Electronic Ladders with SO(5) Symmetry: Phase Diagrams and Correlations at half-filling

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(March 21, 2022)

Abstract

We construct a family of electronic ladder models with SO(5) symmetry which have exact ground states in the form of finitely correlated wave functions. Extensions for these models preserving this symmetry are studied using these states in a variational approach. Within this approach, the zero temperature phase diagram of these electronic ladders at half filling is obtained, reproducing the known results in the weak coupling (band insulator) and strong coupling regime, first studied by Scalapino, Zhang and Hanke. Finally, the compact form of the variational wave functions allows to compute various correlation functions for these systems.

1. INTRODUCTION

The use of symmetries is an important tool to understand the effects of strong correlation in electronic systems. Recently, the SO(3)-symmetry of the antiferromagnetic (AFM) order parameter has been combined with that of d-wave superconductivity to form a five-component vector order parameter. It has been argued that the low energy sector of the resulting theory exhibits an approximate SO(5)-symmetry which allows to explain certain features such as the vicinity AFM order and superconductivity in the phase diagram of the high-$T_c$ materials. Numerical diagonalization studies have been performed and the spectrum
of low lying excitations could in fact be classified according to this symmetry.

A complementary approach has been the attempt to construct microscopic electronic systems with manifest $SO(5)$ invariance and studies of such models to extract the low energy behaviour. Scalapino, Zhang and Hanke succeeded in constructing a two-chain ladder Hamiltonian of this type and studied the strong coupling phase diagram of this system where they were able to identify several distinct phases (Ref. 2, referred to as SZH in the following). The properties of these systems at weak coupling in the metallic regime has been studied by means of bosonization. Such ladder systems, in particular for magnetic insulators have attracted much attention recently due to the existence of various experimental realizations in materials closely related to the high-$T_c$ substances. An interesting observation of Ref. 2 is the existence of an $SO(5)$ superspin phase which has been studied in a variational approach based on finitely correlated matrix product states similar to the ones used for $S = 1$ Haldane magnets. Finitely correlated states have also been considered in electronic systems to describe aspects of the phase diagram of extended Hubbard models and other one-dimensional electronic models.

For $SU(2)$ spin systems the variational approach has been generalized to lattices with ladder geometry and proven to give access to large parts of their phase diagram. This is the motivation for the present work where we extend the matrix product states originally introduced in Ref. 2 to describe the strong coupling physics of the $SO(5)$ superspin phase. We construct manifestly $SO(5)$ invariant many particle wave functions from matrices containing all 16 electronic states on a given rung of the electronic ladder. The relative weight of the six different $SO(5)$ multiplets on a rung is controlled by free parameters which are used to perform a variational study of the zero temperature phase diagram of the ladder at half filling. At strong coupling the results known from Ref. 2 are reproduced within our approach. Furthermore, at weak coupling and sufficiently large interchain hopping amplitude $t_\perp$ the matrix product state correctly describes the gapped ground state of a band insulator corresponding to a filled Fermi sea of electrons with one parity. For intermediate coupling we find a phase with finite amplitude of the $SO(5)$ spinor quartets which are essential for
the presence of a metallic phase of the ladder. The compact form of the variational states allows to study various correlation functions of interest.

In the following section we present the classification of the electronic states of a two-leg ladder system according to the $SO(5)$-symmetry and discuss all possible $SO(5)$ symmetric single rung interactions. In Section III we review the SHZ-model and consider tensor products of rung states to include couplings of neighboring rungs. Section IV deals with various $SO(5)$ symmetric extensions of this model and a general construction routine for systems with exact finitely correlated ground states is given. Section V contains a detailed analysis of the ground state phase diagram of the system in the case of weak and intermediate coupling within a variational approach based on such wave functions. Furthermore we calculate the corresponding correlation functions within this approach. A summary of our results is given in Section VI.

II. ELECTRONIC STATES OF $SO(5)$-SYMMETRIC LADDER MODELS

We consider a two-chain electronic ladder model with canonical creation and annihilation operators $c^\dagger_\sigma(x), c_\sigma(x)$ for electrons (with spin-projection $\sigma = \uparrow, \downarrow$) on sites $x$ of the upper leg and analogous operators $d^\dagger_\sigma(x), d_\sigma(x)$ for the electrons on the lower leg. In order to discuss the $SO(5)$ symmetry of the ladder model and to classify all the 16 possible states on a rung according to this symmetry, these operators are combined into four-dimensional $SO(5)$ spinors:

\[
\Psi_\alpha(x) = \left( c_\uparrow(x), c_\downarrow(x), d^\dagger_\uparrow(x), d^\dagger_\downarrow(x) \right)^T \quad (x \text{ even}) \tag{2.1}
\]

and

\[
\Psi_\alpha(x) = \left( d_\uparrow(x), d_\downarrow(x), c^\dagger_\uparrow(x), c^\dagger_\downarrow(x) \right)^T \quad (x \text{ odd}) \tag{2.2}
\]

Using this definition the ten local generators $L_{ab}$ of the $SO(5)$-algebra on a single rung $x$ are defined as
\[ L_{ab}(x) = -\frac{1}{2} \Psi^\dagger_\alpha(x) \Gamma^{ab}_{\alpha\beta} \Psi_\beta(x), \quad a, b = 1, \ldots, 5. \] (2.3)

Here \( \Gamma^{ab} \) are ten antisymmetric, \( 4 \times 4 \) matrices (their explicit form is given in Appendix A). A convenient basis of the Hilbert space on a single rung is diagonal in the quadratic Casimir charge

\[ C(x) = \sum_{a < b} L^2_{ab}(x). \] (2.4)

In addition we choose to diagonalize the total charge \( Q = \frac{1}{2}(c^\dagger c + d^\dagger d - 2) \) and the \( z \)-component of the spin \( S^z = \frac{1}{2}(c^\dagger \sigma_z c + d^\dagger \sigma_z d) \). Based on the eigenvalues of \( C \) the Hilbert space can be decomposed into six \( SO(5) \) multiplets:

- Three \( SO(5) \) singlets \((C = 0)\), for \( R \) see (A2)

\[
|\Psi_{0,0}^{(1)}\rangle = \left| \frac{c^\dagger d^\dagger}{\sqrt{2}} - \frac{c^\dagger d^\dagger}{\sqrt{2}} \right|_0 = \frac{1}{\sqrt{2}} \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right> - \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right>
\]

\[
|\Psi_{0,0}^{(2)}\rangle = \frac{1}{\sqrt{8}} \Psi^\dagger_\alpha R_{\alpha\beta} \Psi_\beta |\Omega\rangle \sim \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right>
\]

\[
|\Psi_{0,0}^{(3)}\rangle = \frac{1}{\sqrt{8}} \Psi^\dagger_\alpha R_{\alpha\beta} \Psi_\beta |\Omega\rangle \sim \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right>
\] (2.5)

- An \( SO(5) \) vector quintet \((C = 4)\) containing the ferromagnetically polarized state at half filling

\[
|\Psi_{5,\alpha}^{(1)}\rangle \in \left\{ \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right>, \left| \begin{array}{c} \uparrow \downarrow \\ \uparrow \downarrow \end{array} \right>, \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right>, \left| \begin{array}{c} \downarrow \uparrow \\ \downarrow \uparrow \end{array} \right>, \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right> + \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right> \right\} \quad \alpha = 1, \ldots, 5.
\] (2.6)

