Quantum phase transitions in the exactly solved spin-1/2 Heisenberg–Ising ladder

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Abstract
The ground-state behaviour of the frustrated quantum spin-1/2 two-leg ladder with the Heisenberg intra-rung and Ising inter-rung interactions is examined in detail. The investigated model is transformed into the quantum Ising chain with composite spins in an effective transverse and longitudinal field by employing either the bond-state representation or the unitary transformation. It is shown that the ground state of the Heisenberg–Ising ladder can be descended from three exactly solvable models: the quantum Ising chain in a transverse field, the ‘classical’ Ising chain in a longitudinal field or the spin-chain model in a staggered longitudinal–transverse field. The last model serves in evidence of the staggered bond phase with alternating singlet and triplet bonds on the rungs of a two-leg ladder, which appears at moderate values of the external magnetic field and consequently leads to a fractional plateau at a half of the saturation magnetization. The ground-state phase diagram totally consists of five ordered phases and one quantum paramagnetic phase, which are separated from each other either by the lines of discontinuous or continuous quantum phase transitions. The order parameters are exactly calculated for all five ordered phases and the quantum paramagnetic phase is characterized through different short-range spin–spin correlations.

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(Some figures may appear in colour only in the online journal)

1. Introduction
Quantum spin models with competing interactions represent a quite interesting and challenging topic for the current research \cite{1, 2}. Such models show many unusual features in their ground-state properties and are very sensitive to the approximative schemes applied to them. An existence of exact solutions is therefore quite important, since they provide rigorous
information about the complex behaviour of frustrated models. However, exact results for such systems are still limited (see [3] and references cited therein). The simplest examples of rigorously solved quantum spin models are the models with the known dimerized [3–6] or even trimerized [7] ground states. Another example represents frustrated quantum spin antiferromagnets in high magnetic fields with the so-called localized-magnon eigenstates (see e.g. [8] for recent review). It should be nevertheless noted that the aforementioned exact results are usually derived only under certain constraints laid on the interaction parameters, and those models are not tractable generally.

On the other hand, the exact solutions for some spin-1/2 quantum spin ladders with multispin interaction allows us to also find, besides the ground state, thermodynamic properties quite rigorously [9, 10]. Exactly solvable models, which admit the inclusion of frustration, can also be constructed from the Ising models where the decorations of quantum spins are included [11, 12]. The decoration–iteration procedure allows one to calculate exactly all thermodynamic properties of the decorated models when the exact solution for the corresponding Ising model is known. The distinctive feature of these models is that the quantum decorations are separated from each other, so that the Hamiltonian can be decomposed into the sum of commuting parts. The eigenstates of the total Hamiltonian are then simply factorized into a product of the eigenstates of its commuting parts.

New findings of the exactly solvable frustrated quantum spin models with non-trivial (not simply factorizable) ground states are thus highly desirable. This paper deals with the frustrated quantum spin-1/2 two-leg ladder with the Heisenberg intra-rung interaction and the Ising inter-rung interactions between nearest-neighbouring spins from either the same or different leg. Such a model can be regarded as an extension of the spin-1/2 Heisenberg–Ising bond alternating chain, which was proposed and rigorously solved by Lieb et al. [13]. Alternatively, this model can also be viewed as the generalization of the exactly solved quantum compass ladder [14–16] when considering the Heisenberg rather than $XZ$-type intra-rung interaction and accounting for the additional frustrating Ising inter-rung interaction. Moreover, it is quite plausible to suspect that the exact results presented hereafter for the spin-1/2 Heisenberg–Ising two-leg ladder may also bring insight into the relevant behaviour of the corresponding Heisenberg two-leg ladder, which represents a quite challenging and complex research problem in its own right [17, 18]. The frustrated spin-1/2 Heisenberg two-leg ladder has been extensively investigated by employing various independent numerical and analytical methods such as density-matrix renormalization group [19–22], numerical diagonalization [22–26], series expansion [26], bosonization technique [27–29], strong and weak-coupling analysis [30–34], valence-bond spin-wave theory [36], variational matrix-product approach [37, 38] and bond mean-field theory [39–41]. Among the most interesting results obtained for this quantum spin chain, one could mention the existence of the columnar-dimer phase discussed in [32, 33] or the presence of the fractional plateau in the magnetization process examined in [22–25, 34].

The theoretical investigation of two-leg ladder models is motivated not only from the academic point of view, but also from the experimental viewpoint because the two-leg ladder motif captures the magnetic structure of a certain class of real quasi-one-dimensional magnetic materials. The most widespread family of two-leg ladder compounds form cuprates, in which one finds both experimental representatives with the dominating intra-rung interaction, such as SrCu$_2$O$_3$ [42, 43], Cu$_2$((CH$_2$)$_2$N$_2$)$_2$Cl$_4$ [44–47], (C$_5$H$_{12}$N)$_2$CuBr$_4$ [48], (5IAp)$_2$CuBr$_4$ [49], as well as the magnetic compounds with the dominating intra-leg interaction, such as KCuCl$_3$ [50, 51], TiCuCl$_3$ [52–54], NH$_4$CuCl$_3$ and KCuBr$_3$. Understanding the low-temperature magnetism of two-leg ladder models also turns out to be crucial for an explanation of the mechanism, which is responsible for the high-temperature superconductivity of cuprates [55].
Besides the cuprates, other experimental representatives of the two-leg ladder compounds represent vanadates (VO)2P2O7 [56], CaV2O5 and MgV2O5 [57], as well as the polycrystal BIP-BNO [58, 59].

The outline of the paper is as follows. In section 2, the model is defined and the pseudospin representation is considered. The ground-state properties of the model with and without the external field are studied in section 3. The most important findings are summarized in section 4.

