Ground-state phase diagram of an anisotropic $S=\frac{1}{2}$ ladder with alternating rung interactions

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Abstract. Employing mainly numerical methods, we explore the ground-state phase diagram of an anisotropic $S=\frac{1}{2}$ ladder, in which leg interactions are uniform and isotropic, while rung interactions are alternating and have a common Ising-type anisotropy. We determine the phase diagram in the case where $J_{\text{leg}} = 0.2$ (antiferromagnetic), $J_{\text{rung}} = -1.0$ (ferromagnetic) and $|J_{\text{rung}}| \leq 1.0$, the first one being the magnitude of the leg interaction and the second and third ones those of the rung interactions, which are alternating. It is emphasized that the system has a frustration when $J_{\text{rung}}$ is positive. We find that, in the frustrated region, the Haldane state appears as the ground state even when the Ising character of rung interactions is strong. This appearance of the Haldane phase is contrary to the ordinary situation, and it is called the inversion phenomenon concerning the interaction anisotropy. We also find that an incommensurate state becomes the ground state in a portion of the Haldane phase region.

1. Introduction

The frustration effect on the ground-state properties of low-dimensional quantum spin systems with competing interactions has long been a subject of active research. According to a significant amount of theoretical and experimental effort which has been devoted so far, it is now widely known that an interplay between two phenomena of great interest, frustration and quantum fluctuation, leads to various exotic ground states. A typical and long-established example of these ground states is the dimer state accompanying spontaneous translational symmetry breaking in an $S=\frac{1}{2}$ zigzag chain in which antiferromagnetic nearest-neighbor (nn) and next-nearest-neighbor (nnn) interactions are competing with each other [1–3].

The effect of the frustration on the ground-state properties of an $S=\frac{1}{2}$ two-leg ladder system has been extensively studied in the cases where additional leg nnn and/or diagonal interactions are competing with the leg nn and rung interactions [4, 5]. In the present paper, as another example of the frustrated $S=\frac{1}{2}$ two-leg ladder systems, we discuss the case where the rung interactions are alternating [6, 7] and aim at exploring its ground-state phase diagram. We express the Hamiltonian describing this system in the following form:

$$\mathcal{H} = J_{\text{leg}} \sum_{j=1}^{L} \{\vec{S}_{j,a} \cdot \vec{S}_{j+1,a} + \vec{S}_{j,b} \cdot \vec{S}_{j+1,b}\}$$
+ J_{\text{rung}} \sum_{j=1}^{L/2} \gamma \left( S_{2j-1, a}^x S_{2j-1, b}^x + S_{2j-1, a}^y S_{2j-1, b}^y + S_{2j-1, a}^z S_{2j-1, b}^z \right) + J'_{\text{rung}} \sum_{j=1}^{L/2} \gamma \left( S_{2j-1, a}^x S_{2j-1, b}^x + S_{2j-1, a}^y S_{2j-1, b}^y + S_{2j-1, a}^z S_{2j-1, b}^z \right),

where \( \vec{s}_{j,l} = (S_{j,l}^x, S_{j,l}^y, S_{j,l}^z) \) is the spin \( S = 1/2 \) operator acting at the \( (j,l) \) site assigned by rung \( j \) and leg \( l (=a \text{ or } b) \); \( J_{\text{rung}} \) denotes the magnitude of the isotropic leg interaction; \( J_{\text{rung}} \) and \( J'_{\text{rung}} \) denote those of the two kinds of anisotropic rung interactions which are alternating, the XXZ-type anisotropy being controlled by the parameter \( \gamma \) in common with both interactions; \( L \) is the total number of spins in each leg, which is assumed to be even. It is emphasized that this system has a frustration when \( J_{\text{rung}} J'_{\text{rung}} < 0 \) irrespective of the sign of \( J_{\text{rung}} \).