- Two \( SO(5) \) spinor quartets \((C = 5/2)\) for an odd number of electrons on a given rung

\[
|\Psi_{4,\alpha}^{(1)}\rangle \sim \sqrt{2} \Psi^\dagger_\alpha |\Omega\rangle \in \left\{ \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right>, \left| \begin{array}{c} \uparrow \downarrow \\ \uparrow \downarrow \end{array} \right>, \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right>, \left| \begin{array}{c} \downarrow \uparrow \\ \downarrow \uparrow \end{array} \right> \right\} \quad \alpha = 1, \ldots, 4,
\] (2.7)

\[
|\Psi_{4,\alpha}^{(2)}\rangle \sim \sqrt{2} \Psi^\dagger_\alpha |\Omega\rangle \in \left\{ \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right>, \left| \begin{array}{c} \uparrow \downarrow \\ \uparrow \downarrow \end{array} \right>, \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right>, \left| \begin{array}{c} \downarrow \uparrow \\ \downarrow \uparrow \end{array} \right> \right\} \quad \alpha = 1, \ldots, 4.
\]
We label the states $|\Psi_{d,\alpha}^{(k)}\rangle$ on a rung by the dimension $d$ of the corresponding multiplet $(\alpha = 1, \ldots, d)$ and an additional index $k$. Similarly, we can characterize product states on two rungs (see Sect. III). Alternatively, the vector quintet (2.6) can be constructed from $SO(5)$ spinors $|\Psi_{5,1(2)}^{(1)}\rangle = \frac{1}{\sqrt{2}}(n_1 \pm n_5)|\Omega\rangle$, $|\Psi_{5,3(4)}^{(1)}\rangle = \frac{1}{\sqrt{2}}(n_2 \pm n_3)|\Omega\rangle$ and $|\Psi_{5,5}^{(1)}\rangle = n_4|\Omega\rangle$, with the superspin vector

$$n^a(x) \equiv \frac{1}{2} \Psi^{\dagger}_\alpha(x) \Gamma^a_{\alpha\beta} \Psi_\beta(x), \ a = 1, \ldots, 5.$$ (2.8)

Again, the explicit form of the $4 \times 4$ Dirac $\Gamma$-matrices $\Gamma^a$ is given in Appendix A.

Any electronic ladder model with a local $SO(5)$-symmetry on a rung has to preserve the degeneracy of the energy within the states of each single multiplet. The invariant Hamiltonian on a single rung can therefore be written as a sum over projection operators on these states:

$$h_x = \lambda_5 \sum_{\mu=1}^{5} |\Psi_{5,\mu}^{(1)}\rangle \langle \Psi_{5,\mu}^{(1)}| + \sum_{k,l=1}^{2} \lambda_{4}^{(k,l)} \sum_{\mu=1}^{4} |\Psi_{4,\mu}^{(k)}\rangle \langle \Psi_{4,\mu}^{(l)}| + \sum_{k,l=1}^{3} \lambda_{0}^{(k,l)} |\Psi_{0,0}^{(k)}\rangle \langle \Psi_{0,0}^{(l)}|,$$ (2.9)

where $\lambda_{d}^{(k,l)} = (\lambda_{d}^{(l,k)})^*$ because of the hermiticity of $h_x$. All $SO(5)$-symmetric terms on a rung can be expressed using linear combinations of these projection operators, e.g., the projection operator on the first singlet $|\Psi_{0,0}^{(1)}\rangle$ is

$$\hat{P}^{1,1}_{0,0} = |\Psi_{0,0}^{(1)}\rangle \langle \Psi_{0,0}^{(1)}| = -\frac{1}{3} S^c(x) S^d(x) + \frac{4}{3} (S^c(x) S^d(x))^2,$$ (2.10)

with $\hat{P}^{k,l}_{d,\mu} = |\psi_{d,\mu}^{(k)}\rangle \langle \psi_{d,\mu}^{(l)}|$ and $S^c(x) = \frac{1}{2} \epsilon^c(x) \bar{\sigma} c(x)$. A complete classification of these terms is given in Appendix B. As a simple example we choose

$$\lambda_0 = \begin{pmatrix} -\frac{7}{2} U - 3V & 2\sqrt{2}t_\perp & -2\sqrt{2}t_\perp \\ 2\sqrt{2}t_\perp & U - V & 0 \\ -2\sqrt{2}t_\perp & 0 & U - V \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & -2t_\perp & * \\ * & 0 & * \\ -2t_\perp & * & 0 \end{pmatrix} \quad \text{and} \quad \lambda_5 = \frac{U}{2} + V,$$

which leads to the Hubbard-type Hamiltonian with an $SO(5)$-symmetry introduced by SZH.
where \( J = 4(U+V) \). This condition on the exchange amplitude guarantees the degeneracy between the states in the \( SO(5) \)-quintet and therefore the local \( SO(5) \)-symmetry of the system. We will discuss this model and \( SO(5) \) symmetric extensions in the following sections.

### III. COUPLING OF NEIGHBORING RUNGS

In order to describe an extended quasi-one dimensional electronic system one has to include coupling of neighboring rungs in addition to single rung interactions considered in the previous section. The simplest possible term is an \( SO(5) \) symmetric hopping term between adjacent rungs

\[
-2t_\parallel \sum_{\langle x,y \rangle} \left[ c_\sigma^\dagger(x)c_\sigma(y) + d_\sigma^\dagger(x)d_\sigma(y) + H.c. \right],
\]

which can be brought into a manifestly \( SO(5) \)-symmetric form using the alternating definitions of the spinors \( (2.1), (2.2) \). This hopping term together with the local rung interactions \( (2.11) \) yield the complete SZH-model. The ground state phase diagram of this system in the limit of strong coupling \( (U,V \gg t_\perp, t_\parallel) \) has been determined by SZH using perturbation theory (see Fig. 2). Four different phases have been established at half-filling:

In phase I (occurring for \( 0 \leq V \leq -2U \)) the model can be mapped onto an Ising-like system in a magnetic field: phase \( I_a \) \( (V \geq -U/3) \) is a CDW phase and \( I_b \) \( (V \leq -U/3) \) corresponds to the disordered Ising phase. Phase II is a spin-gap \( d \)-wave phase (product of rung singlets), emerging for \( V \geq -U, U \geq 0 \) and for \( V \geq -2U, U \leq 0 \). The phase III \( (V \leq -U, V \leq 0) \) is the superspin-phase where the \( SO(5) \)-quintet is dominant. For a further examination of this superspin phase, SZH have used the finitely correlated wave function.
\[ |\Psi_0^{SZH}\rangle = \text{Tr} \left( \prod_{x=1}^{L} \Gamma^a n_a |\Omega\rangle \right) \] (3.2)

(summation over the index \(a\) is implied and the trace is taken in the \(4 \times 4\) matrix space where the \(\Gamma^a\) are defined). In this form periodic boundary conditions have been imposed. By adding many particle interactions to their original Hubbard-type Hamiltonian this state (3.2) can be made to be the exact ground state of the resulting model. This state has been argued to capture the essential physics of the superspin phase — similar to the rôle of the AKLT-model as a representative for a Haldane-gapped spin-1 chain. The wave function (3.2) will be the starting point for constructing a generalized matrix product wave function including all 16 states on a rung (see section [V]) and later be used for a variational study of the ground state phase diagram of the SZH model and its various SO(5) symmetric extensions beyond strong coupling (see section [V]). The hopping term (3.1) is one of many possibilities to include interactions between two adjacent rungs of the ladder but the requirement for a local SO(5)-symmetry puts constraints on the explicit form of these terms. Explicit expressions for some of the interaction terms are listed in terms of electron operators in Appendix [B]. For a classification of these additional interactions we consider products of wave functions on two neighboring rungs \(x\) and \(y\). A decomposition into SO(5)-multiplets similar to (2.3 – 2.7) gives 50 different multiplets invariant under the action of the SO(5) generators \(L_{ab}(x, y) = L_{ab}(x) + L_{ab}(y)\). Tensor products containing a singlet factor on one of the rungs are trivial leading to simple product states, e.g. the SO(5) singlets \(|\Psi_{0,0}^{(i)}\rangle_x |\Psi_{0,0}^{(j)}\rangle_y\).

