16 C. Gazza, G. B. Martins, J. Riera, E. Dagotto, Phys. Rev. B 59, 709 (1999).

17 T. Siller, M. Troyer, T. M. Rice, S. R. White, Phys. Rev. B 63, 195106 (2001).

18 T. F. A. Müller, T. M. Rice, Phys. Rev. B 58, 3425 (1998).

19 S. Rommer, S. R. White, D. J. Scalapino, Phys. Rev. B 61, 13424 (2000).

20 D. Poilblanc, D. J. Scalapino, W. Hanke, Phys. Rev. B 52, 6796 (1995).

21 E. Dagotto, G. B. Martins, J. Riera, A. L. Malvezzi, C. Gazza, Phys. Rev. B 58, 12063 (1998).

22 J. Riera, D. Poilblanc, E. Dagotto, Eur. Phys. J. B 7, 53 (1999).

23 D. Poilblanc, O. Chiappa, J. Riera, S. R. White, D. J. Scalapino, Phys. Rev. B 62, R14633 (2000).
24. K. Tsutsui, D. Poilblanc, S. Capponi, cond-mat/0106389.
25. C. A. Hayward, D. Poilblanc, R. M. Noack, D. J. Scalapino, W. Hanke, Phys. Rev. Lett. 75, 926 (1995).
26. C. A. Hayward, D. Poilblanc, Phys. Rev. B 53, 11721 (1996).
27. J. Oitmaa, C. J. Hamer, Z. Weihong, Phys. Rev. B 60, 16364 (1999).
28. M. Sigrist, T. M. Rice, F. C. Zhang, Phys. Rev. B 49, 12058 (1994).
29. Y. L. Lee, Y. W. Lee, C.-Y. Mou, Z. Y. Weng, Phys. Rev. B 60, 13418 (1999).
30. A. Läuchli, Diploma thesis, ETH Zürich (1999).
31. H. Lin, L. Balents, M. P. A. Fisher, Phys. Rev. B 58, 1794 (1998).
32. I. Bose and S. Gayen, J. Phys.: Cond. Mat. 11, 6427 (1999).
33. G. Sierra, M. A. Martin-Delgado, J. Dukelsky, S. R. White, D. J. Scalapino, Phys. Rev. B 57, 11666 (1998).
34. S. Sachdev and R. N. Bhatt, Phys. Rev. B 41, 9323 (1990).
35. A. V. Chubukov, Pis'ma Zh. Eksp. Teor. Fiz. 49, 108 (1989); [JETP Lett. 49, 129 (1989)].
36. A. V. Chubukov and Th. Jolicoeur, Phys. Rev. B 44, 12050 (1991).
37. O. A. Starykh, M. E. Zhitomirsky, D. I. Khomskii, R. R. P. Singh, and K. Ueda, Phys. Rev. Lett. 77, 2558 (1996).
38. W. Brenig, Phys. Rev. B 56, 14441 (1997).
39. T. Barnes, E. Dagotto, J. Riera, and E. S. Swanson, Phys. Rev. B 3196 (1993).
40. M. Reigrotzki, H. Tsunetsugu, and T. M. Rice, J. Phys.: Condens. Matter 6, 9235 (1994).
41. C. Jurecka and W. Brenig, Phys. Rev. B 61, 14307 (2000).
42. Very recently Park and Sachdev used this representation for a mean-field theory of two-dimensional antiferromagnets and spin ladders at finite doping.
43. O.P. Sushkov and V.N. Kotov Phys. Rev. Lett. 81, 1941 (1998).
44. V. N. Kotov, O. P. Sushkov, Z. Weihong, and J. Oitmaa, Phys. Rev. Lett. 80, 5790 (1998).
45. V. N. Kotov, O. P. Sushkov, and R. Eder, Phys. Rev. B, 6266 (1999).
46. C. Jurecka, V. Grützun, A. Friedrich, W. Brenig, Eur. Phys. J 21, 469 (2001).
47. Schmitt-Rink and C.M. Varma, Phys. Rev. Lett. 60, 2793 (1988).
48. C. L. Kane, P. A. Lee, N. Read, Phys. Rev. B 39, 6880 (1989).
49. G. Martinez, P. Horsch, Phys. Rev. B 44, 317 (1991).
50. Z. Liu, E. Manousakis, Phys. Rev. B 45, 2425 (1992).
51. S. Gopalan, T. M. Rice, M. Sigrist, Phys. Rev. B 49, 8901 (1994).
52. A. Luther and V.J. Emery, Phys. Rev. Lett. 33, 589 (1974);
V.J. Emery, in Highly Conducting One-Dimensional Solids, edited by J.T. Devreese et al. (Plenum, New York, 1979).
53. F.D.M. Haldane, Phys. Rev. Lett. 45, 1358 (1980); J. Phys. C 14, 2585 (1981).
54. M. Greven, R. J. Birgeneau, and U. -J. Wiese, Phys. Rev. Lett. 77, 1865 (1996).