2. Heisenberg–Ising two-leg ladder

Let us define the spin-1/2 Heisenberg–Ising ladder through the following Hamiltonian:

$$
H = \sum_{i=1}^{N} \left[ J_1 (s_{1,i} \cdot s_{2,i})_{\Lambda} + J_2 (s_{1,i}^x s_{2,i+1}^x + s_{1,i}^y s_{2,i+1}^y + s_{1,i}^z s_{2,i+1}^z) + J_3 (s_{1,i}^y s_{2,i+1}^y + s_{1,i}^z s_{2,i+1}^z) - h (s_{1,i}^z + s_{2,i}^z) \right],
$$

(1)

where \((s_{1,i} \cdot s_{2,i})_{\Lambda} = s_{1,i}^x s_{2,i}^x + s_{1,i}^y s_{2,i}^y + s_{1,i}^z s_{2,i}^z\) are three spatial projections of spin-1/2 and \(J_1, J_2, J_3\) are three Heisenberg (Ising) bonds. These states are the eigenstates of the Heisenberg coupling between two spins located on the \(i\)th rung, i.e., \(|\phi_{0,0}^i\rangle\) is the singlet-bond state, \(|\phi_{1,0}^i\rangle\) and \(|\phi_{1,\pm}^i\rangle\) are triplet states. Following

*Figure 1. Quantum spin-1/2 Heisenberg–Ising two-leg ladder. Thick (thin) lines denote the Heisenberg (Ising) bonds.*

It can be checked that the z-projection of total spin on a rung \(S_z^i = s_{1,i}^z + s_{2,i}^z\) commutes with the total Hamiltonian \([S_z^i, H] = 0\) and, hence, it represents a conserved quantity. For further convenience, it is therefore advisable to take advantage of the bond representation, which has been originally suggested by Lieb et al for the Heisenberg–Ising chain [13]. Let us introduce the bond-state basis consisting of four state vectors:

$$
|\phi_{0,0}^i\rangle = \frac{1}{\sqrt{2}} (|\downarrow, \uparrow, \uparrow, \downarrow\rangle - |\uparrow, \downarrow, \downarrow, \uparrow\rangle), \quad |\phi_{1,0}^i\rangle = \frac{1}{\sqrt{2}} (|\downarrow, \downarrow, \uparrow, \uparrow\rangle + |\uparrow, \uparrow, \downarrow, \downarrow\rangle),
$$

$$
|\phi_{1,-}^i\rangle = \frac{1}{\sqrt{2}} (|\downarrow, \uparrow, \downarrow, \uparrow\rangle - |\uparrow, \downarrow, \uparrow, \downarrow\rangle), \quad |\phi_{1,+}^i\rangle = \frac{1}{\sqrt{2}} (|\downarrow, \uparrow, \downarrow, \uparrow\rangle + |\uparrow, \downarrow, \uparrow, \downarrow\rangle).
$$

(2)

These states are the eigenstates of the Heisenberg coupling between two spins located on the \(i\)th rung, i.e., \(|\phi_{0,0}^i\rangle\) is the singlet-bond state, \(|\phi_{1,0}^i\rangle\) and \(|\phi_{1,\pm}^i\rangle\) are triplet states. Following
two subspaces can be singled out in the bond space: (i) $|\phi_{0,0}\rangle$, $|\phi_{1,0}\rangle$ and (ii) $|\phi_{1,+}\rangle$, $|\phi_{1,-}\rangle$. The first and second subspaces correspond to $(S_z)^2 = 0$ and $(S_z)^2 = 1$, respectively, and the Hamiltonian can be diagonalized separately in each subspace. We can introduce the index of subspace at the $i$th site: $n_i = 0(1)$ if the given state is in the subspace with $(S_z)^2 = 0 ((S_z)^2 = 1)$ spanned by states $|\phi_{0,0}\rangle$, $|\phi_{1,0}\rangle$, $|\phi_{1,+}\rangle$, $|\phi_{1,-}\rangle$. According to [13], let us also call the bond states purity (impurity) states if $n_i = 0(1)$. If one makes pseudospin notations for the states $|\phi_{0,0}\rangle = |\uparrow\rangle_0$, $|\phi_{1,0}\rangle = |\uparrow\rangle_1$, the action of the spin-1/2 operators in the subspace $n_i = 0$ can be expressed in terms of new raising and lowering operators:

$$
s_i^+ = -\frac{1}{2}(a_i^+ + a_i) = -\tilde{s}_i^+, \quad s_i^- = \frac{1}{2}(a_i^+ + a_i) = \tilde{s}_i^-,
$$

$$
(s_1 \cdot s_2)_\Delta = a_1^+ a_2 - \frac{2 + \Delta}{4} = \tilde{s}_i^+ - \frac{\Delta}{4}.
$$

The operators $a_i^+$ and $a_i$ satisfy the Pauli algebra $\{a_i, a_i^+\} = 0, \{a_i, a_j\} = \{a_i^+, a_j^+\} = 0, [a_i, a_j] = [a_i, a_i^+] = [a_i^+, a_i^+] = 0$ for $i \neq j$, and half of their sum can be identified as a new pseudospin operator $\tilde{s}_i^+$. Analogously, one can consider the pseudospin representation of the subspace $n_i = 1$ with $|\phi_{1,+}\rangle = |\downarrow\rangle_1$, $|\phi_{1,-}\rangle = |\downarrow\rangle_0$ and find the action of spin operators in it as follows:

$$
s_i^+ = \frac{1}{2}(a_i^+ + a_i) = \tilde{s}_i^+, \quad s_i^- = \frac{1}{2}(a_i^+ + a_i) = \tilde{s}_i^-,
$$

$$
(s_1 \cdot s_2)_\Delta = a_1^+ a_2 - \frac{2 + \Delta}{4} = \tilde{s}_i^+ - \frac{\Delta}{4}.
$$

Combining (3) and (4) we find the general expressions for the pseudospin representation of these operators, which are valid in both subspaces:

$$
s_i^+ = (2n_i - 1)\tilde{s}_i^+, \quad s_i^- = \tilde{s}_i^-, \quad (s_1 \cdot s_2)_\Delta = (1 - n_i)\tilde{s}_i^+ + \frac{\Delta}{4}(2n_i - 1).
$$