Altogether there are nine singlets, 12 quartets and six quintets of this form. The remaining 169 states are obtained by forming tensor products of quartets (2.7) and quintets (2.6). The decomposition of these products into irreducible representations of SO(5) reads

\[
\begin{align*}
4 \otimes 4 &= 1 \oplus 5 \oplus 10, \\
4 \otimes 5 &= 4 \oplus 16, \\
5 \otimes 5 &= 1 \oplus 10 \oplus 14
\end{align*}
\]
(numbers denote the dimension of the corresponding $SO(5)$ irrep). For example, one of four $SO(5)$-singlets in the tensor product of quartet states (2.7) is

$$|\Psi_{0,0}^{(10)}(x,y)\rangle \equiv \frac{1}{2} \left( -|\Psi_{4,1}^{(1)}|\Psi_{4,3}^{(2)}\rangle - |\Psi_{4,2}^{(1)}|\Psi_{4,4}^{(2)}\rangle + |\Psi_{4,3}^{(1)}|\Psi_{4,1}^{(2)}\rangle + |\Psi_{4,4}^{(1)}|\Psi_{4,2}^{(2)}\rangle \right). \quad (3.3)$$

Similar combinations of the rung states appear in the other states, the Casimir charges of the new multiplets are $C = 6$ for the decuplets, $C = 10$ for the 14-dimensional and $C = 15/2$ for the 16-dimensional representations. The multiplets can be classified further according to the different eigenvalues of $Q$ and $S^z$ on their member states. In Fig. [1] the state content of the various multiplets is shown. In the following we use this classification of the $SO(5)$-multiplets to construct ladder systems with exact ground states including different $SO(5)$ symmetric nearest neighbor interactions.

**IV. EXTENSIONS OF SZH**

As mentioned in the Introduction the finitely correlated wave functions originally introduced to discuss the spin-liquid phases arising in one-dimensional higher spin Heisenberg models have recently been generalized to more general lattices. In particular, ladder models whose ground states are of this form have been constructed. In these spin systems the ground state is of the form $|\Psi_0\rangle = \prod_{x=1}^{L} g_x$ where $g_x$ is a $(2 \times 2)$ matrix containing the different states on a single site or rung $x$ (e.g. spin-1 states for the AKLT model, singlet and triplet states for a two-leg $S = 1/2$ ladder, etc.). Different properties under translation in the extended direction can be realized by an appropriate choice of the free parameters appearing in $g_x$ (e.g. an alternation to introduce dimerization [19]). Within a transfer matrix approach it is straightforward to compute various ground state correlation functions for different boundary conditions, periodic ones correspond to taking the trace of the matrix product wave function [22].

For a further analysis of the SZH-model and the construction of $SO(5)$-symmetric ladder systems with exact ground states in matrix product form we have extended the wave function (3.2) to include the three $SO(5)$-singlets (2.5) and the two $SO(5)$ spinor quartets (2.7).
\[ |\Psi_0\rangle = \text{Tr} \left( \prod_{x=1}^{L} g_x(\{p_i\}) \right). \] (4.1)

Now \( g_x \) is a 5 \( \times \) 5-matrix and \( p_i \) (\( i = 1, \ldots, 6 \)) are variational parameters assigning different weights to the multiplets (2.4) - (2.7) on a rung (see Appendix A). We restrict ourselves to the translational invariant case, where the parameters \( p_i \) are chosen to be independent of the rung position \( x \). In this case the matrix product wave function on two neighboring rungs contains two \( SO(5) \) singlets, two quartets, one quintet and one decuplet. The 14-dimensional and 16-dimensional representations are absent by construction. The states of the matrix product are linear combinations of the basis in Sect. III above, their explicit form is rather complicated. With respect to the spin-\( SU(2) \) subalgebra the remaining multiplets present in the matrix product contain spin singlet, doublet and triplet states only (states with total spin polarization \( S^z > 1 \) are members of the 14 and 16-dimensional representation, see Fig. III). An immediate consequence is that the ansatz cannot be expected to describe the formation of ferromagnetic domains with higher spin states. An analogous argument holds for higher values of the charge \( Q \), corresponding to strong local deviations from half filling.

There is a simple way to construct spin ladder systems with matrix product wave functions as ground states\( ^3 \) and a generalization to electronic ladder models with an \( SO(5) \)-symmetry is straightforward. The starting point is a general \( SO(5) \)-symmetric Hamilton operator on two neighboring rungs

\[
h_{x,x+1} = \sum_{k,l=1}^{4} \lambda_{16}^{(k,l)} \sum_{\mu=1}^{16} \hat{P}_{16,\mu}^{k,l} + \sum_{\mu=1}^{14} \lambda_{14} \hat{P}_{14,\mu}^{k,l} + \sum_{k,l=1}^{5} \lambda_{10}^{(k,l)} \sum_{\mu=1}^{10} \hat{P}_{10,\mu}^{k,l} + \sum_{k,l=1}^{10} \lambda_{5}^{(k,l)} \sum_{\mu=1}^{5} \hat{P}_{5,\mu}^{k,l} + \sum_{k,l=1}^{16} \lambda_{4}^{(k,l)} \sum_{\mu=1}^{4} \hat{P}_{4,\mu}^{k,l} + \sum_{k,l=1}^{14} \lambda_{0}^{(k,l)} \hat{P}_{0,0}^{k,l}, \] (4.2)

where \( \hat{P}_{d,\mu}^{k,l} = |\psi_{d,\mu}^{(k)}\rangle\langle\psi_{d,\mu}^{(l)}| \) are projection operators on all possible \( SO(5) \)-multiplets (see section III). The states \( |\psi_{d,\mu}^{(k)}\rangle \) are product wave functions on two rungs, \( k \) and \( l \) label the multiplet, \( \mu \) the states in the multiplet and \( d \) is the corresponding dimension of this
irreducible representation. The hermiticity of \( h_{x,x+1} \) requires \( \lambda_d^{(k,l)} = (\lambda_d^{(l,k)})^* \) for the coupling constants, leaving altogether 322 free parameters in the Hamiltonian. A Hamiltonian \( H = \sum_x h_{x,x+1} \) has a finitely correlated ground state \( |\Psi_0\rangle = \prod_x g_x \) with zero energy provided that the following conditions are satisfied:

- \( h_{x,x+1} \) has to annihilate all states contained in the matrix elements of the product \( g_x g_{x+1} \)

- all other eigenstates of \( h_{x,x+1} \) have positive energy

Starting with an ansatz for \( g_x \) in (4.1), one has to identify all multiplets \( |\psi_{d,i_d}\rangle \) contained in the product wave function \( g_x g_{x+1} \). These multiplets are labelled by indices \( i_d = 1, ..., g_d \) where the maximum number \( g_d \) is the number of multiplets with an equal Casimir-charge \( (d \) is the dimension of the irreducible representation), e.g. \( g_{10} = 2 \) if the product wave function on two neighboring rungs contains two independent \( SO(5) \) decuplets. After the determination of the multiplet content of \( |\Psi_0\rangle \) the corresponding parameters \( \lambda_d^{(k,i_d)} \) in \( h_{x,x+1} \) are set to zero to fulfill the first condition. The remaining operators in (4.2) will now project on states not included in the matrix product wave function, which leads to zero energy for the ansatz. To satisfy now the second condition the reduced matrices \( \lambda_d^{(k,l)} \) (\( l \neq i_d \)) have to be chosen positive definite (i.e. positive eigenvalues) such that (4.1) will be the lowest energy state of the system.

