Elementary excitations in one-dimensional spin-orbital models: neutral and charged solitons and their bound states

A. K. Kolezhuk and H.-J. Mikeska
Institut für Theoretische Physik, Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany
U. Schollwöck
Sektion Physik, Ludwig-Maximilians Universität München, Theresienstr. 37, D-80333 München, Germany
(August 22, 2000)

We study, both numerically and variationally, the interplay between different types of elementary excitations in the model of a spin chain with anisotropic spin-orbit coupling, in the vicinity of the “dimer line” with an exactly known dimerized ground state. Our variational treatment is found to be in qualitative agreement with the exact diagonalization results. Soliton pairs are shown to be the lowest excitations only in a very narrow region of the phase diagram near the dimer line, and the phase transitions are always governed by magnon-type excitations which can be viewed as soliton-antisoliton bound states. It is shown that when the anisotropy exceeds certain critical value, a new phase boundary appears. In the doped model on the dimer line, the exact elementary charge excitation is shown to be a hole bound to a soliton. Bound states of those “charged solitons” are studied; exact solutions for \( N \)-hole bound states are presented.

75.10.Jm, 75.30.Kz, 72.10.Fk, 71.70.Ej

I. INTRODUCTION

One-dimensional systems with coupled spin and orbital degrees of freedom have been attracting considerable attention during the last two years. This interest is partly motivated by the progress in the experimental study of the quasi-one-dimensional spin-gap materials Na\(_2\)Ti\(_2\)Sb\(_2\)O and NaV\(_2\)O\(_5\), which are believed to be described by a two-band orbitally degenerate Hubbard model at quarter filling. Orbital degrees of freedom may be described with the help of pseudospin-1/2 variables; the corresponding effective Hamiltonian for the dimer may be described with the help of pseudospin-1/2 operators at the site. Generally, the model has an SU(2) \( \times \) SU(2) symmetry, so that the total spin \( (S, S^z) \) of the \( S \)-chain, as well as the \( z \)-projection \( \tau^z \) of the total spin of the \( \tau \)-chain are good quantum numbers. Under certain simplifying assumptions (neglecting Hund’s rule coupling, nearest neighbor hopping between the same type of orbitals only, and only one Coulomb on-site repulsion constant), one obtains the above Hamiltonian with \( \varepsilon = \varepsilon' = 0 \), \( J_s, J_\tau = \frac{1}{4} K \) which possesses the hidden SU(4) symmetry. At this special point, the model is Bethe ansatz solvable and gapless. Depending on the microscopic details of the interaction, this high symmetry can be broken in several ways. For example, finite Hund’s rule coupling or existence of more than one Coulomb repulsion constant makes \( J_s \) and \( J_\tau \) different, and local crystal fields can induce considerable anisotropy in the orbital sector.

The phase diagram of the isotropic (\( \varepsilon = \varepsilon' = 0 \)) SU(2) \( \times \) SU(2) version of the model in the vicinity of the SU(4) point was analytically studied recently by several authors. Extensive density matrix renormalization group (DMRG) studies of the phase diagram established the form of phase boundaries and the quantum numbers of the lowest-lying excitations.

Moving away off the SU(4) point towards larger \( J_s, J_\tau \), one runs into the spontaneously dimerized phase with a finite gap and twofold degenerate ground state. The structure of the elementary excitation spectrum in the dimerized phase is known rather incompletely. The weak coupling (\( J_{s,\tau} \gg K \)) region of the dimerized phase is known to be a realization of the so-called non-Haldane spin liquid, where magnons become incoherent excitations since they are unstable against the decay into soliton-antisoliton pairs. Variational study for a special “dimer line” \( J_s = J_\tau = \frac{1}{4} K \), where the exact ground state in the form of a simple valence bond solid state is known, confirms that solitons are the lowest excited states also in case of strong coupling. However, recent DMRG results revealed a complicated pattern of the change in quantum numbers of the lowest-lying excited states in the vicinity of this special point; the standard DMRG technique provides only the information about the quantum numbers and energy of the lowest excited state, but not the information on the entire...
spectrum. Recent work using the so-called dynamical DMRG method contains data for the dynamical structure factor, but for only one point in the dimerized phase, namely for the dimer point.

Further, realistic material-relevant models are generically anisotropic \((\varepsilon, \varepsilon' \neq 0)\) and asymmetric \((J_s \neq J_t)\). The anisotropic model of the same type arises also as an effective Hamiltonian for a spin tube. Thus we think it is of interest to get insight into the properties of the elementary excitations in the dimerized phase of the more general asymmetric/anisotropic model, which is the aim of the present paper.

In section II we introduce briefly the “dimer line” in the space of model parameters where the exact twofold degenerate spontaneously dimerized ground state is known. Based on this picture of the ground state, in section III we present the variational study of the interplay between different types of elementary excitations, namely, between soliton-antisoliton pairs and their bound states (magnons). We show that soliton pairs are the lowest excitations only in a narrow region of the phase diagram, and away from the dimer line the low-energy physics is determined by magnon-type localized excitations which are essentially soliton-antisoliton bound states.