The effective Hamiltonian can be rewritten in terms of new operators as follows:

$$
H = \sum_{i=1}^{N} \left\{ J_1(1 - n_i)\tilde{s}_i^+ - 2hn_0\tilde{s}_i^+ + \frac{J_1\Delta}{4}(2n_i - 1)
+ [4J_2n_in_{i+1} - 2(J_2 - J_3)(n_i + n_{i+1} - 1)]\tilde{s}_i^+\tilde{s}_{i+1}^+ight\}.
$$

It is noteworthy that equation (5) can be considered as some nonlinear spin transformation from $s_i^+$ to new operators $\tilde{s}_i^+$, $\tilde{s}_i^-$, where e.g. $s_i^+ = (n_i - \frac{1}{2})$, $\tilde{s}_i^+ = \frac{n_i}{2}$. The transformation can be generated by the following unitary operator:

$$
U = \prod_{i=1}^{N} \exp\left[-\frac{\pi}{2}(s_i^+ + s_{i+1}^-)\right] \exp\left(i\pi s_i^+ s_{i+1}^-\right) \exp\left(-\frac{\pi}{2}s_i^+\right) \exp\left(i\pi s_{i+1}^+\right).
$$

The crucial point is the second factor, which introduces the nonlinearity. Other terms are the rotation in spin space, they are used to adjust the transformed operators to the form of (5). Finally, the spin operators are transformed as follows:

$$
U s_1^+ U^+ = s_1^+, \quad U s_1^- U^+ = 2s_1^+ s_2^-, \quad U s_1^+ U^+ = 2s_1^+ s_2^-.
$$

$$
U s_2^+ U^+ = 2s_1^+ s_2^-, \quad U s_2^- U^+ = -2s_1^+ s_2^-, \quad U s_2^+ U^+ = s_2^-.
$$

The transformed Hamiltonian has the form of the quantum Ising chain with composite spins in an effective longitudinal and a transverse magnetic field:

$$
UHU^+ = \sum_{i=1}^{N} \left\{ \frac{J_1}{2}(1 - 2s_i^+)s_{i+1}^+ + \frac{J_1\Delta}{2}s_i^+ + J_2(4s_i^+ s_{i+1}^+ + 1)
+ 2J_3(s_i^+ + s_{i+1}^-)s_i^+ s_{i+1}^- - h(1 + 2s_i^+)s_{i-1}^+ + h(s_{i+1}^+ - h(s_i^+ s_{i+1}^-)s_i^+ s_{i+1}^-).
$$

(9)
The straightforward correspondence $s^i_1 = n_i - \frac{1}{2}$, $s^i_2 = s^i$ leads to the equivalence between the Hamiltonians (6) and (9). It should be noted that such a representation also remains valid in the case of the asymmetric ladder having both diagonal (crossing) Ising interactions different from each other.

3. Ground state of the Heisenberg–Ising two-leg ladder

The Hamiltonian (6) can also be rewritten in the following more symmetric form:

$$ H = \sum_{i=1}^{N} \left\{ J_1 (1 - n_i) s^i_1 - 2 h n_i s^i_1 + \frac{J_1 \Delta}{4} (2 n_i - 1) ight\} + [2 (J_2 + J_3) n_i n_{i+1} + 2 (J_2 - J_3) (1 - n_i) (1 - n_{i+1})] \hat{s}_i \hat{s}_{i+1}. $$

(10)

This form serves as evidence that the effective model splits at the $i$th site into two independent chains provided that two neighbouring bonds are in different subspaces, i.e. $n_i \neq n_{i+1}$. The uniform Hamiltonians, when all $n_i = 0$ or all $n_i = 1$, read

$$ H^0 = \sum_{i=1}^{N} \left[ J_1 (s^i_1 - \Delta/4) + 2 (J_2 - J_3) \hat{s}_i \hat{s}_{i+1} \right]. $$

(11)

$$ H^1 = \sum_{i=1}^{N} \left[ 2 (J_2 + J_3) \hat{s}_i \hat{s}_{i+1} - 2 h \hat{s}_i + \frac{J_1 \Delta}{4} \right]. $$

(12)

If all bonds are in purity states ($n_i = 0$), one obtains the effective Hamiltonian of the Ising chain in the transverse field that is exactly solvable within Jordan–Wigner fermionization [60, 61]. If all bonds are in impurity states ($n_i = 1$), one comes to the Ising chain in the longitudinal field that is solvable by the transfer-matrix method (see e.g. [62]). Accordingly, the ground-state energy of the model in $n_i = 0$ subspace is given by [61]

$$ e^0_i = \lim_{N \to \infty} \frac{E^0_i (N)}{N} = - (J_1 + |J_2 - J_3|) \frac{\pi}{2} \text{E} \left( \sqrt{1 - \gamma^2} \right) - \frac{J_1 \Delta}{4}, $$

(13)

where $\gamma = \frac{J_2 - J_3}{J_2 + J_3}$ and $\text{E} (\kappa) = \int_0^\pi d\theta \sqrt{1 - \kappa^2 \sin^2 \theta}$ is the complete elliptic integral of the second kind.

The ground-state energy of the model in $n_i = 1$ subspace is given by the ground-state energy of the effective Ising chain in the longitudinal field:

$$ e^1_i = \lim_{N \to \infty} \frac{E^1_i (N)}{N} = \begin{cases} \frac{J_1 \Delta}{4} + \frac{J_2 + J_3}{2} - |h|, & \text{if } |h| > (J_2 + J_3), \\ \frac{J_1 \Delta}{4} - \frac{J_2 + J_3}{2}, & \text{if } |h| \leq (J_2 + J_3). \end{cases} $$

(14)

The upper (lower) case corresponds to the ferromagnetically (antiferromagnetically) ordered state being the ground state at strong (weak) enough magnetic fields.