In principle a general Hamiltonian where our ansatz (4.1) is the exact ground state, can be built by operators projecting on the other remaining \( SO(5) \)-multiplets (e.g. the 14-dimensional and the four 16-dimensional representations) and it has 249 free coupling constants \( \lambda_d^{(k,l)} \) (\( l \neq i_d \)). We give explicit expressions for some of these operators in terms of electron operators in Appendix B3. In general however, the structure of these projection operators is quite complicated making it difficult to motivate these exactly solvable systems on physical grounds.
V. VARIATIONAL STUDIES OF THE PHASE DIAGRAM

An examination of the SZH model beyond strong coupling can be done by using (4.1) as a variational wave function. This wave function leads to the variational energy

\[ E_{\text{rung}} = \langle \Psi_0 | H_{\text{Coulomb}} | \Psi_0 \rangle \sim \left( p_2^2 + p_3^2\right)\left(U/2 - V\right) + 5p_6^2(U/2 + V) - p_1^2\left(\frac{7}{2}U + 3V\right) \]

for the spin and charge interaction on a rung (see equation 2.12). Here \( p_6 \) is the parameter corresponding to the \( SO(5) \)-quintet, \( p_1 \) is the weight of the singlet \( |\Omega\rangle \) and \( p_{2,3} \) of the symmetric and antisymmetric linear combinations of the other \( SO(5) \)-singlets (2.5). The variational energy corresponding to the hopping term on a rung is

\[ E_{t_\perp} = \langle \Psi_0 | H_{\text{Hopping}} | \Psi_0 \rangle \sim t_\perp \left[ 8p_1p_2 + 2\left(\frac{p_5^2}{h_2} - p_4^2\right) \right] (w - h_1) \]

and between two neighboring rungs (see equation 3.4) it is

\[ E_{t_\parallel} \sim t_\parallel \left[ p_4p_5\left(25p_6^2 + p_1^2 - p_2^2 - p_3^2\right) + h_2\left(p_2p_3 - 5p_1p_6\right) + \left(p_4^2 - p_5^2\right)\left(5p_2p_6 - p_1p_3\right) \right]. \]

where \( h_1 = 5p_6^2 + p_1^2 + p_2^2 + p_3^2, h_2 = p_4^2 + p_5^2 \) and \( w = \sqrt{h_1^2 + 16h_2^2} \).

In the strong coupling limit one can neglect these hopping terms (5.2, 5.3). Minimizing the energy with respect to the \( p_i \) reproduces exactly the phase diagram calculated by SZH within perturbation theory (Fig. 2) where the phases are fixed by the largest amplitude \( p_i \) of the corresponding state and the crossover is continuous. The phase I is dominated by the bonding singlet state with amplitude \( p_2 \), phase III is the superspin phase (\( p_6 \)) and phase II consists of products of rung singlets (\( p_1 \)). In this approach with translationally invariant \( p_i \) the crossover between the two Ising-phases can not be reproduced. We now extend this analysis of the phase diagram of the SZH model to weak and intermediate coupling.

A. Weak coupling phase diagram

The band structure of the non-interacting system at half-filling is well known. For \( U = V = 0 \) there are two energy bands, given by
\[ \epsilon_{\pm}(k) = \pm 2t_\perp - 4t_\parallel \cos(k), \quad -\pi \leq k \leq \pi \] (5.4)

and two different cases have to be distinguished:

For \( t_\perp < 2t_\parallel \) the Fermi energy intersects the two bands (see Fig. 3(a)) and for \( t_\perp \geq 2t_\parallel \) they are separated by an energy gap (see Fig. 3(b)). The gapless system \((t_\perp < 2t_\parallel)\) has been studied using bosonization of the low lying modes in the vicinity of the four Fermi points to obtain the phase diagram for weak coupling \((U, V \ll t_\perp, t_\parallel)\): Lin et al.\(^4\) found that at half filling the system is driven towards an integrable SO(8)-symmetric Gross-Neveu model in a weak coupling renormalization group analysis and predicted the occurrence of additional phases compared to the strong coupling case. The ongoing debate of these results (see the criticism of Ref. 23) cannot be clarified within the present ansatz: Using finitely correlated wave functions always leads to an exponential decay of correlation functions, indicating the existence of an energy gap between the ground state and the first excited state.

**B. Phase diagram for \( t_\perp \geq 2t_\parallel \)**

For \( t_\perp \geq 2t_\parallel \) the variational ansatz gives the exact ground state for the non-interacting system \((U = V = 0)\):

Choosing \( p_1 = -\frac{1}{\sqrt{2}}, p_2 = \frac{1}{\sqrt{2}} \) and \( p_i \equiv 0 \) for \( i = 3, \ldots, 6 \) we find

\[ |\Psi_0\rangle \sim \prod_{x=1}^{L} \left(-c^\dagger_x d^\dagger_x + c^\dagger_x d^\dagger_x - d^\dagger_x d^\dagger_x - c^\dagger_x c^\dagger_x\right)(x) |0\rangle, \] (5.5)

which corresponds to complete filling of the modes with energy \( \epsilon_-(k) \) in (5.4), the band insulator. Consequently, we expect the variational approach to give reasonable results for the weak coupling phase diagram in this regime of hopping amplitudes. The quality of the approach can be measured by the mean deviation \( \sqrt{\langle (\Delta H)^2 \rangle} = \sqrt{\langle H^2 \rangle - \langle H \rangle^2} \) of the energy. For \( U, V \ll t_\perp, t_\parallel \) the mean deviation stays small compared to the energy so that the ansatz should give reliable results.

We find that only two phases are present in the weak coupling case (see Fig. 4): the Ising phase I \((p_2)\) and the spin-gap d-wave phase II \((p_1)\) already known from the strong
coupling diagram (see Fig. 2). The superspin phase disappears and also the $SO(5)$-quartets have no significant weight ($p_4, p_5, p_6 \sim 0$) as expected for a band insulator.

Considering the complete ground state phase diagram (see Fig. 4) we find an additional phase for intermediate coupling ($U, V \approx t_\perp, t_\parallel$) where the $SO(5)$-quartets have the largest weight, in particular the rung-symmetric one $|Q_α^+⟩$ (A5). Apart from these, the symmetric singlet state $⟨Ψ^{α}_RΨ^{β}_R − Ψ^{α}_LΨ^{β}_L|Ω⟩$ — which determines the ground state in phase $I$ — has a significant weight. Due to the resonating structure of the ansatz and the relatively large variational value of $⟨(ΔH)^2⟩$ the phase boundaries are not very accurate — for a more detailed study of this question the present work should be complemented by a numerical approach. As discussed earlier it is not possible within this approach to determine the position of the crossover line between the two Ising phases, or even whether this transition still occurs for the case of weak or intermediate coupling.

C. Ground State Correlations

The physics in the ground state is determined by ground state correlation functions, which are easily computed from matrix product wave functions. The matrix product ansatz (4.1) with the six free parameters $p_i$ represents the ground state for a large class of models. We have calculated various correlation functions explicitly in the thermodynamic limit ($L \to \infty$) for this variety of models (a detailed list is given in Appendix C) and we determined the correlation length and the amplitude of different ground state correlations for the SZH-model when we used the ansatz as a variational wave function.

The two-point correlations in matrix product states are always short-ranged (if not vanishing) and have the following form

$$⟨O^{\dagger}(r)O(0)⟩ = A(\{p_i\}) e^{-rt}$$

They exhibit an exponential decay with the correlation length $\xi$ and amplitude $A(\{p_i\})$. As an example we consider the correlation length and amplitude of the expectation value of the
spin-spin correlation function \( \langle \vec{S}_{c,d}(r) \vec{S}_{c,d}(0) \rangle \) (see Fig. 3) and of field correlators \( \langle c^\dagger_\alpha(r)c_\beta(0) \rangle \), \( \alpha, \beta \in \{ g, u \} \) (Fig. 3) for the SZH-model on a circle in the \( U-V \)-plane (with \( U^2 + V^2 = 3 \)) intersecting the phases I, II and the quartet phase (see Fig. 4).

The spin-spin correlation function \( \langle \vec{S}_{c,d}(r) \vec{S}_{c,d}(0) \rangle \) in Fig. 3 is non-vanishing only in the quartet phase but with an extremely small correlation length indicating strong nearest neighbor correlations. For the electron-electron correlation in Fig. 6 with \( c_{g,u}(x) = (c_\uparrow(x) + c_\downarrow(x)) \pm (d_\uparrow(x) + d_\downarrow(x)) \) the correlation length \( \xi \) is small for all angles \( \phi \) but with a very large amplitude \( A \) except in the quartet phase.

The sharp peak in both diagrams at \( \phi \sim \frac{5}{8}\pi \) indicate the crossover of the phases II and I in Fig. 4 where the correlation length diverges. Calculating these correlations in the strong coupling limit the phase boundaries in Fig. 4 are denoted by very sharp peaks in the electron-electron correlation length \( \xi_{(c^\dagger g,u(r)c_{g,u}(0))} \) with a non-vanishing amplitude. The spin-spin correlations are zero in the whole phase diagram and give no further hints of an underlying structure in the system.