In the vicinity of the dimer line, the elementary excitations can be studied variationally. There are essentially two types of excitations: (i) solitons connecting the two degenerate spontaneously dimerized ground states (exactly speaking, soliton pairs), and (ii) magnons which are localized excitations and can be viewed as soliton-antisoliton bound states. The variational results give an upper bound for the dispersion at the dimer line where the ground state is exact, and one may expect that they provide a reasonably good approximation in the vicinity of this line.

II. EXACT GROUND STATES

In addition to the \(SU(4)\) model, there are several other particular points in the phase diagram of \(\mathbb{N}\), for which exact results are available. Particularly, at the point \(J_s = J_t = 3K/4\) the exact ground state is a product of checkerboard-ordered spin and orbital singlets (see Fig. 1), so that the spin and orbital degrees of freedom are completely decoupled in the ground state. This ground state is spontaneously dimerized and thus twofold degenerate in case of periodic boundary conditions (for open boundaries the degeneracy would be 8-fold).

One can show that the same ground state persists in a finite range of anisotropy in the case of the special choice \(\varepsilon = \varepsilon'\). In this case, up to a constant term, the model \(\mathbb{N}\) can be recast in the form

\[
\hat{H} = \sum_n (S_n S_{n+1} + J_s) (\tau_n \tau_{n+1} + \varepsilon \tau_n^z \tau_{n+1}^z + J_s),
\]

where we have set \(K\) to be the unit energy scale. Then it is easy to see that the choice \(J_s = 3/4, J_t = (3 + \varepsilon)/4\) makes the checkerboard-type singlet product wave function an eigenstate, and one can prove that it stays the ground state as long as \(-2 < \varepsilon < \infty\). Thus, in the 3D phase space \((J_s, J_t, \varepsilon)\) one has a line with an exactly known ground state; in what follows we will call it the “dimer line” for the sake of brevity. This line ends at the multicritical point \(\varepsilon = -2\), where the ground state becomes degenerate with infinitely many other states; e.g., changing any of the orbital \((\tau)\) singlets into a triplet with \(\tau^z = \pm 1\) does not change the energy. The point \(\varepsilon = +\infty\) is another multicritical point where the triplets with \(\tau^z = 0\) can be created with no energy cost. For \(\varepsilon < -2\) the ground state is also exactly known and is a product of the ferromagnetic state in \(\tau\)-sector and the antiferromagnetic Bethe-ansatz state in the \(S\)-sector. The energy of ferromagnons softens at \(k = \pi\) when \(\varepsilon\) tends to \(-2\).

We have also checked that \(\mathbb{N}\) at \(J_t = 3/4, J_s = (3 + \varepsilon)/4\) is the only nontrivial model with exactly known ground state (within the physically relevant subspace of Hamiltonians defined by \(\mathbb{N}\)) which can be found within the matrix-product based optimum ground states approach (see e.g. Ref. 15 and references therein), at least if one uses a rather general matrix-product ansatz

\[
|\Psi\rangle = \mathrm{Tr}(g_1(C)g_2(C) \cdots g_{N-1}(C)g_N(C))
\]

where \(C \equiv \{x, y, x', y', p, q\}\), and the elementary matrix \(g_n(C)\) has the following form:

\[
g_n(C) = \begin{pmatrix}
|x| \uparrow \downarrow \rangle_n + |y| \downarrow \uparrow \rangle_n \\
q|\uparrow \uparrow \rangle_n \\
-\overline{p} |\downarrow \downarrow \rangle_n \\
x' |\uparrow \downarrow \rangle_n + y' |\downarrow \uparrow \rangle_n
\end{pmatrix}.
\]

Here \(n\) denotes the rung of the “ladder,” and the first and second arrows denote the states of \(S\) and \(\tau\) spins, respectively.

III. VARIATIONAL STUDY OF THE ELEMENTARY EXCITATIONS

In the vicinity of the dimer line, the elementary excitations can be studied variationally. There are essentially two types of excitations: (i) solitons connecting the two degenerate spontaneously dimerized ground states (exactly speaking, soliton pairs), and (ii) magnons which are localized excitations and can be viewed as soliton-antisoliton bound states. The variational results give an upper bound for the dispersion at the dimer line where the ground state is exact, and one may expect that they provide a reasonably good approximation in the vicinity of this line.
A. Solitons

For a single soliton excitations one can use the variational ansatz of the type introduced in Ref. [3]

\[ |\alpha; p\rangle = \sum_n \left\{ e^{ip_n^x} |L\rangle_n^{\sigma^+} + e^{-ip_n^x} |R\rangle_n^{\sigma^-} \right\}. \]  

(3)

Here the states \( |L\rangle_n^{\sigma^+}, |R\rangle_n^{\sigma^-} \) are shown schematically in Fig. 1, and \( x_n^L = 2n + \frac{1}{2}, x_n^R = 2n + \frac{3}{2} \) are the effective “center of mass” coordinates of \( |L\rangle \) and \( |R\rangle \) states, respectively, and \( \alpha \) is a variational parameter. This soliton state has the quantum numbers \( S^z = \sigma, \tau^z = \tau \) and may be combined in pair with the corresponding antisoliton state to get states with \( (S, \tau^z) = (1, \pm 1), (0, 0), (1, 0) \) or \( (0, \pm 1) \). Since there are no diagonal exchange interactions in our “ladder”, the variational energy of a single soliton does not depend on \( (\sigma, \tau) \) so that we omit the corresponding index in what follows.