3.1. Ground-state phase diagram in a zero field

If the external field vanishes ($h = 0$), it is sufficient to show that the inequality $E^0_i (N_1) + E^0_i (N_2) \geq E^0_i (N_1 + N_2)$ holds for any finite transverse Ising chain with free ends in order to prove that the ground state always corresponds to a uniform bond configuration. Here, $E^0_i (N)$ denotes the ground-state energy of the Hamiltonian:

$$ H^0 (N) = 2 (J_2 - J_3) \sum_{i=1}^{N-1} \hat{s}_i \hat{s}_{i+1} + J_1 \sum_{i=1}^{N} \left( \hat{s}_i - \Delta/4 \right), $$

(15)
Indeed, two independent chains of sizes $N_1$ and $N_2$ can be represented by the following Hamiltonian:

$$H^0(N_1, N_2) = 2(J_2 - J_3) \sum_{i=1}^{N_1-1} \hat{s}_i^x \hat{s}_{i+1}^x + 2(J_2 - J_3) \sum_{i=N_1}^{N_1+N_2-1} \hat{s}_i^x \hat{s}_{i+1}^x + J_1 \sum_{i=1}^{N_1+N_2} \left( \hat{s}_i^z - \frac{\Delta}{4} \right).$$

$$= H^0(N_1 + N_2) - 2(J_2 - J_3) \hat{s}_{N_1}^z \hat{s}_{N_1+1}^z. \quad (16)$$

If $E^0_0(N)$ and $|\psi^N_0\rangle$ are the lowest eigenvalue and eigenstate of $H^0(N)$, then $E^0_0(N_1, N_2) = E^0_0(N_1) + E^0_0(N_2)$ and $|\psi^N_0\rangle = |\psi^N_0\rangle|\psi^N_0\rangle$ are the lowest eigenvalue and eigenstate of $H^0(N_1, N_2)$. Now, it is straightforward to show that

$$E^0_0(N_1) + E^0_0(N_2) = \langle \psi^N_0|H^0(N_1 + N_2)|\psi^N_0\rangle - 2(J_2 - J_3)\langle\psi^N_0|\hat{s}_{N_1}^z|\psi^N_0\rangle\langle\psi^N_0|\hat{s}_{N_1+1}^z|\psi^N_0\rangle \geq E^0_0(N_1 + N_2). \quad (17)$$

Here, we have used that $\langle \psi^N_0|\hat{s}_{N}^z|\psi^N_0\rangle = 0$ for any finite chain $[13, 61]$, and that the lowest mean value of the operator $H^0(N_1 + N_2)$ is achieved in its ground state.

It is easy to show by straightforward calculation that the same property is valid for the Ising chain with free ends in zero longitudinal field, i.e.

$$E^0(N_1 + N_2) = E^0(N_1) + E^0(N_2) + \frac{|J_2 + J_3|}{2} \leq E^0_0(N_1) + E^0_0(N_2). \quad (18)$$

Now, let us prove that the ground state of the whole model may correspond only to one uniform bond configuration. It can be readily understood from (10) that the effective Hamiltonian does not contain an interaction between spins from two neighbouring bonds if they are in different subspaces $[63]$. It means that the effective model splits into two independent parts at each boundary (domain wall) between the purity and impurity states. Thus, the Heisenberg–Ising ladder for any given configuration of bonds can be considered a set of independent chains of two kinds and of different sizes. Then, the ground-state energy of any randomly chosen bond configuration will be as follows:

$$E = E^0_0(N_1) + E^0_0(N_2) + \cdots + E^0_0(M_1) + E^0_0(M_2) + \cdots \geq E^0_0(N_1 + N_2 + \cdots) + E^0_0(M_1 + M_2 + \cdots). \quad (19)$$

It is quite evident from equations (17) and (18) that the one uniform configuration, which corresponds to the state with lower energy than the other one, must be according to inequality (19) the lowest energy state (i.e. ground state). Therefore, the model may show in the ground state the first-order quantum phase transition when the lowest eigenenergies in both subspaces becomes equal $e^0_1 = e^0_0$. Besides, there also may appear the more striking second-order (continuous) quantum phase transition at $|J_1| = |J_2 - J_3|$ in the ground state, which is inherent to the pure quantum spin chain $[61]$. From this perspective, the Heisenberg–Ising ladder can show a variety of quantum phase transitions in its phase diagram.

The ground-state phase diagram of the spin-1/2 Heisenberg–Ising ladder in a zero magnetic field is shown in figure 2. It reflects the symmetry of the model, i.e. it is invariant under the exchange of the Ising interactions $J_2$ and $J_3$, as well as under the simultaneous change of the signs of $J_2$ and $J_3$. Altogether, five different ground states can be recognized in figure 2.

(i) Quantum paramagnetic (QPM) state for $e^0_0 < e^0_1$, and $|J_1| > |J_2 - J_3|$: the equivalent transverse Ising chain (11) is in the gapped disordered state with no spontaneous magnetization $\langle \hat{s}_i^z \rangle = 0$ and non-zero magnetization $\langle \hat{s}_i^z \rangle \neq 0$ induced by the effective transverse field. For the initial Heisenberg–Ising ladder, it means that the rung singlet dimers are dominating on Heisenberg bonds in the ground state. Although each bond may
possess the antiferromagnetic order, the interaction along legs demolishes it and leads to the disordered quantum paramagnetic state.

(ii) *Stripe Leg (SL) state* for $e_0^L < e_0^P$ and $|J_1| < J_1 - J_2$: the equivalent transverse Ising chain exhibits the spontaneous ferromagnetic ordering with $\langle \hat{S}^z_i \rangle \neq 0$. Due to relations (3) and (4), one obtains for the Heisenberg–Ising ladder $\langle \hat{S}^z_{i,1} \rangle = \langle \hat{S}^z_{i,1} \rangle = -\langle \hat{S}^z_{i,2} \rangle = -\langle \hat{S}^z_{i,2} \rangle \neq 0$. This result is taken to mean that the Heisenberg–Ising ladder shows a ferromagnetic order along legs and antiferromagnetic order along rungs, i.e. the magnetizations of chains are opposite. The staggered magnetization as the relevant order parameter in this phase is non-zero and it exhibits evident quantum reduction of the magnetization given by $m^*_{SL} = \frac{1}{N} \sum_{i=1}^{N} (\langle \hat{S}^z_{i,1} \rangle - \langle \hat{S}^z_{i,2} \rangle) = \frac{1}{2} [1 - J_1^2 / (J_1 - J_2)^2]^{1/2}$. Here, we used the result for the spontaneous magnetization of transverse Ising chain [61].