D. Variational examination of \( SO(5) \)-symmetric extensions

Our variational approach is also suitable to study the phase diagrams of various \( SO(5) \)-symmetric extensions of the SZH model. We have considered additional interactions on a single rung and between two neighboring rungs, using the construction routine of section IV and V.

1. Single rung interactions

All single rung interactions can be constructed using the projection operators of Sect. I and a detailed list of all possible terms can be found in the Appendix I. Taking into account the operators \( \hat{P}^{k,l}_{d,\mu} \) with the coupling constants \( \lambda^{(k,l)}_d \) leads to the following contributions to the variational energy (5.1), calculated with the ansatz (4.1)
\[ \langle \hat{P}_{1,(0,0)}^{1,1} \rangle = \frac{p_1^2}{w} \]  
\[ \langle \hat{P}_{2,(0,0)}^{2,2} \rangle = \frac{1}{2w} (p_2 + p_3)^2 \]  
\[ \langle \hat{P}_{3,(0,0)}^{3,3} \rangle = \frac{1}{2w} (p_2 - p_3)^2 \]  
\[ \langle \hat{P}_{1,(0,0)}^{1,2} + \hat{P}_{2,(0,0)}^{2,1} \rangle = \frac{\sqrt{2}}{w} p_1 (p_3 + p_2) \]  
\[ \langle \hat{P}_{1,(0,0)}^{1,3} + \hat{P}_{3,(0,0)}^{3,1} \rangle = \frac{\sqrt{2}}{w} p_1 (p_3 - p_2) \]  
\[ \langle \hat{P}_{2,(0,0)}^{2,3} + \hat{P}_{3,(0,0)}^{3,2} \rangle = \frac{1}{w} (p_2^2 - p_3^2) \]  
\[ \sum_{\mu} \langle \hat{P}_{(4,\mu)}^{1,1} \rangle = \frac{w - h_1}{2wh_2} (p_4 - p_5)^2 \]  
\[ \sum_{\mu} \langle \hat{P}_{(4,\mu)}^{2,2} \rangle = \frac{w - h_1}{2wh_2} (p_4 + p_5)^2 \]  
\[ \sum_{\mu} \langle \hat{P}_{(4,\mu)}^{1,2} + \hat{P}_{(4,\mu)}^{2,1} \rangle = \frac{w - h_1}{wh_2} (p_4^2 - p_5^2) \]  
\[ \sum_{\mu} \langle \hat{P}_{(5,\mu)}^{0,0} \rangle = \frac{5p_6^2}{w} \]  

These modifications of the model cause some changes in the ground state phase diagram, e.g. the simple terms like (a) and (j) will only shift the phase boundaries without changing the general structure of the phase diagram. Other interactions like the pair hopping term (f)

\[ t_{\text{pair}} \left( d_\uparrow \dagger c_\uparrow c_\downarrow + \text{h.c.} \right) \sim \hat{P}_{(0,0)}^{2,3} + \hat{P}_{(0,0)}^{3,2} \]  

will dramatically change the phase diagram (see Fig. 7).

For small negative values of \( t_{\text{pair}} \) (\(| t_{\text{pair}} | \leq t_{||} \)) the Ising-phase I of the phase diagram in Fig. 4 with the amplitude \( p_2 \) splits into two singlet phases: a symmetric (\( p_2 \)) and an antisymmetric phase (\( p_3 \)) (see Fig. 4a, \( t_{\text{pair}} = -1 \)), where the crossover line has the same gradient (\( U = -2V \)). Increasing the amplitude of \( t_{\text{pair}} \) leads to a pure antisymmetric phase (see Fig. 4b, \( t_{\text{pair}} = -4 \)) in I and also to a strong change of the shape of the quartet phase. For small positive values of \( t_{\text{pair}} \) the general structure of the phase diagram is preserved (like Fig. 4). In the regime of the coupling constants with \( t_{\text{pair}} \gg t_{||} \) the quartet phase vanishes (see Fig. 8).
Other interactions also exhibit strong effects on the phase diagram, e.g. including a quartet term like (i) which contains a hopping term on a rung and a bond-charge interaction (see App. B).

\[
t_{\text{quar}} \left[ (c_{\uparrow}^\dagger d_{\uparrow} + h.c.) (1 - (n_{c_{\downarrow}} - n_{d_{\downarrow}})^2) + \uparrow\leftrightarrow\downarrow \right]
\]  \quad (5.8)
leads to different phase diagrams, depending on the coupling constant. For positive values of \( t_{\text{quar}} \) the quartet phase vanishes with increasing values of the coupling constant (like in Fig. 8) until there are only the three known phases (see Fig. 8a). For \( t_{\text{quar}} < 0 \) the quartet phase grows (see Fig. 8b), dominated by the symmetric combination \( (p_4) \) of the states.

The mean deviation in the weak coupling limit in these two special cases (5.7, 5.8) is small compared to the energy (calculated on a circle with radius \( R = 0.1 \) around \( U = V = 0 \)) except for the value \( t_{\text{quar}} \leq -1 \). The ansatz also provides very good results in the strong coupling limit \( (R \geq 100) \), except for the crossover lines to the superspin phase where the mean deviation is very large. The same problem occurs in the intermediate coupling regime in the quartet phase where the ansatz is not a good eigenstate of the system.

We expect that including the other interactions on a rung will lead to similar changes in the ground state phase diagram.

2. Two-rung interactions

In most cases the \( SO(5) \)-symmetric interactions between two neighboring terms have a very complex structure but for some of them we can give simple expressions (see Appendix B). For them we can calculate the corresponding variational energy, e.g. the two-pair hopping term leading to an \( SO(5) \) singlet-singlet transition

\[
t_{2\text{-pair}} \left[ d_{\uparrow}(x)d_{\uparrow}(y)d_{\downarrow}(x)d_{\downarrow}(y)c_{\uparrow}(x)c_{\uparrow}(y)c_{\downarrow}(x)c_{\downarrow}(y) + h.c \right]
\]  \quad (5.9)
giving \( E_{2\text{-pair}} \sim 2t_{2\text{-pair}} (p_2 + p_3)^2 (p_3 - p_2)^2 \). The other \( SO(5) \)-singlet interactions on two rungs lead to similar expressions, which will change the phase diagram (Fig. 4) in the Ising phase according to the value of the coupling constant \( t_{2\text{-pair}} \).
Including an $SO(5)$-quartet interaction in the SZH-model (see eqn. (B18)) gives the variational energy

$$E = t_{qxy} \frac{w - h_1}{2wh_2 (w + h_1)} \left( p_2^2 - p_3^2 \right) \left( p_4^2 - p_5^2 \right).$$

The phase diagrams obtained for different values of the coupling constant $t_{qxy}$ are very similar to the phase diagram in Fig. 4. The additional interaction has no significant effect except for minor changes of the crossover lines.

\section*{VI. SUMMARY AND OUTLOOK}

We have constructed a large class of electronic ladder models with $SO(5)$ symmetry having finitely correlated ground states and, consequently, correlation functions exhibiting exponential decay. These matrix product states have been used to perform a variational study of the ground state phase diagram of the SZH model for $t_{\perp} \geq 2t_{\parallel}$. For vanishing coupling the ground state of the band insulator is found to be in the class of variational states and at strong coupling the phases identified by SZH are reproduced. In the intermediate coupling regime signatures of a new phase dominated by local $SO(5)$-quartets are found, and at weak coupling the $SO(5)$ superspin phase is absent. Within our approach it is possible to compute various correlations giving further insights into the nature of the phases which have been identified. Finally, we have introduced various $SO(5)$ symmetric extensions to the SZH model and discussed their impact on the phase diagram. In the future we will include dimerization in the matrix product ansatz for further studies of the Ising transition in phase I and the possibility of spontaneous breaking of translational invariance in exactly solvable models.