It is easy to see that there exist a couple of useful symmetry properties. Upon the operation of interchanging upper and lower leg \( (S \leftrightarrow \tau) \) the \( R \) and \( L \) soliton states transform as \( |L\rangle_n \rightarrow |R\rangle_{n-1/2}, |R\rangle_n \rightarrow |L\rangle_{n+1/2} \), so that

\[ |\alpha; p\rangle \rightarrow \alpha |(\alpha^{-1}; p). \]  

(4)

That means that if the variational energy of the state \( |\alpha\rangle \) calculated with the Hamiltonian \( H \) has a minimum at a certain \( \alpha = \alpha_0 \), then the energy of the same state calculated with the Hamiltonian with interchanged \( S \) and \( \tau \) operators should have a minimum at \( \alpha' = 1/\alpha \). An important consequence is that in the symmetric case \( \varepsilon = 0 \), \( J_s = J_r \) the minimum should always occur at \( \alpha = \pm 1 \). (It should be remarked that this property was missed in our earlier treatment [5] the variational parameter \( \zeta = \alpha e^{i\varphi} \) used in Ref. [3] was erroneously assumed to be real, which forced the minimum to be at \( \zeta = \pm 1 \).

Upon a reflection \( x \rightarrow -x \) the soliton states transform as \( |L\rangle_n \rightarrow |R\rangle_{N-n}, |R\rangle_n \rightarrow |L\rangle_{N-n} \), so that one has

\[ |\alpha; p\rangle \rightarrow \alpha e^{i\varphi(2n+1)} |(\alpha^{-1}; -p). \]  

(5)

where the asterisk denotes complex conjugation. The energies of two states with mutually conjugate wave functions should be equal, therefore replacing \( \alpha \) by \( 1/\alpha^* \) should not change the variational energy, which means that the minimum is reached on a subspace with \( |\alpha|^2 = 1 \). Thus, we can set \( \alpha = e^{i\varphi} \) in our variational ansatz [3].

Essentially simple but tedious calculation of the variational dispersion yields

\[ E_{\text{sol}}(p) = \frac{F_0(p) + F_c(p) \cos \varphi + F_s(p) \sin \varphi}{24(25 - 16 \cos^2 p)(5 + 4 \cos \varphi \cos p)}, \]  

(6)

where we have used the notation

\[ F_0(p) = |J_r(\varepsilon + 3) + 3J_s| (383 - 392 \cos 2p) + (\varepsilon + 3)(48 \cos 4p + 180 \cos 2p - 93), \]

\[ F_c(p) = 4 \cos p(33 - 32 \cos 2p) (2J_r - 3(\varepsilon + 3) + 6J_s), \]

\[ F_s(p) = 20 \sin p(25 - 16 \cos^2 p) \{ J_r(\varepsilon + 3) - 3J_s \}. \]  

(7)

It is now easy to minimize the expression \( \varphi(p) \) in \( \varphi \) and to obtain the final variational soliton energy. The equation \( dE_s/d\varphi = 0 \) always has two roots, \( \varphi_0 \) and \( \pi - \varphi_0 \), and one of them yields the minimum for \( 0 < p < \pi \), and the other does so for \( \pi < p < 2\pi \). In this way, though one cannot see that from Eq. [3] directly, the final minimized soliton energy \( E_{\text{sol}}^{\min}(p) \) is symmetric with respect to the shift \( p \rightarrow p + \pi \), in full agreement with the fact that the Brillouin zone in the dimerized phase is halved.

For certain special cases the variational soliton dispersion can be sufficiently simplified. It is easy to see that under the following condition of “generalized symmetry”:

\[ J_s = J(1 + \varepsilon/3), \quad J_r = J, \]  

(8)

the function \( F_s(p) \) identically vanishes, so that the minimum of \( \varphi(p) \) is reached at \( \varphi = 0 \) or \( \pi \) (i.e., \( \alpha = \pm 1 \)), and one obtains

\[ E_{\text{sol}}^{\text{sym}} = (3 + \varepsilon)/24 \times \frac{62J + 12 \cos 2p + 3 - (64J + 12)}{5 - 4|\cos p|}. \]  

(9)

At the dimer line, i.e., for \( J = \frac{3}{4} \), the above expression simplifies further to

\[ E_{\text{sol}}^{\text{dimer}} = \frac{3 + \varepsilon}{16} (5 - 4|\cos p|). \]  

(10)

The energy gap at the dimer line occurs always at \( p = 0, \pi \). One can check that the gap which follows from \( \varphi_0(p) \) coincides with the result given in Ref. [3] however, for general \( p \) the formula \( \varphi(p) \) yields the lower energy and is in addition much simpler than the corresponding expression in Ref. [3].