(iii) *Néel state* for $e_0^L < e_0^P$ and $|J_1| < J_2 - J_3$: the effective transverse Ising chain shows the spontaneous antiferromagnetic ordering with $\langle \hat{S}^z_i \rangle = (-1)^i m^*_i \neq 0$. For the Heisenberg–Ising ladder, one consequently obtains $\langle \hat{S}^z_{i,1} \rangle = -\langle \hat{S}^z_{i,1} \rangle = -\langle \hat{S}^z_{i,2} \rangle = -\langle \hat{S}^z_{i,2} \rangle \neq 0$. Hence, it follows that the nearest-neighbour spins both along legs and rungs exhibit predominantly antiferromagnetic ordering. The dependence of staggered magnetization as the relevant order parameter is quite analogous to the previous case $m^*_{AF} = \frac{1}{N} \sum_{i=1}^{N} (-1)^i (\langle \hat{S}^z_{i,1} \rangle - \langle \hat{S}^z_{i,2} \rangle) = \frac{1}{2} [1 - J_1^2 / (J_2 - J_3)^2]^{1/2}$.

(iv) *Stripe Rung (SR) state* for $e_0^L < e_0^P, J_2 > 0, J_3 > 0$. The model shows classical ordering in this phase with the antiferromagnetically ordered nearest-neighbour spins along legs and the ferromagnetically ordered nearest-neighbour spins along rungs.

(v) *Ferromagnetic (FM) state* for $e_0^L < e_0^P, J_2 < 0, J_3 < 0$. The ground state corresponds to the ideal fully polarized ferromagnetic spin state.
Figure 3. Zero-temperature variations of: (a) the order parameters; (b) the nearest-neighbour spin–spin correlation along legs as a function of the Ising intra-leg interaction $J_2$ for $J_1 = 1$, $\Delta = 1$ and three different values of the crossing Ising interaction $J_3 = 0$, 0.6, 1.2.

The results displayed in figure 2(a) demonstrate that the Heisenberg–Ising ladder is in the disordered QPM phase whenever a relative strength of both Ising interactions $J_2$ and $J_3$ is sufficiently small compared to the Heisenberg intra-rung interaction $J_1$. It is noteworthy, moreover, that the QPM phase reduces to a set of fully non-correlated singlet dimers placed on all rungs (the so-called rung singlet-dimer state) along the special line $J_2 = J_3$ up to $e_0^2 < e_0^1$, which is depicted in figure 2 by dotted lines. Under this special condition, the intra-rung spin–spin correlation represents the only non-zero pair correlation function and all the other short-ranged spin–spin correlations vanish and/or change their sign across the special line $J_2 = J_3$. It should be remarked that the completely identical ground state can also be found in the symmetric Heisenberg two-leg ladder with $J_2 = J_3$ (see figure 2(b)). To compare, the rung singlet-dimer state is the exact ground state of the symmetric Heisenberg–Ising ladder with $\Delta = 1$ for $J_1 > J_2$, while the symmetric Heisenberg ladder displays this simple factorizable ground state for $J_1 > 1.4015J_2$ [35, 36]. (For clarity, this horizontal line is not shown in figure 2(b) as it coincides exactly with the ground-state boundary of the Heisenberg–Ising ladder extended over larger parameter space.) It should be stressed, however, that the short-range spin–spin correlations become non-zero in QPM whenever $J_2 \neq J_3$ even if this phase still preserves its disordered nature with the prevailing character of the rung singlet-dimer state. To support this statement, the zero-temperature dependences of the order parameters and the nearest-neighbour spin–spin correlation along legs are plotted in figure 3. The relevant order parameters evidently disappear in QPM, whereas the nearest-neighbour correlation function changes its sign when passing through the special line $J_2 = J_3$ of the rung singlet-dimer state.

Note furthermore that the Heisenberg–Ising ladder undergoes the second-order quantum phase transition from the disordered QPM phase to the spontaneously long-range-ordered Néel or SL phase, which predominantly appears in the parameter region where one from both Ising couplings $J_2$ and $J_3$ is antiferromagnetic and the other one is ferromagnetic. The significant quantum reduction of staggered order parameters implies an obvious quantum character of both Néel and SL phases in which the antiferromagnetic correlation on rungs still dominates (see figure 3). Thus, the main difference between both the quantum long-range-ordered phases emerges in the character of the nearest-neighbour correlation along legs, which is ferromagnetic.
in the SL phase but antiferromagnetic in the Néel phase. The continuous vanishing of the order parameters depicted in figure 3(a) provides direct evidence of the second-order quantum phase transition between the disordered QPM phase and the ordered SL (or Néel) phase, which is also accompanied by the weak-singular behaviour of the nearest-neighbour correlation function visualized in figure 3(b) by black dots. Here, it should be noted that the $zz$ correlation function of the Heisenberg–Ising ladder can be easily derived from the result of the $xx$ correlation function of the transverse Ising chain calculated in [61]. Last but not least, the strong enough Ising interactions $J_2$ and $J_3$ may break the antiferromagnetic correlation along rungs and lead to the presence of the fully ordered ferromagnetic rung states FM or SR depending on whether both Ising interactions are ferromagnetic or antiferromagnetic, respectively. It should be noted that this change is accompanied by a discontinuous (first-order) quantum phase transition on behalf of a classical character of both FM and SR phases, which can also be clearly seen in figure 3 from an abrupt change of the order parameters as well as the nearest-neighbour correlation function.