\section*{ACKNOWLEDGEMENTS}

This work has been supported in parts by the Deutsche Forschungsgemeinschaft under Grant No. Fr 737/3–1.
APPENDIX A: THE GAMMA MATRICES AND THE VARIATIONAL WAVE FUNCTION

For the construction of the $SO(5)$-invariant quantities, we have used the representation of the matrices in Ref. 2. The five Dirac $\Gamma$-matrices have the following form

$$
\begin{align*}
\Gamma^1 &= \begin{pmatrix} 0 & -i\sigma_y \\ i\sigma_y & 0 \end{pmatrix}, \\
\Gamma^{2,3,4} &= \begin{pmatrix} \bar{\sigma} & 0 \\ 0 & \bar{\sigma} \end{pmatrix}, \\
\Gamma^5 &= \begin{pmatrix} 0 & \sigma_y \\ \sigma_y & 0 \end{pmatrix}, \\
\end{align*}
$$

(A1)

where $\bar{\sigma}$ are the Pauli matrices. The matrices $\Gamma^{ab}$ are defined by $\Gamma^{ab} \equiv -i/2 [\Gamma^a, \Gamma^b]$ and the matrix $R$ is given by

$$
R \equiv \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}.
$$

(A2)

Using these definitions, it is simple to construct the matrix $g_x$ of the variational wave function (4.1). It has the following structure

$$
g_x = \begin{pmatrix} p_0 \Gamma^a n_a |\Omega\rangle + \sum_{i=1}^{3} p_i |\tilde{\Psi}^{(i)}_{0,0}\rangle \mathbb{1} \\ -|q_3\rangle - |q_4\rangle & |q_1\rangle & |q_2\rangle & 0 \end{pmatrix}
$$

(A3)

The three $SO(5)$-singlets are included in this ansatz only on the main diagonal elements. $|\tilde{\Psi}^{(1)}_{0,0}\rangle \equiv |\Psi^{(1)}_{0,0}\rangle$ from (2.3) and $|\tilde{\Psi}^{(2,3)}_{0,0}\rangle$ are the symmetric and an antisymmetric combinations of the two other singlets

$$
|\tilde{\Psi}^{(2,3)}_{0,0}\rangle \sim \left( \Psi^\dagger_{\alpha} R_{\alpha\beta} \Psi^\dagger_{\beta} \mp \Psi_{\alpha} R_{\alpha\beta} \Psi_{\beta} \right)|\Omega\rangle.
$$

(A4)

The quartets enter the matrix $g_x$ in $|q_\alpha\rangle = p_4 |Q^{+}_\alpha\rangle + p_5 |Q^{-}_\alpha\rangle$ where $|Q^{\pm}_\alpha\rangle$ are the symmetric and antisymmetric combinations of (2.7)

$$
|Q^{\pm}_\alpha\rangle \sim \left\{ \left| \begin{array}{c} \uparrow \\ \downarrow \end{array} \right| \pm \left| \begin{array}{c} \downarrow \\ \uparrow \end{array} \right| , \left| \begin{array}{c} \uparrow \\ \uparrow \end{array} \right| \mp \left| \begin{array}{c} \downarrow \\ \downarrow \end{array} \right| \left| \begin{array}{c} \uparrow \downarrow \\ \uparrow \downarrow \end{array} \right|, \left| \begin{array}{c} \downarrow \\ \downarrow \end{array} \right| \pm \left| \begin{array}{c} \uparrow \downarrow \\ \uparrow \downarrow \end{array} \right| \right\}.
$$

(A5)
They are arranged in the right column and the lowest row of $\begin{bmatrix} A_3 \end{bmatrix}$ in such a way that in the product $g_x g_{x+1}$ one has $SO(5)$-singlets on the diagonal only.

**APPENDIX B: $SO(5)$-SYMMETRIC OPERATORS ON ONE RESP. TWO RUNGS**

We present here a selection of various $SO(5)$-symmetric terms on a single and on two rungs (B1,B2). Furthermore, a list of terms is given for which our matrix product ansatz (4.1) would be the lowest energy state (B3).

1. **Single rung interactions**

We now present all possible $SO(5)$-symmetric terms on a rung. Their general construction is done in terms of projection operators on the different $SO(5)$-multiplets. Expressed through electronic operators most of them are already known from the SZH-model (2.11) and an additional biquadratic exchange. As a shorthand notation we introduce

$$U, V, J, \alpha \equiv U \left( (n_{c\uparrow}(x) - \frac{1}{2})(n_{c\downarrow}(x) - \frac{1}{2}) + (c \rightarrow d) \right) + V (n_c(x) - 1)(n_d(x) - 1) + J \vec{S}_c(x)\vec{S}_d(x)$$

$$+ \alpha (\vec{S}_c(x)\vec{S}_d(x))^2$$

In addition we find various single electron and pair hopping terms together with bond-charge type interactions. Using the notation of Sect. I for the projection operators on a rung we obtain the following terms by projection on the singlets

$$\hat{P}_{0,0}^{1,1} = |\Psi_{0,0}^{(1)}\rangle\langle\Psi_{0,0}^{(1)}| = \begin{bmatrix} 0, 0, -\frac{4}{3}, \frac{4}{3} \end{bmatrix}$$

$$\hat{P}_{0,0}^{2,2} = \begin{bmatrix} \frac{1}{2}, 1, \frac{2}{3}, \frac{4}{3} \end{bmatrix} + \frac{1}{2} \left[ n_{d\uparrow}n_{d\downarrow}(1 - n_c) - c \leftrightarrow d \right]$$

$$\hat{P}_{0,0}^{3,3} = \begin{bmatrix} \frac{1}{2}, 1, \frac{2}{3}, \frac{4}{3} \end{bmatrix} - \frac{1}{2} \left[ n_{d\uparrow}n_{d\downarrow}(1 - n_c) - c \leftrightarrow d \right]$$

$$\hat{P}_{0,0}^{1,2} + \hat{P}_{0,0}^{2,1} = \frac{1}{\sqrt{2}} \left[ (c_{\uparrow}d_{\uparrow} + h.c.) n_{d\downarrow}(n_{c\downarrow} - 1) + \uparrow\downarrow \rightarrow \downarrow\uparrow \right]$$

$$\hat{P}_{0,0}^{1,3} + \hat{P}_{0,0}^{3,1} = -\frac{1}{\sqrt{2}} \left[ (c_{\uparrow}d_{\uparrow} + h.c.) n_{c\downarrow}(n_{d\downarrow} - 1) + \uparrow\downarrow \rightarrow \downarrow\uparrow \right]$$

$$\hat{P}_{0,0}^{2,3} + \hat{P}_{0,0}^{3,2} = d_{\downarrow}d_{\downarrow}c_{\uparrow}c_{\uparrow} + h.c.$$
The projection operators on the quartet states read

\[
\sum_{\mu=1}^{4} \hat{P}_{1,\mu}^{4,1} = \left[ 0, 0, -\frac{8}{3}, -\frac{16}{3} \right] + (1 - n_{c\uparrow}n_{c\downarrow})n_{d\uparrow} + n_{d\downarrow}n_{d\uparrow}(n_{c} - 2) \tag{B8}
\]

\[
\sum_{\mu=1}^{4} \hat{P}_{2,\mu}^{4,2} = \left[ 0, 0, -\frac{8}{3}, -\frac{16}{3} \right] + (1 - n_{d\uparrow}n_{d\downarrow})n_{c\uparrow} + n_{c\downarrow}n_{c\uparrow}(n_{d} - 2) \tag{B9}
\]

\[
\sum_{\mu=1}^{4} \hat{P}_{1,\mu}^{4,1} + \hat{P}_{2,\mu}^{4,2} = \left[ (c_{\uparrow}^\dagger d_{\uparrow} + h.c.)(1 - (n_{c\downarrow} - n_{d\downarrow})^2) + \uparrow\leftrightarrow\downarrow \right], \tag{B10}
\]

and finally, projection on the quintet gives

\[
\sum_{\mu=1}^{5} \hat{P}_{5,\mu}^{5} = \left[ 1, \frac{1}{2}, \frac{13}{3}, \frac{20}{3} \right]. \tag{B11}
\]