Although materials corresponding to the present model have been neither yet found nor synthesized so far, we believe that it is a physically realistic model. In fact, for example, Yamaguchi \textit{et al.} \cite{8, 9} have recently demonstrated the modulation of magnetic interactions in spin ladder systems by using verdazyl-radical crystals. The flexibility of molecular arrangements in such organic-radical materials is expected to realize spin ladder systems with alternating rung interactions.

In the following discussions, we confine ourselves to the case where \( J_{\text{rung}} \) is ferromagnetic, and we put \( J_{\text{rung}} = -1 \), choosing \(|J_{\text{rung}}|\) as the unit of energy. We also consider, for simplicity, only the case where \( J_{\text{rung}} = 0 \), \(|J_{\text{rung}}| \leq 1 \) and \( 0 \leq \gamma < 1 \), that is, we assume that \( J_{\text{rung}} \) is antiferromagnetic and relatively weak, and that the anisotropy of the rung interactions is of the Ising-type. Determining the ground-state phase diagram on the \( \gamma \) versus \( J'_{\text{rung}} \) plane, we mainly employ the numerical methods such as the exact-diagonalization (ED) method and the density-matrix renormalization-group (DMRG) method \cite{10, 11} with the help of physical considerations as well as already-known results for some special cases.

2. Special cases

We discuss here some special cases for which the ground states have already been clarified or for which they are reasonably anticipated by physical considerations.

2.1. Case where \( J_{\text{rung}} = J'_{\text{rung}} (=-1) \)

In this case where \( J_{\text{rung}} \ll |J_{\text{rung}}| = |J'_{\text{rung}}| \), by the use of the degenerate perturbation theory, the present system can be mapped onto the \( S=1 \) chain in the following way. The eigenstates of an isolated \( J_{\text{rung}} \)- or \( J'_{\text{rung}} \)-rung are given by \( \phi_{j}^{1, +} = \alpha_{j,a} \alpha_{j,b} \), \( \phi_{j}^{1, 0} = \left( \alpha_{j,a} \beta_{j,b} + \beta_{j,a} \alpha_{j,b} \right) / \sqrt{2} \), \( \phi_{j}^{1, -} = \beta_{j,a} \beta_{j,b} \) and \( \phi_{j}^{0, 0} = \left( \alpha_{j,a} \beta_{j,b} - \beta_{j,a} \alpha_{j,b} \right) / \sqrt{2} \), where \( \alpha_{j,l} \) denotes the \( S_{j,l}^z = +1/2 \) state and \( \beta_{j,l} \) the \( S_{j,l}^z = -1/2 \) state. The corresponding energies are, respectively, \( E^{1, +} = -1/4 \), \( E^{1, 0} = (1-2\gamma)/4 \), \( E^{1, -} = -1/4 \) and \( E^{0, 0} = (1+2\gamma)/4 \), for all \( j \)'s. Then, it is easy to see that when \( \gamma \) is sufficiently large, the state \( \phi_{j}^{0, 0} \) can be neglected. We introduce the pseudo \( S=1 \) operator \( \tilde{T}_j \) for rung \( j \), and make the \( T_j^+ = +1 \), \( 0 \) and \( -1 \) states correspond to \( \phi_{j}^{1, +} \), \( \phi_{j}^{1, 0} \) and \( \phi_{j}^{1, -} \), respectively. The relation \( T_j^+ = \tilde{T}_{j,a} + \tilde{T}_{j,b} \) holds, as is readily shown by comparing the matrix elements of both operators \( T_j^+ \) and \( \tilde{T}_{j,l} \) with respect to \( \phi_{j}^{1, +} \), \( \phi_{j}^{1, 0} \) and \( \phi_{j}^{1, -} \). Thus, the Hamiltonian \( (1) \) for the \( S=1/2 \) operator \( \tilde{T}_{j,l} \) can be mapped onto the effective Hamiltonian \( \mathcal{H}_{\text{eff}} \) for the \( S=1 \) operator \( T_j^+ \), which is given by