Finally, let us also provide a more detailed comparison between the ground-state phase diagrams of the Heisenberg, Heisenberg–Ising and Ising two-leg ladders, all depicted in figure 2(b). One can note that the displayed ground-state phase diagrams of the Heisenberg and Heisenberg–Ising two-leg ladders have several similar features. The phase boundary between the classically ordered SR phase and three quantum phases (QPM, SL and Néel) of the Heisenberg–Ising ladder follows quite closely the first-order phase boundary between the Haldane-type phase and the dimerized phase of the pure Heisenberg ladder obtained using the series expansion and exact diagonalization [26]. Of course, the most fundamental difference lies in the character of SR and Haldane phases because the former phase exhibits a classical long-range order contrary to a more spectacular topological order of the pure quantum Haldane-type phase with a non-zero string order parameter [31] even though the ferromagnetic intra-rung correlation is common for both phases. The difference between the ground states of the Heisenberg–Ising and pure Heisenberg two-leg ladder becomes much less pronounced in the parameter region with the strong intra-rung interaction $J_1$, which evokes the quantum phases in the ground state of both these models. In the case of a sufficiently strong frustration $J_2 \sim J_3$, the ground state of the Heisenberg–Ising ladder forms the disordered QPM phase, whereas the antiferromagnetic or ferromagnetic (Néel or SL) long-range order emerges along the legs if the diagonal coupling $J_1$ is much weaker or stronger than the intra-leg interaction $J_2$. Note that the quantum Néel and SL phases have several common features (e.g. predominant antiferromagnetic correlations along rungs) with the disordered QPM phase from which they evolve when crossing continuous quantum phase transitions given by the set of equations:

$$J_3 = J_2 - J_1 \quad \text{(for } J_3 < J_2) \quad \text{and} \quad J_3 = J_2 + J_1 \quad \text{(for } J_3 > J_2).$$

It cannot be definitely ruled out whether or not these quantum-ordered phases may become the ground state of the pure Heisenberg ladder because they are also predicted by the bond-mean-field approximation [39–41], but have not been found by most of the numerical methods. Further numerical investigations of the Heisenberg ladder are therefore needed to clarify this unresolved issue.

### 3.2. Ground-state phase diagram in a non-zero field

When the external field $h$ is switched on, the inequality for the ground states of the Ising chain in the longitudinal field (18) is generally valid only for $J_1 + J_2 \leq 0$ or $J_1 + J_2 \geq 2|h|$. Hence, it is necessary to modify the procedure of finding the ground states inside the region where the relation (18) is broken. However, one may use, with success, the method suggested by Shastry and Sutherland [64, 25] in order to find the ground states inside this parameter region. Let us
represent our effective Hamiltonian (10) in the form

\[ H = \sum_{i=1}^{N} H_{i,i+1}, \]

\[ H_{i,i+1} = \frac{1}{2} \sum_{l=0}^{i+1} \left\{ J_{1}(1 - n_{l})\hat{s}_{l}\cdot\hat{s}_{l}' + \frac{J_{1}\Delta}{4}(2n_{l} - 1) \right\} + [2(J_{2} + J_{3})n_{l}n_{l+1} + 2(J_{2} - J_{3})(1 - n_{l})(1 - n_{l+1})]\hat{s}_{l}\cdot\hat{s}_{l+1}. \] (20)

Then, one can employ the variational principle implying that \( E_{0} \geq \sum_{l=1}^{N} E_{0}(l, l+1) \), where \( E_{0}(l, l+1) \) is the lowest eigenenergy of \( H_{i,i+1} \).

Looking for the eigenenergies of \( H_{i,i+1} \), it is enough to find the lowest eigenstate of each bond configuration:

- \( n_{i} = n_{i+1} = 0, E_{0}^{0,0}(i, i+1) = -\frac{1}{2}\sqrt{J_{1}^{2} + (J_{2} - J_{3})^{2}} - \frac{J_{1}\Delta}{4}, \)
- \( n_{i} = n_{i+1} = 1, \quad E_{0}^{1,1}(i, i+1) = \begin{cases} \frac{J_{1}\Delta}{4} + \frac{J_{2} + J_{3}}{2} - |h|, & \text{if } |h| > (J_{2} + J_{3})(FM), \\ \frac{J_{1}\Delta}{4} - \frac{J_{2} + J_{3}}{2}, & \text{if } |h| \leq (J_{2} + J_{3})(AF). \end{cases} \)
- \( n_{i} = 0, n_{i+1} = 1 (n_{i} = 1, n_{i+1} = 0), E_{0}^{0,1}(i, i+1) = E_{0}^{1,0}(i, i+1) = -\frac{J_{2} - |h|}{2}. \)

The phase corresponding to the alternating bond configuration \( n_{i} = 0, n_{i+1} = 1 \) will be hereafter referred to as the staggered bond (SB) phase. It should be mentioned that in the SB phase there does not exist any correlations between spins from different rungs, and the overall energy comes from the intra-rung spin–spin interactions and the Zeeman energy of the fully polarized rungs [63]. It can be easily seen from a comparison of \( E_{0}^{0,1}(i, i+1) \) and \( E_{0}^{1,1}(i, i+1) \) that the eigenenergy of the SB phase \( E_{0}^{0,1}(i, i+1) \) always has lower energy than the lowest eigenenergy of the fully polarized state \( E_{0}^{1,1}(i, i+1) \) inside the stripe:

\[ J_{2} + J_{3} - \frac{J_{1}(1 + \Delta)}{2} \leq |h| \leq J_{2} + J_{3} + \frac{J_{1}(1 + \Delta)}{2}. \] (21)

Note that the ferromagnetic ordering is preferred for external fields above this stripe \( |h| \geq J_{2} + J_{3} + \frac{J_{1}(1 + \Delta)}{2} \), while the antiferromagnetic ordering becomes the lowest energy state below this stripe \( |h| \leq J_{2} + J_{3} - \frac{J_{1}(1 + \Delta)}{2} \).