2. Interactions between neighboring rungs

Equivalently, the \(SO(5)\)-symmetric expressions on two rungs can be classified. The choice of the basis on the two-rung system is very important for the structure of the \(SO(5)\)-symmetric terms. Using the simplest combination the product of an \(SO(5)\)-singlet on one rung and another \(SO(5)\) multiplet on the other gives for a projection operator e.g.

\[
\sum_{\mu=1}^{5} \hat{P}_{5,\mu}^{5,1}(x, y) = \hat{P}_{0,0}^{1,1}(x) \sum_{\mu=1}^{5} \hat{P}_{5,\mu}(y) \tag{B12}
\]

for the product of an \(SO(5)\)-singlet on rung \(x\) and an \(SO(5)\)-quintet on \(y\), where \(\hat{P}_{k,l}^{d,\mu}\) is defined in section [II]. The numbers \(k\) and \(l\) in \(\hat{P}_{k,l}^{d,\mu}\) depend on the way the different multiplets on the rungs are labelled. Another example is an operator projecting on an \(SO(5)\)-singlet on each of the rungs

\[
\hat{P}_{0,0}^{2,2}(x, y) = |\Psi_{0,0}^{(2)}(x, y)\rangle\langle\Psi_{0,0}^{(2)}(x, y)| = \hat{P}_{0,0}^{1,1}(x)\hat{P}_{0,0}^{2,2}(y). \tag{B13}
\]

(see equation (2.3) for the definition of the wave functions). All projection operators of states consisting of at least one \(SO(5)\)-singlet on a rung can be decomposed in the same manner. For some of these operators a compact representation in terms of electron operators is possible. As an example consider the operator

\[
20
\]
\[ c_\uparrow(x)c_\downarrow(x)d_\uparrow(y)d_\downarrow(y)c_\uparrow(y)c_\downarrow(y)d_\uparrow(x)d_\downarrow(x) + h.c. \] (B14)

describing pair exchange between two neighboring rungs. It causes a transition between two \( SO(5) \) singlet states and can be written as

\[ \sim \hat{P}^{3,2}_{0,0}(y)\hat{P}^{3,2}_{0,0}(x) + h.c. \] (B15)

Other \( SO(5) \) singlet-singlet transitions of this type are

\[
d_\uparrow(x)d_\downarrow(y)d_\uparrow(x)d_\downarrow(y)c_\uparrow(x)c_\downarrow(y)c_\uparrow(y)c_\downarrow(y) + h.c ,
\]

\[
N_d(y)n_{c\uparrow}(y)n_{c\downarrow}(y) \left[ d_\uparrow(x)d_\downarrow(x)c_\uparrow(x)c_\downarrow(x) + h.c. \right] , \tag{B16}
\]

\[
N_c(x)n_{d\uparrow}(x)n_{d\downarrow}(x) \left[ c_\uparrow(y)c_\downarrow(y)d_\uparrow(y)d_\downarrow(y) + h.c \right] ,
\]

where

\[ N_\alpha(y) = \left( 1 - n_{\alpha\uparrow}(y) - n_{\alpha\downarrow}(y) + n_{\alpha\uparrow}(y)n_{\alpha\downarrow}(y) \right), \quad \alpha \in \{c, d\} \] (B17)

Similar terms are obtained from projection operators on direct products of an \( SO(5) \)-singlet on one and an \( SO(5) \)-quartet on the other rung, e.g.

\[
\left[ (n_{c\uparrow}(x) - n_{d\uparrow}(x))^2 - 1 \right] c_\uparrow(x)c_\downarrow(x)c_\uparrow(y)c_\downarrow(y)d_\uparrow(x)d_\downarrow(x)d_\uparrow(y)d_\downarrow(y) + h.c \] (B18)

The projection operators on the remaining 169 states with a structure similar to (3.3) cannot easily be decomposed in this way. They are significantly more complex, generically their expansion into electronic operators produces complicated bond-charge interaction terms. Still, forming suitable linear combinations of such terms can lead to simpler \( SO(5) \)-symmetric terms on two rungs, e.g. the pair hopping term in (3.1) or a diagonal hopping term

\[
\sum_{(x,y)} \left[ d_\uparrow(x)c_\sigma(y) - c_\uparrow(x)d_\sigma(y) + h.c. \right] . \tag{B19}
\]
3. SO(5)-symmetric Hamiltonians with exact Ground States

At the end of section IV we claimed that a general Hamiltonian where our ansatz \((4.1)\) is the ground state of the system is given by

\[
h_{x,x+1} = \sum_{k,l=1}^{4} \lambda_{16}^{(k,l)} \sum_{\mu=1}^{16} \hat{P}_{16,\mu} + \sum_{\mu=1}^{14} \lambda_{14} \hat{P}_{14,\mu} + \text{additional terms.} \quad \text{(B20)}
\]

The coupling constants have to be chosen such that \(\lambda_{14} > 0\) and the matrix \(\lambda_{16}\) of coupling constants is positive definite. This implies that \(E = 0\) is a lower bound on the spectrum and therefore the state \((4.1)\) — having zero energy by construction — will be a ground state. The additional terms in \((B20)\) are the projection operators on the remaining multiplets not present in the matrix product wave function. For example the projection operator on one of the \(SO(5)\)-singlets not present in this product reads

\[
\lambda_{0}^{(k,l)}\left[-c^{\dagger}_x(x)c^{\dagger}_y(y)c^{\dagger}_x(x)c^{\dagger}_y(y)d^{\dagger}_x(x)d^{\dagger}_y(y) + n_{d\uparrow}(x)n_{d\uparrow}(y)n_{d\downarrow}(x)n_{d\downarrow}(y)N_c(x)N_c(y) \right] \quad \text{(B21)}
\]

Just as \(\lambda_{16}\) above the matrices \(\lambda_{d}\) \((d = 0, 4, 5, 10)\), coupling the projection operators on the remaining multiplets have to be chosen to be positive definite.

APPENDIX C: CORRELATION FUNCTIONS

The calculation of expectation values between matrix product states is straightforward using a transfer matrix method (see e.g. Ref. 22):

To this end we define a \(25 \times 25\) transfer matrix \(G\) on a rung

\[
G_{\alpha_1,\alpha_2} \sim G_{(i_1,j_1),(i_2,j_2)} \equiv g^{\dagger}_{(i_1,i_2)}g_{(j_1,j_2)} \quad \text{(C1)}
\]

with the indices

\[
\alpha_1 = 1, \ldots, 25 \leftrightarrow (11), \ldots, (15), (21), \ldots, (55).
\]

In terms of \(G\) the norm of the ground state can be written as
\[ \langle \Psi_0 \mid \Psi_0 \rangle = \text{Tr} \ G^L = \sum_{i=1}^{25} \lambda_i^L \]  

where \( \lambda_i \) are the eigenvalues of \( G \). In the thermodynamic limit \((L \to \infty)\) the largest eigenvalue \( \lambda_1 \) dominates this expression and we obtain \( \langle \Psi_0 | \Psi_0 \rangle \sim \lambda_1^L \). Similarly, one-point correlators of an operator \( O \) are

\[ \langle O \rangle = \frac{1}{\lambda_1} \langle e_1 | Z(O) | e_1 \rangle \]  

and a two-point correlation function reads

\[ \langle O_1^\dagger O_r \rangle = \sum_{n=1}^{25} \frac{1}{\lambda_n^2 \lambda_1} \left( \frac{\lambda_n}{\lambda_1} \right)^r \langle e_1 | Z(O_1) | e_n \rangle \langle e_n | Z(O_r) | e_1 \rangle. \]  

Here \( | e_n \rangle \) are the eigenvectors with eigenvalue \( \lambda_n \) of \( G \) and \( Z(O_i) \sim g^\dagger O_i g \) is the transfer matrix related to the operator \( O_i \). With the matrix \([A3]\) the largest eigenvalue of \( G \) is given by

\[ \lambda_1 = \frac{1}{2} (h_1 + w) \]  

with \( h_1 = 5p_6^2 + p_1^2 + p_2^2 + p_3^2, \ h_2 = p_4^2 + p_5^2 \) and \( w = \sqrt{h_1^2 + 16h_2^2} \).