The energy of the continuum of soliton-antisoliton scattering states is given by

\[ E_{\text{pair}}(k, q) = E_s(k/2 + q) + E_a(k/2 - q), \]  

where \( k \) and \( q \) are respectively the total and relative momentum. All momenta here are defined for the original non-dimerized chain, and the Brillouin zone is in fact halved, so that \( k \in [-\pi/2, \pi/2] \).

B. Magnons

We understand “magnons” as localized excitations which do not break the dimer order (in contrast to solitons). In a crude approximation, one could imagine that a magnon state corresponds to exciting one of the singlet bonds on the \( S \) or \( \tau \) chains to a triplet and making it propagate along the chain. One may speak about \( S \)- or \( \tau \)-magnons, respectively. In turns out, however, that
such a crude single-mode approximation overestimates considerably the magnon energy. A simple reason is that a state $|t_{n\mu}\rangle$ shown in Fig. 3 is not an eigenstate of the Hamiltonian even at the dimer line, and under the action of the Hamiltonian it gets mixed with other states. In the vicinity of the dimer line the largest contribution to the first-order matrix elements (i.e., of the $\langle \psi | \hat{H} | t_{n\mu}\rangle$ type) comes from the action of the local Hamiltonian $\hat{h}_n$ coupling the sites $(2n + 1)$ and $(2n + 2)$ (see Fig. 2). The other first-order contributions are proportional to small parameters $\lambda_\tau = J_s - \frac{3\pi}{4}$, $\lambda_s = J_s - \frac{3\pi}{4}$, measuring the deviations from the dimer line, and we neglect them for the sake of consistency (see below). Thus, it looks reasonable to take a linear combination of the two orthogonal states $|t_{n\mu}\rangle$ and $|\hat{h}_n|t_{n\mu}\rangle - \langle t_{n\mu}|\hat{h}_n|t_{n\mu}\rangle|t_{n\mu}\rangle$ (see Fig. 2) as a simplest variational ansatz. The magnon state with momentum $k$ can be written as

$$|m; k\rangle = \sum_n e^{ik(2n + 1)} \left\{ \cos \chi |t_{n\mu}\rangle + \sin \chi |\Delta^{(1)} t_{n\mu}\rangle \right\},$$

where $|\Delta^{(1)} t_{n\mu}\rangle$ is assumed to be normalized, and $\chi$ is a variational parameter. After minimization in $\chi$, the magnon dispersions take the following form:

$E_S(k) = e_{0, s} + (1/8)(3 + \varepsilon - 4J_s) \cos(2k),$  
$$E_0(k) = e_{0, s}^0 + (1/8)(1 + \varepsilon - 4J_s) \cos(2k),$$

where the superscripts for $\tau$-magnons indicate the value of $\tau$. One may observe that the inclusion of the above-mentioned contributions to $|\Delta^{(1)} t_{n\mu}\rangle$ which are proportional to $\lambda_{s, \tau}$ would lead to corrections of the order $O(\lambda_{s, \tau}^2)$ in both the bandwidth and the self-energy of magnons. To be consistent, we have to omit those contributions, since we have already implicitly neglected the corrections to the ground state energy which are also $O(\lambda_{s, \tau}^2)$ in the leading order. (This does not mean, of course, that our calculation will have the accuracy $O(\lambda_{s, \tau}^2)$, since the contributions from the higher-order matrix elements of the type $\langle \psi | (\hat{H})^n | t_{n\mu}\rangle$ do not contain any small parameter. The ansatz (12) should be considered as purely variational, sort of “one-step Lanczos” trick).

The self-energies for $\tau$-magnons can be compactly written as

$$e_{0, \tau}^S = 3J_s/4 + J_\tau - \frac{2(1 + \eta \varepsilon) + 2\{1 + \eta \varepsilon\}^2 + 48J^2_\tau}{16}^{1/2},$$

where $\eta = 1$ for $\mu = \pm 1$ and $\eta = -1$ for $\mu = 0$. The expression for the self-energy of an $S$-magnon is somewhat cumbersome due to the fact that the state $|\Delta^{(1)} t_{n\mu}\rangle$ in case of the $S$-magnons does not have a certain value of the total orbital momentum $T$ and is a mixture of states with $T = 0$ and 2:

$$e_{0, S} = J_s + J_\tau - \frac{4J_\tau(3 - \varepsilon) + 3(1 + \varepsilon) + \sqrt{Z}}{16(\varepsilon^2 + 2\varepsilon + 3)},$$

$$Z = 16J^2_\tau(\varepsilon^2 + 2\varepsilon + 2)[\varepsilon^4 + 4\varepsilon^3 + 27(\varepsilon^2 + 2\varepsilon + 2)] + 8J_\tau\varepsilon^2(4\varepsilon + 6\varepsilon^3 + 21\varepsilon^2 + 32\varepsilon + 24) + \varepsilon^6 + 6\varepsilon^5 + 21\varepsilon^4 + 44\varepsilon^3 + 36(2\varepsilon^2 + 2\varepsilon + 1).$$

One can observe that the ansatz for a magnon state which we have used above is in fact equivalent to the simplest possible ansatz for a bound state of soliton and antisoliton, where only the configurations of the type $|L\rangle_n|\bar{L}\rangle_{n + \frac{1}{2}}$, $|R\rangle_n|\bar{R}\rangle_{n + \frac{1}{2}}$, $|L\rangle_n|\bar{R}\rangle_{n + \frac{1}{2}}$, $|R\rangle_n|\bar{L}\rangle_{n + \frac{1}{2}}$ with soliton and antisoliton being nearest neighbors are taken into account. Here the bars denote antisoliton states; note that for fixed boundary conditions, solitons and antisolitons live on different sublattices, e.g. the free spin in the $\tau$ chain (see Fig. 3) is placed on the odd (even) rung for solitons (antisolitons), respectively, which is reflected in the above notation.