If one compares the respective eigenenergies of the staggered bond phase \( E_{0}^{0,1}(i, i+1) \) and the uniform purity phase \( E_{0}^{0,0}(i, i+1) \) \( (n_{i} = n_{i+1} = 0) \), one obtains another condition implying that \( E_{0}^{0,1}(i, i+1) \) becomes lower than \( E_{0}^{0,0}(i, i+1) \) only if

\[ |h| \geq \sqrt{J_{2}^{2} + (J_{2} - J_{3})^{2}} - \frac{J_{1}(1 - \Delta)}{2}. \] (22)

This means that the SB phase with the overall energy \( E_{0}^{0,1} = -N(J_{1} + 2|h|)/4 \) becomes the ground state inside the region confined by conditions (21) and (22). The lowest field, which makes the SB phase favourable, can also be found as

\[ |h_{\text{min}}| = \frac{J_{1}(1 + \Delta)}{2}. \] (23)

Similarly, one may also find the condition under which two eigenenergies corresponding to the uniform impurity configuration \( E_{0}^{1,1}(n_{i} = n_{i+1} = 1) \) become lower than the respective eigenenergy of the uniform purity configuration \( E_{0}^{0,0}(n_{i} = n_{i+1} = 0) \). The ferromagnetic state...
of the uniform impurity configuration becomes lower if the external field exceeds the boundary value:

$$|h| \geq \frac{1}{2} \left[ J_2 + J_3 + J_1 \Delta + \sqrt{J_1^2 + (J_2 - J_3)^2} \right]$$

whereas the condition for the antiferromagnetic state of the uniform impurity configuration is independent of the external field:

$$J_1 \Delta + \sqrt{J_1^2 + (J_2 - J_3)^2} \leq (J_2 + J_3).$$

It is worth noting that it is not possible to find the ground state outside the boundaries (22), (24) and (25) using the variational principle. However, it is shown in the appendix that the bond configuration, which corresponds to the ground state, cannot exceed period 2. Therefore, one has to search for the ground state just among the states that correspond to the following bond configurations: all $n_i = 0$; all $n_i = 1$; $n_{2i-1} = 0$, $n_{2i} = 1$ ($n_{2i-1} = 1$, $n_{2i} = 0$). In this respect, two phases are possible inside the stripe given by (21). The ground state of the Heisenberg–Ising ladder forms the SB phase if $e_0^{(0)} < e_0^{(1)}$:

$$|h| \geq \frac{2(J_1 + |J_2 - J_3|)}{\pi} E(\sqrt{1 - \gamma^2}) - \frac{J_1(1 - \Delta)}{2}$$

Several ground-state phase diagrams are plotted in figures 4–6 for a non-zero magnetic field. The most interesting feature stemming from these phase diagrams is that the SB phase may become the ground state for the magnetic field $h \geq \frac{J_1(1 + \Delta)}{2}$, which is sufficiently strong to break the rung singlet-dimer state. It can be observed from figure 4 that the SB phase indeed evolves along the line of the rung singlet-dimer state and replaces the QPM phase in the ground-state phase diagram. The external magnetic field may thus cause an appearance of another peculiar quantum SB phase with the translationally broken symmetry, i.e. the alternating singlet and fully polarized triplet bonds on the rungs of the two-leg ladder. Hence, it follows that the SB phase emerges at moderate values of the external magnetic field and it consequently leads to the presence of the intermediate magnetization plateau at a half of the saturation magnetization. It is quite apparent from figures 5(a) and 6(a) that the Heisenberg–Ising ladder without the frustrating diagonal Ising interaction $J_3 = 0$ exhibits this striking
magnetization plateau just for the particular case of the antiferromagnetic Ising intra-leg interaction $J_2 > 0$. On the other hand, the fractional magnetization plateau inherent to the presence of the SB phase is substantially stabilized by the spin frustration triggered by the non-zero diagonal Ising interaction $J_3 \neq 0$ and hence, the plateau region may even extend over a relatively narrow region of the ferromagnetic Ising intra-leg interaction $J_2 < 0$ as well (see figure 5(b)).

It should be noted that the same mechanism for the appearance of the magnetization plateau has also been predicted for the spin-1/2 Heisenberg two-leg ladder by making use of
exact numerical diagonalization and DMRG methods [22–25, 34]. Let us therefore conclude our study by comparing the respective ground-state phase diagrams of the Heisenberg–Ising and Heisenberg two-leg ladders in the presence of the external magnetic field displayed in figure 6. According to this plot, both models give essentially the same magnetization process in the strong-coupling limit of the Heisenberg intra-rung interaction $J_1 \gtrapprox 1.5$, where two subsequent field-induced transitions in the following order QPM–SB–FM can be observed and, consequently, the magnetization exhibits two abrupt jumps at the relevant transition fields. On the other hand, the fundamental differences can be detected in the relevant magnetization process of the Heisenberg–Ising and Heisenberg ladders in the weak-coupling limit of the intra-rung interaction $J_1$. At low fields, the quantum Haldane-like phase constitutes the ground state of the pure Heisenberg ladder in contrast to the classical SR phase, which is the low-field ground state of the Heisenberg–Ising ladder. In addition, the Heisenberg–Ising ladder still exhibits a magnetization plateau corresponding to a gapped SB phase at intermediate values of the magnetic field in this parameter space, while a continuous increase of the magnetization can be observed in the pure Heisenberg ladder due to the presence of the gapless Luttinger-liquid phase at moderate fields. Finally, it is also noteworthy that the saturation fields towards FM phase are also quite different for the Heisenberg–Ising and Heisenberg ladders in the weak-coupling limit of the Heisenberg intra-rung interaction.

4. Conclusions

The frustrated Heisenberg–Ising two-leg ladder was considered within the rigorous approach using the fact that the $z$-projection of total spin on a rung is a conserved quantity. By means of the pseudospin representation of bond states, we have proved the exact mapping correspondence between the investigated model and some generalized spin-1/2 quantum Ising chain with the composite spins in an effective longitudinal and a transverse fields. We have also found the unitary transformation which reproduces the analogous mapping between the models. While the bond-state representation has more transparent physical interpretation, the unitary transformation gives the complete relation between spin operators of both models, and it might be useful for searching quantum spin ladders which admit exact solutions.

It has been shown that the ground state of the model under investigation must correspond to a regular bond configuration not exceeding the period 2. Hence, the true ground state will be the lowest eigenstate of either the transverse Ising chain, the Ising chain in the longitudinal field, or the non-interacting spin-chain model in the staggered longitudinal–transverse field.