\[
\mathcal{H}_{\text{eff}} = 0.1 \sum_{j=1}^{L} \tilde{T}_j^+ \cdot \tilde{T}_{j+1} + D \sum_{j=1}^{L} (T_{j}^z)^2, \quad D = (\gamma - 1)/2,
\]

where the on-site anisotropy \( (D^-) \) term comes from the difference between \( E^{1, +} = E^{1, -} \) and \( E^{1, 0} \).
Figure 1. Schematic pictures of the AFstN (left panel), Haldane (center panel) and F-SD (right panel) phases. Each of the small open circles denotes an $S = 1/2$ spin. Two $S = 1/2$ spins in each ellipse form a singlet dimer. An $S = 1/2$ spin with an upward arrow and that with a downward arrow are, respectively, in the $S^z = +1/2$ ($\alpha$) and $S^z = -1/2$ ($\beta$) states.

It has already been clarified by Chen et al. [13] that in the $S = 1$ chain governed by the effective Hamiltonian (2), the phase transition from the Néel to the Haldane state takes place at $D \sim -0.04$ as $D$ increases. This suggests that in the present $S = 1/2$ ladder, the ground state is the antiferromagnetic stripe Néel (AFstN) state, sketched in the left panel of Fig. 1, or the Haldane state, sketched in the center panel of Fig. 1, depending upon whether $\gamma < \gamma_c^{(\text{AFstN,H})}$ or $\gamma_c^{(\text{AFstN,H})} < \gamma < 1$ with $\gamma_c^{(\text{AFstN,H})} \sim 0.9$. (It is noted that the Néel state in the $S = 1$ chain corresponds to the AFstN state in the $S = 1/2$ ladder.)

2.2. Case where $|J_{\text{rung}}| (=1) \gg J'_{\text{rung}} > 0$

In this case, the procedure discussed in the previous subsection can be applied to the $J_{\text{rung}}$-rung only. Thus, the Hamiltonian (1) can be mapped onto an anisotropic ‘$S = 1$’-$S = 1/2$’ diamond chain. Hida and Takano [12] have studied the ground state of this chain. By using their results, we may conclude that, when $\gamma \to 1.0$, the ground state in this case is the Haldane state if $J'_{\text{rung}} \lesssim 0.26$.

2.3. Case where $J'_{\text{rung}} \sim -J_{\text{rung}} (=1)$

In this case where $0 < J_{\text{rung}} \ll |J_{\text{rung}}| \sim |J'_{\text{rung}}|$, the lowest-energy state of an isolated $J'_{\text{rung}}$-rung is the singlet dimer state $\phi_2^{(1,0)}$, while that of the ferromagnetic $J_{\text{rung}}$-rung is one of the ferromagnetic states $\phi_2^{(1,+)}$ and $\phi_2^{(1,-)}$. The effective interaction between the neighboring $J_{\text{rung}}$-rungs through the in-between $J'_{\text{rung}}$-rung can be obtained by carrying out a third-order perturbation calculation. The resulting effective interaction is considered to be antiferromagnetic judging from the numerical result discussed below (see the right panel of Fig. 4). Therefore, the $J_{\text{rung}}$-rung in the $\phi_2^{(1,+)}$ (or $\phi_2^{(1,-)}$) state and that in the $\phi_2^{(1,-)}$ ($\phi_2^{(1,+)}$) state arrange alternatively. Thus, the ground state in the present case is anticipated to be the ‘ferromagnetic’-singlet dimer’ (F-SD) state sketched in the right panel of Fig. 1.