This indicates that magnons should be viewed as bound soliton-antisoliton states, rather than as independent excitations. Our simple ansatz can capture only the short-range physics of the tightly bound states with quantum numbers $(S, \tau^z) = (1, 0), (0, 0), (0, \pm 1)$; it will miss, however, possibly existing higher-lying loosely bound states as well as states with $(S, \tau^z) = (1, \pm 1)$.

It is interesting to remark that solitons themselves can be viewed as bound states of two spinors belonging to the $S$ and $\tau$ chains, respectively, which should unfold when one moves towards the exactly solvable SU(4) point. Therefore on the way from the SU(4) point to the dimer line there should exist an interesting hierarchy of bound states, which would be an interesting subject of the future studies.

C. Crossover between solitons and magnons

The minimum of the lower boundary of the soliton continuum is at $k = 0$ in the immediate vicinity of the dimer line. When $J_s$, $J_\tau$ decrease below certain values, the second equivalence minimum splits off and starts to move towards $\pi/2$. The magnon gap always lies either at $J = 0$ or at $k = 0$. Fig. 4 illustrates the behavior of the gap along the “generalized symmetric line” $J_s = J(1 + \varepsilon/3)$, $J_\tau = J$ for a few choices of $\varepsilon$.

One can observe the following important feature: the solitons are the lowest excitations only in a limited region of the phase space. Even at the dimer line line solitons cease to be the lowest excited states if the anisotropy is sufficiently strong: the $\tau^\pm$-magnons become the lowest
excitations for $\varepsilon < -59/33$ and soften at the phase transition point $\varepsilon = -2$ (respectively, $\tau^0$-magnons become the lowest excitations for $\varepsilon > 59/7$ and the corresponding gap saturates at the finite value of $\frac{3}{\pi}$ at $\varepsilon \to +\infty$). One can see that whenever the variational gap closes while moving from the dimer line, the magnon gap touches zero first, so that the phase transitions are always governed by magnons.

Three branches of $\tau$-magnons are degenerate at $\varepsilon = 0$, and for $\varepsilon > 0$ ($\varepsilon < 0$) the $\tau^\pm$-magnons ($\tau^0$-magnons) become lower in energy, respectively; the $S$-branch lies always in between the $\tau^\pm$ and $\tau^0$ branches. In this connection, we would like to make a remark concerning Fig. 4 of Ref. 20 which shows the behavior of the $S$-magnon gap (the lowest excitation in the $(S^z, \tau^z) = (1, 0)$ sector) across one of the phase boundaries in the model $4\pi$ with $\varepsilon = -1$. We think the behavior of $S$-gap is not relevant as a proof of the first order transition, because another excitation, namely that of the $(0, 1)$ sector, should be responsible for the transition.

Away from the dimer line our description should become progressively worse since the pure dimer state is too far from the correct ground state. Thus the present approach cannot be used for estimation of the shape of the phase boundaries, except when they become close to the dimer line (see below).

Another observation is that though the gap of the soliton continuum can be at incommensurate $k$, the lowest excited state almost always (actually except for very narrow regions, whose existence may well be an artifact of our approximation) occurs at the commensurate values of $k = 0$ or $\pi/2$ (see Fig. 3), which is consistent with the results of Refs. 3,9. However, the contribution from solitons can be observed in the dynamic structure factor $S(k, \omega)$. Unfortunately, the only existing dynamical DMRG study provides data only for one point in the dimerized phase (namely, for the point $J_s = \frac{3}{4}, J_r = \frac{3}{4}, \varepsilon = 0$) where no incommensurability is expected.

One can see that if $\varepsilon$ tends towards the multicritical points $\varepsilon = -2$ or $\varepsilon = +\infty$, then there are two transitions along the generalized symmetry line in the vicinity of the point $J = \frac{3}{4}$ belonging to the dimer line: one at $J < \frac{3}{4}$, and another at $J > \frac{3}{4}$. This indicates that if the anisotropy exceeds a certain critical value, an additional transition boundary should appear in the $(J_r, J_s)$ plane. Note that in this case the variational phase boundaries lie close to the dimer line, so that this statement can be considered reliable.

D. Comparison with numerical results

We have studied the spectrum of low-lying excitations of the model $4\pi$ by means of the exact diagonalization (Lanczos) method, using a chain consisting of 12 sites (i.e., having 12 spin and 12 pseudospin degrees of freedom).