The most interesting results to emerge from this study are closely related to the extraordinary diversity of the constructed ground-state phase diagrams and the quantum phase transitions between different ground-state phases. In the absence of the external magnetic field, the ground-state phase diagram constitute four different ordered phases and one quantum paramagnetic phase. The disordered phase was characterized through short-range spin correlations, which indicate a dominating character of the rung singlet-dimer state in this phase. On the other hand, the order parameters have been exactly calculated for all the four ordered phases, two of them having classical character and two purely quantum character as evidenced by the quantum reduction of the staggered magnetization in the latter two phases. Last but not least, it has been demonstrated that the external magnetic field of a moderate strength may cause the appearance of the peculiar SB phase with the alternating character of singlet and triplet bonds on the rungs of two-leg ladder. This latter finding is consistent with the presence of the fractional magnetization plateau at a half of the saturation magnetization in the relevant magnetization process.
Using this procedure we can reduce the number of sites in impurity clusters to 2, i.e. only \( \Delta_1 \) bond inbetween. If condition (21) is valid, such a configuration can achieve a lower energy. If \( \epsilon \) contains the cluster of more than two impurity bonds, its energy can be lowered by adding pure bond inbetween. If condition (21) is valid, such a configuration can achieve a lower energy. The same result can be analogously obtained for \( E_0(N, 1) \) or \( E_0(N, 2) \) can correspond to the ground state.

Define the energy per spin for each configuration as

\[
E = E_0(N_1, M_1) + E_0(N_2, M_2) + \cdots + E_0(N_L, M_L),
\]

where \( E_0(N_i, M_i) = E_0^1(N_i) + E_0^2(M_i) \) is the lowest energy of the complex of two independent spin chains which correspond to the purity and impurity bond states, \( N_1 + M_1 + N_2 + M_2 + \cdots + N_L + M_L = N \). If \( E_0(N_i, M_i) = E_0(N_i, M_i)/(N_i + M_i) \) corresponds to the lowest energy per spin among other clusters, it is evident that the ground-state configuration is alternating purity and impurity clusters of length \( N_i \) and \( M_i \).

Let us first consider the case when \( \hbar \) is restricted under condition (21). If the configuration contains the cluster of more than two impurity bonds, its energy can be lowered by adding pure bond inbetween. If condition (21) is valid, such a configuration can achieve a lower energy. Using this procedure we can reduce the number of sites in impurity clusters to 2, i.e. only \( E_0(N, 1) \) or \( E_0(N, 2) \) can correspond to the ground state.

Define the energy per spin for each configuration as

\[
e_0(N, 1) = \frac{E_0^1(N) + E_0^1(1)}{N + 1}, \tag{A.2}
\]

\[
e_0(N, 2) = \frac{E_0^1(N) + E_0^1(2)}{N + 2}. \tag{A.3}
\]

If \( e_0(1, 1) < e_0(2, 1) \) and so on \( (e_0(N, 1) < e_0(N + 1, 1)) \), the ground state corresponds to the staggered bond configuration. Suppose that for some \( N \),

\[
\Delta e_0(N - 1) = e_0(N, 1) - e_0(N - 1, 1)
\]

\[
= \frac{1}{N(N + 1)}(N E_0^1(N) - (N + 1) E_0^1(N - 1) - E_0^1(1)) < 0. \tag{A.4}
\]

Consequently, it is clear that

\[
\Delta e_0(N) = \frac{1}{(N + 1)(N + 2)}((N + 1) E_0^1(N + 1) - (N + 2) E_0^1(N) - E_0^1(1)) < 0, \tag{A.5}
\]

if \( E_0^1(N + 1) - 2 E_0^1(N) + E_0^1(N - 1) < 0 \), i.e. the ground-state energy of finite transverse Ising chain is a convex function of \( N \). The last condition is ensured by non-increasing \( \Delta E_0^1(N) = E_0^1(N + 1) - E_0^1(N) \) \( (\Delta E_0^1(N) \geq \Delta E_0^1(N + 1)) \) that can be shown by numerical calculations for finite chains (see figure A1) using the numerical approach [65]. For \( J_2 = J_1 \), we obtain the free spin Hamiltonian and \( E_0^1(N) \) depends linearly on \( N \). Conditions (A.4) and (A.5) together mean that \( e_0(N, 1) \) may have only one extremum and it is the maximum. Therefore, \( e_0(N, 1) \) may take the minimal value only in two limiting cases \( N = 1, N \to \infty \).

The same result can be analogously obtained for \( e_0(N, 2) \). Now, we can compare the energies of \( (N, 1) \) and \( (N, 2) \) configurations. For \( |h| \geq \frac{J_1 + J_2}{2} \),

\[
e_0(1, 1) - e_0(1, 2) = \frac{1}{6} \left( -\frac{J_1(1 + \Delta)}{2} - (J_2 + J_3) + |h| \right) < 0, \tag{A.6}
\]
due to the upper boundary of condition (21). To summarize, the ground-state configuration in the region confined by (21) can correspond to either staggered bond or uniform purity configuration.

Let us consider the ground state for $|h| > J_2 + J_3 + J_1 (1 + \Delta_1)/2$. Similar to the previous case we can prove that $e_0(N, M)$ is a convex function of $N$ and $M$ if the ground-state energies of the uniform chains have the following properties:

$$E_0^0(N + 1) - 2E_0^0(N) + E_0^0(N - 1) \leq 0,$$

$$E_1^1(N + 1) - 2E_1^0(N) + E_1^0(N - 1) \leq 0. \tag{A.7}$$

One can find that $E_1^1(N + 1) - E_1^0(N) = \frac{|h - \Delta|}{2}$ and $E_1^1(N + 1) - 2E_1^0(N) + E_1^1(N - 1) = 0$. That is why the minimal value of the ground state can be achieved in one of three cases: staggered bond, purity and impurity configuration. The staggered bond configuration should be excluded from this list for $|h| > J_2 + J_3 + J_1 (1 + \Delta_1)/2$, since it cannot be the ground state due to the variational principle.

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Figure A1. $\Delta E_0^0(N) = E_0^0(N + 1) - E_0^0(N)$ as a function of system size $N$ for the transverse Ising chain with free ends (15): $J_1 = 1$, $\Delta = 0$, $|J_2 - J_3| = 0, 0.2, 0.4, \ldots, 4$ from top to bottom.
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