This enables us to calculate the expectation values of any operator acting on a single or two rungs, respectively. For example, we find

\[ \langle \vec{S} \rangle = 0, \quad \langle (S^i)^2 \rangle = \frac{w - h_1 + 8p_6^2}{4w} \]  

for local magnetic moments and

\[ \langle c_{g(u)}^\dagger(x) c_{g(u)}(x) \rangle = \frac{1}{w} \left[ \frac{w - h_1}{h_2} (p_6^2 + 3p_4^2) + 2h_1 + 4p_1 p_2 \right] \]  

\[ \langle c_\alpha^\dagger(x) c_\beta(x) \rangle = \frac{1}{w} \left[ \frac{w - h_1}{h_2} (2p_4 p_5 - 4p_2 p_3) \right], \quad \alpha \neq \beta \]  

for electronic expectation values. Here, \( \alpha, \beta \in \{g, u\} \) and \( c_{g(u)}(x) = (c_\uparrow(x) + c_\downarrow(x)) \pm (d_\uparrow(x) + d_\downarrow(x)) \).

Correlations between the total spin on two rungs decay exponentially

\[ \langle \vec{S}_1 \vec{S}_r \rangle = -\frac{3}{4w(h_1 + w)} \left( \frac{h_1 - 4p_6^2}{\lambda_1} \right)^r \left( \frac{w - h_1 + 8p_6^2}{h_1 - 4p_6^2} \right)^2 \]
as expected for finitely correlated states. Spin-spin correlations between individual sites on
rungs separated by a distance \( r \) can be expressed as

\[
\langle \vec{S}_\alpha(r) \vec{S}_\beta(0) \rangle = A_{\alpha\beta}(\{p_i\}) \left( \frac{h_1 - 4p_6^2}{\lambda_1} \right)^r + B_{\alpha\beta}(\{p_i\}) \left( \frac{h_1 - 8p_6^2}{\lambda_1} \right)^r,
\]

\[(C10)\]

where the amplitudes \( A_{\alpha\beta}(\{p_i\}) \) and \( B_{\alpha\beta}(\{p_i\}) \) depend on the choice of \( \alpha \) and \( \beta \), i.e. whether
correlators of spins on the same or on different legs of the ladder are considered. Analogously,
one can study electronic correlations, e.g.

\[
\langle c^\dagger_g(r) c^\dagger_u(r) c_g(0) c_u(0) \rangle = -\frac{8}{3} \langle \vec{S}_1 \vec{S}_r \rangle
\]

\[
\langle c^\dagger_{g,u}(r) c_{g,u}(0) \rangle = C_{g,u}(\{p_i\}) \left( \frac{h_2}{\lambda_1} \right)^r + D_{g,u}(\{p_i\}) \left( -\frac{h_2}{\lambda_1} \right)^r.
\]

\[(C11)\]

with the amplitudes \( C_{g,u} \) and \( D_{g,u} \).
REFERENCES

1 S. Zhang, Science 275, 1089 (1997).

2 D. Scalapino, S. Zhang, and W. Hanke, Phys. Rev. B 58, 443 (1998).

3 D. G. Shelton and D. Sénéchal, Phys. Rev. B 58, 6818 (1998).

4 H. Lin, L. Balents, and M. Fisher, Phys. Rev. B 58, 1794 (1998).

5 E. Dagotto and T. M. Rice, Science 271, 618 (1996).

6 I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Phys. Rev. Lett. 59, 799 (1987).

7 M. Fannes, B. Nachtergaele, and R. Werner, Europhys. Lett. 10, 633 (1989).

8 A. Klümper, A. Schadschneider, and J. Zittartz, J. Phys. A 24, L955 (1991).

9 M. Nakamura, Phys. Rev. B 61, 16377 (2000).

10 M. Nakamura, K. Itoh, and N. Muramoto. [cond-mat/0003413].

11 D. Dmitriev, V. Krivnov, and A. Ovchinnikov, Phys. Rev. B 61, 14592 (2000).

12 E. H. Kim, G. Sierra, and D. Duffy, Phys. Rev. B 60, 5169 (1999).

13 A. Kolezhuk and H.-J. Mikeska, Int. J. Mod. Phys. B 12, 2325 (1998).

14 S. Brehmer, A. K. H.-J. Mikeska, and U. Negebauer, J. Phys.: Condens. Matter 10, 1103 (1998).

15 U. Negebauer and H.-J. Mikeska, Z. Phys. B 99, 151 (1996).

16 K. Totsuka and M. Suzuki, J.Phys.: Condens. Matter 7, 1639 (1995).

17 S. Rabello, H. Kohno, E. Demler, and S.-C. Zhang, Phys. Rev. Lett. 80, 3586 (1998).

18 A. Kolezhuk and H.-J. Mikeska, Phys. Rev. B 56, R11380 (1997).

19 A. Kolezhuk and H.-J. Mikeska, Eur. Phys. J. B 5, 543 (1998).
20 S. Brehmer, H.-J. Mikeska, and U. Neugebauer, J. Phys. Condens. Matter 8, 7161 (1996).

21 A. Koleshuk and H.-J. Mikeska, Phys. Rev. Lett. 80, 2709 (1998).

22 A. Klümper, A. Schadschneider, and J. Zittartz, Z. Phys. 87, 281 (1992).

23 V. Emery, S. Kivelson, and O. Zachar, Phys. Rev. B 59, 15641 (1999).
FIG. 1. The irreducible $SO(5)$ representations appearing on a pair of rungs decomposed corresponding to the eigenvalues of $Q$ and $S^z$: (a) the quartet (with Casimir charge $C = 5/2$), (b) the quintet ($C = 4$), (c) the ten-dimensional ($C = 6$), (d) the 14-dimensional ($C = 10$) and (e) 16-dimensional ($C = 15/2$) irrep (double circle indicate two states with identical eigenvalues).
FIG. 2. Strong coupling phase diagram, $U$ and $V$ measured in units of $t_{\parallel}$

FIG. 3. Band structure of a two-leg ladder model for (a) $t_{\perp} = t_{\parallel}$ and (b) $t_{\perp} = 2t_{\parallel}$
FIG. 4. Phase diagram for $t_{\perp} = 2t_{\parallel}$ ($t_{\parallel} = 1$): the phase boundaries were calculated by comparing the amplitudes of the different multiplets.

FIG. 5. Correlation length and amplitude for the spin-spin correlation function, the full line corresponds to $\langle \vec{S}_{c(d)}(r)\vec{S}_{c(d)}(0) \rangle$ and the dotted to $\langle \vec{S}_{c(d)}(r)\vec{S}_{d(c)}(0) \rangle$. 
FIG. 6. The correlation length and amplitude of the expectation value \( \langle c_{g,u}^\dagger(r)c_{g,u}(0) \rangle \), the full line corresponds to \( \langle c_{g(u)}^\dagger(r)c_{g(u)}(0) \rangle \) and the dotted to \( \langle c_{g(u)}^\dagger(r)c_{u(g)}(0) \rangle \).

FIG. 7. Phase diagram for \( t_\perp = 2t_\parallel \) including pair hopping for (a) \( t_{\text{pair}} = -t_\parallel \) and (b) \( t_{\text{pair}} = -4t_\parallel \) with \( t_\parallel = 1 \).
FIG. 8. Phase diagram for $t_\perp = 2t_\parallel$ including pair hopping for $t_{\text{pair}} = 4t_\parallel$ with $t_\parallel = 1$.

FIG. 9. Phase diagram for $t_\perp = 2t_\parallel$ including a quartet term with (a) $t_{\text{quar}} = +4t_\parallel$ and (b) $t_{\text{quar}} = -4t_\parallel$ with $t_\parallel = 1$. 