Fig. 4 illustrates the behavior of the elementary excitations spectrum for a few choices of $J_s, J_r, \varepsilon$, in comparison with the variational results. For each value of the momentum $k$, the energies of four lowest-lying eigenstates in each of the subspaces with $(S^z, \tau^z) = (0, 0)$, $(1, 1), (1, 0)$, and $(0, 1)$ were calculated. (The subspaces are denoted in Fig. 4 respectively with circles, diamonds, down and up triangles). One can see that our simple variational ansatz is in a qualitative agreement with the Lanczos data for the lowest excited states in the vicinity of the dimer line. It explains the main feature of the Lanczos data, namely, the rather flat dispersions observed nearly everywhere in the dimerized phase. One can also observe the tendency of solitons to have a spectrum with the minimum at an incommensurate value of $k$ when $J_s, J_r$ decrease below certain value (see Fig. 3).

Identification of different types of excitations can be done as follows: Free soliton-antisoliton pairs can have any of the four above-mentioned $(S^z, \tau^z)$ combinations, whose energy would be exactly degenerate in the infinite system; that allows one to identify the soliton states in Fig. 4a-d as highly degenerate (in reality, nearly degenerate) points where several different symbols are sitting on top of each other. $S$-magnons appear as degenerate combination of circle and down triangle, $\tau^0$-magnons should be circles, and $\tau^\pm$-magnons must be up triangles.

The agreement concerning the higher-lying excitations is considerably worse. Only for $\varepsilon = 0$ (see Fig. 4a,b) one can see the isolated magnon branch; for high anisotropies in the vicinity of the multicritical point (Fig. 4f) a large number of states appears immediately above the lowest-lying states appears, which may mean that actually many bound states split from the soliton continuum, and we are able to capture only the lowest-lying, most tightly bound states due to the short-range nature of the magnon ansatz $4\pi$.

IV. DOPED SPIN-ORBITAL MODEL: CHARGED SOLITONS AND THEIR BOUND STATES

It is interesting to study the behavior of the spin-orbital model doped with holes (i.e., away from the quarter filling). In this case one has to consider the corresponding $t$-$J$ model, adding the appropriate hopping term to the Hamiltonian $H(J_s, J_r, \varepsilon)$ determined by Eq. 3:

$$\tilde{H} = \tilde{H}(J_s, J_r, \varepsilon) + t \sum_{l,\sigma\tau} (c^\dagger_{l,\sigma\tau} c_{l+1,\sigma\tau} + \text{h.c.}) \quad (16)$$

Here $c_{l,\sigma\tau}$ are the electron Fermi-operators at the site $l$, $\sigma$ and $\tau$ are the corresponding spin and orbital quantum numbers, and the condition of no double occupancy is implicitly assumed. We also assume, in a similar fashion as in the course of derivation of $4\pi$, that hopping exists only between the nearest neighbors with the same type
of orbitals; the hopping amplitude $t$ is chosen to be negative for the sake of definiteness. One may also wish to add the nearest-neighbor Coulomb repulsion term

$$\widetilde{H} \rightarrow \widetilde{H} + V \sum_i \tilde{n}_i \tilde{n}_{i+1},$$

where $\tilde{n}_i = \sum_{\sigma} c^\dagger_{i,\sigma} c_{i,\sigma}$.

Consider a single hole in this system. If one is on the dimer line $J_x = 3/4$, $J_y = (3 + \varepsilon)/4$, where the checkerboard-type singlet state is exact, it is easy to show that the hole state $|h; n\rangle$ shown schematically in Fig. 8 gets hopped to the neighboring site without disturbing the structure of the ground state, so that the corresponding translational invariant state with momentum $k$ is an exact eigenstate with the energy

$$E_{1h}(k) = 2e_0 + 2t \cos(k), \quad e_0 = \frac{3(3 + \varepsilon)}{16}. \quad (17)$$

Such a state connects two regions with different dimerization pattern, so that it can be viewed as a \"charged soliton\", or a hole bound on a soliton. One can straightforwardly see that a hole state which does not disturb the dimer order is not able to move and has to decay into a \"charged soliton\" and an antisoliton.

The two-hole problem can be also easily studied. The general two-hole state with a total momentum $k$ can be written as

$$\Psi(k) = \sum_{n_1 < n_2} e^{ik(n_1 + n_2)/2} f(n_2 - n_1) |n_1, n_2\rangle, \quad (18)$$

and from the Schrödinger equation one obtains the following system of equations for the function $f(r)$:

$$2t \cos \frac{k}{2} [f(r + 1) + f(r - 1)] = (E_{2h} - 4e_0) f(r), \quad r \geq 2,$$

$$2t \cos \frac{k}{2} f(2) = (E_{2h} - 3e_0 - V) f(1). \quad (19)$$

Setting $f(r) = Ae^{iqr} + Be^{-iqr}$, with the parameter $q$ (having the meaning of the relative momentum) being real, one obtains the continuum of scattering states with the energy

$$E_{2h}(k, q) = 4e_0 + 4t \cos(k/2) \cos(q/2). \quad (20)$$

There is also a bound state solution with $f(r) = f_0 e^{-\kappa r}$; the parameter $\kappa > 0$ is determined by the equation

$$e^{\kappa} = \frac{V - e_0}{2t \cos(k/2)}. \quad (21)$$

This solution describes a localized state with the energy

$$E_{2bh}(k) = 3e_0 + V - \frac{2t^2}{e_0 - V} (1 + \cos k). \quad (22)$$

The spectrum of the 2-hole problem is schematically shown in Fig. 9. One can see that for $V < e_0 - 2|t|$, the energy of this state lies below the lower boundary of the two-hole continuum in the whole range of $k$. When $e_0 < V < e_0 - 2|t|$, the bound state exists only in a certain interval $[k_0, \pi]$ where $k_0$ is determined from (21) by demanding that $\kappa$ is positive; $k_0$ tends to $\pi$ as $V$ tends to $e_0$. For $V > e_0$ the energy of the localized state (22) lies above the upper boundary of the continuum, so that the states are \"antibound.\" Thus, the \"charged solitons\", which are themselves bound states of a hole and a soliton, tend, in their turn, to form bound states, if the condition $e_0 > V$ is satisfied.

One can observe that the general $N$-hole problem is equivalent to that of the XXZ ferromagnet with $J_z = e_0 - V$ and $J_{xy} = 2t$, in external magnetic field $h = e_0 + \tilde{V}$ along the $z$ axis, and thus can be treated by means of the Bethe ansatz. In fact, one can use the known result for the energy of $N$-spin bound complex (21) to translate it into the corresponding formula for our problem:

$$E_N(k) = (e_0 + V) N + \{ (e_0 - V)^2 - 4t^2 \}^{1/2} \times \left\{ \tanh(N/N_0) + \frac{2}{\sinh(2N/N_0)} \sin^2(k/2) \right\},$$

where $N_0$ is defined by the relation

$$\cosh(2/N_0) = (V - e_0)/2t.$$

One can straightforwardly check that (22) is the particular case of (23) for $N = 2$. For large $N$ such a $N$-hole complex corresponds to a classical soliton state in the XXZ ferromagnetic chain. The expression (23) is valid for $|V - e_0| > 2|t|$. It is known (22) that for $|V - e_0| < 2|t|$ only bound (respectively antibound) states with $N = 2$ exist, and the energies of states with larger $N$ fall into the continuum. For $V - e_0 < -2|t|$ the $N$-hole bound complex is stable against the decay into smaller composite particles, i.e.,

$$E_N(k) < \min\{ E_{N-M}(k) + E_M(k') \} ,$$

and the opposite inequality (meaning respectively instability) is fulfilled if $V - e_0 > 2|t|$. Thus, for $V - e_0 < -2|t|$ the ground state of the model (10) at finite doping represents a condensate in which all holes are bound in a single \"particle\" with zero total momentum, i.e., in the intermediate regime $-2|t| < V - e_0 < 2|t|$ only the two-hole bound states are stable, and for $V - e_0 > 2|t|$ all bound states become unstable.

V. SUMMARY

We have studied, by means of the combination of variational and exact results, as well as numerically, the interplay between different types of elementary excitations in the model of an anisotropic spin-orbital chain. We analyze the vicinity of the special \"dimer line\" in the phase
space of the model where the spontaneously dimerized ground state is known exactly. Solitons in the dimer order are shown to be the lowest excitations only in a narrow region of the phase diagram, and the phase transitions are always governed by magnon-type excitations which can be viewed as soliton-antisoliton bound states. It is suggested that an additional phase boundary appears when the anisotropy exceeds certain critical value.

We have considered also a $t$-$J$ version of the doped spin-orbital model. The elementary charge excitation is shown to be a “charged soliton”, or a soliton bound on a hole. We have studied the conditions under which the “charged solitons” tend to form bound states; the exact expression for the energy of the $N$-hole bound complex, based on the known results from the Bethe Ansatz, is presented.

ACKNOWLEDGMENTS

This work was initiated during the “Quantum Magnetism” conference at the Institute for Theoretical Physics, Santa Barbara, and HJM wishes to acknowledge the hospitality and support of the ITP during this conference. AK acknowledges the hospitality of Hannover Institute for Theoretical Physics. This work was supported by the German Federal Ministry for Research and Technology (BMBFT) under the contract 03MI5HAN5.

---

* On leave of absence from the Institute of Magnetism, 36(b) Vernadskii avenue, 03142 Kiev, Ukraine.

1. E. Axtell, T. Ozawa, S. Kauzlarich, and R.R.P. Singh, J. Solid State Chem. 134, 423 (1997).
2. M. Isobe and Y. Ueda, J. Phys. Soc. Jpn. 65, 1178 (1996); Y. Fujii, H. Nakao, T. Yoshihama, M. Nishi, K. Nakajima, K. Kakurai, M. Isobe, Y. Ueda, and H. Sawa, ibid. 66, 326 (1997).
3. I. Kugel and D. I. Khomskii, Sov. Phys. JETP 37, 725 (1973); Sov. Phys. Usp. 25, 231 (1982).
4. Y. Q. Li, M. Ma, D. N. Shi, and F. C. Zhang, Phys. Rev. Lett. 81, 3527 (1998).
5. Y. Yamashita, N. Shibata, and K. Ueda, Phys. Rev. B 58, 9114 (1998).
6. G. V. Uimin, JETP Lett. 12, 225 (1970); C. K. Lai, J. Math. Phys. 15, 1675 (1974); B. Sutherland, Phys. Rev. B 12, 3795 (1975).
7. P. Azaria, A. O. Gogolin, P. Lecheminant, and A. A. Nersesyanyan, Phys. Rev. Lett. 83, 624 (1999); P. Azaria, E. Boulat, and P. Lecheminant, Phys. Rev. B 61, 12112 (2000).
8. C. Itoi, S. Qin, and I. Affleck, Phys. Rev. B 61, 6747 (2000).
9. Yu-Li Lee and Yu-Wen Lee, Phys. Rev. B 61, 6765 (2000).
10. S. K. Pati, R. R. P. Singh, and D. I. Khomskii, Phys. Rev. Lett. 81, 5406 (1998).
11. Y. Yamashita, N. Shibata, and K. Ueda, J. Phys. Soc. Jpn. 69, 242 (2000).
12. A. A. Nersesyanyan and A. M. Tsvelik, Phys. Rev. Lett. 78, 3939 (1997).
13. A. K. Kolezhuk and H.-J. Mikeska, Phys. Rev. Lett. 80, 2709 (1998).
14. W. Yu and S. Haas, cond-mat/0005528.
15. D. Sa and C. Gros, cond-mat/0004023.
16. E. Orignac, R. Citro, and N. Andrei, Phys. Rev. B 61, 11533 (2000).
17. K. Itoh, J. Phys. Soc. Jpn. 68, 322 (1999).
18. M. J. Martins and B. Nienhuis, cond-mat/0004238 (2000).
19. A. K. Kolezhuk and H.-J. Mikeska, Int. J. Mod. Phys. B, 12, 2325 (1998).
20. S. K. Pati and R. R. P. Singh, Phys. Rev. B 61, 5868 (2000).
21. A. A. Ovchinnikov, Sov. Phys. JETP Lett. 5, 38 (1967).
22. A. M. Kosevich, B. A. Ivanov, and A. S. Kovalev, Phys. Rep. 194, 117 (1990).
23. I. G. Gogev, Sov. Phys. JETP 34, 892 (1972).
24. C.N. Yang and C. P. Yang, Phys. Rev 151, 258 (1966).
FIG. 1. The single soliton states $|L\rangle_{\sigma\tau}^n$, $|R\rangle_{\sigma\tau}^n$ used in Eq. (3). The lower and the upper chains correspond to real spins ($S$) and orbital pseudospins ($\tau$), respectively. Thick solid lines denote singlet bonds. The soliton connects two degenerate spontaneously dimerized states which are exact ground states of the model (2) at $J_\tau = 3/4$, $J_s = (3 + \varepsilon)/4$.

\[
|t_{\mu\mu}\rangle = \begin{array}{c}
\text{FIG. 2. Magnon states used in Eqs. (11), (12). Here } \omega = 0 \text{ for } \tau\text{-magnons (i.e., when the upper leg here is the } \tau \text{ chain) and } \\
\omega = \varepsilon \text{ for } S\text{-magnons (the upper leg is the } S \text{ chain).}
\end{array}
\]

\[
|\Delta t_{\mu\mu}\rangle = \begin{array}{c}
\end{array}
\]
FIG. 3. Variational results for the behavior of the gaps for different types of excitations, along the “generalized symmetry line” $J_s = J(1 + \varepsilon/3)$, $J_\tau = J$, for a few values of the anisotropy $\varepsilon$. Magnon gaps (shown by dashed lines) are straight lines. The gap of soliton-antisoliton pair excitations (shown by a solid line) is a straight line while the minimum of the soliton dispersion lies at $k = 0$, and it starts to deviate from a straight line for $J$ below certain threshold value, when the minimum occurs at an incommensurate value of $k$. 
FIG. 4. Behavior of the soliton and magnon excitations along the line $J_s = J_r (1 + \varepsilon/3)$ in the $(J_s, J_r)$ plane for fixed $\varepsilon$. Solid lines indicate the boundaries of the soliton continuum, and isolated long-dashed lines correspond to the magnon-type excitations which can be viewed as soliton-antisoliton bound states. In (f), additional dashed lines near $k = 0$ and $k = \pi$ show the lower boundary of the magnon continuum formed by two $\tau^{+1}$ magnons. Symbols denote the exact diagonalization (Lanczos) data for a system of the length 12 (rungs); circles, diamonds, up and down triangles correspond to the states with the quantum numbers $(S^z, \tau^z) = (0, 0), (1, 1), (0, 1), \text{and} (1, 0)$, respectively. (For $\varepsilon = 0$, up and down triangles are degenerate and thus for the sake of simplicity, only up triangles are displayed).
FIG. 5. A “charged soliton” state $|h; n\rangle$ corresponding to a hole localized on a soliton in the dimer order.

FIG. 6. The spectrum of the two-hole problem, for fixed $e_0$ and $t$, at several different values of $V$, as discussed in the main text. Shaded region denotes the continuum of scattering states formed by a “charged soliton” and “charged antisoliton”; isolated solid and dashed lines correspond to the bound and antibound states, respectively.