3. Ground-state phase diagram

We denote, respectively, by $E_0^{(p)}(L, M)$ and $E_1^{(p)}(L, M)$ the lowest and second-lowest energy eigenvalues of the Hamiltonian (1) under periodic boundary conditions within the subspace characterized by $L$ and the total magnetization $M \equiv \sum_{j=1}^{L}(S_{j,\alpha}^{z} + S_{j,\beta}^{z})$. It is noted that $E_0^{(p)}(L, 0)$ always gives the ground-state energy for the finite-$L$ system. Then, the excitation energy gap $\Delta_{00}(L)$ within the $M = 0$ subspace is given by

$$\Delta_{00}(L) = E_1^{(p)}(L, 0) - E_0^{(p)}(L, 0).$$

(3)

We also define the site magnetization $m_{j,l}(L)$ as

$$m_{j,l}(L) = \langle S_{j,l}^{z} \rangle_{L} ,$$

(4)

3
Figure 2. Ground-state phase diagram on the $\gamma$ versus $J'_\text{rung}$ plane. Here, F-SD, H and AFstN stand, respectively, for ‘ferromagnetic’-‘singlet dimer’, Haldane and antiferromagnetic stripe Néel. The solid lines are the second-order (2D Ising) phase boundary lines. The dotted lines, being the Lifshitz lines, separate the commensurate and incommensurate regions; the region between these lines is the incommensurate one.

where $\langle \cdots \rangle_L$ denotes the ground-state expectation value for the system with $L$ rungs.

Figure 2 shows our final result for the ground-state phase diagram on the $\gamma$ versus $J'_\text{rung}$ plane. It consists of the F-SD, Haldane and AFstN phases. The solid lines are the 2D Ising phase boundary line between the F-SD and Haldane phases and that between the Haldane and AFstN phases. On the other hand, the dotted lines, which are often called the Lifshitz lines, separate the commensurate and incommensurate regions; the latter region is between them. The most striking feature of this phase diagram is the fact that an incommensurate region appears within the Haldane phase region, which can be attributed to the frustration effect. The fact that the Haldane state appears as the ground state even at the $\gamma \to 0$ limit is also interesting. This is because the Haldane state is known to become the ground state mainly in the case of the XY-type anisotropy in the $S = 1$ XXZ chain [13]. This phenomenon is called the inversion phenomenon concerning the interaction anisotropy [14–17].

Let us turn to a discussion on the determination of the phase diagram. In Fig. 3 we plot the $J'_\text{rung}$-dependence of the excitation energy gap $\Delta_{00}(L)$ for $\gamma = 0.6$, calculated by the ED method. This figure demonstrates that the ground state is doubly degenerate when

![Figure 4](image-url)  
Figure 4. Plots of the site magnetizations $m_{j,l}(96)$ ($l=a, b$) versus $j$ with $\gamma$ fixed at $\gamma = 0.6$; the left, center and right panels are, respectively, for $J'_\text{rung} = 0.1$, 0.3 and 0.5. The red circles and the blue crosses show, respectively, $m_{j,a}(96)$ and $m_{j,b}(96)$.
\[ -1 \leq J'_{\text{ring}} \leq 0.22 \text{ and when } 0.43 \leq J'_{\text{ring}} \leq 1, \text{ while it is unique when } 0.22 \leq J'_{\text{ring}} \leq 0.43. \]  From these results together with the physical considerations discussed in section 2, we may expect that, when \(-1 \leq J'_{\text{ring}} \leq 0.22, 0.22 \leq J'_{\text{ring}} \leq 0.43 \text{ and } 0.43 \leq J'_{\text{ring}} \leq 1,\) the ground states are, respectively, the AFstN, Haldane and F-SD states. In order to ascertain these expectations, we have performed DMRG calculations for the finite-size system with \(2L=192\) spins under open boundary conditions to evaluate the site magnetization \(m_{j,0}(96)\) for various values of \(J'_{\text{ring}}\). As examples, the results for the cases of \(J'_{\text{ring}}=0.1, 0.3\) and 0.5 are depicted in Fig. 4. We see from this figure that in all cases \(m_{j,0}(96)\) and \(m_{j,b}(96)\) are almost equal to each other. In the first case, \(m_{j-1,0}(96) \approx -m_{j,0}(96)\), which shows that the ground state in this case is the AFstN state. In the second case, the edge states clearly exist; this is one of the most representative features of the Haldane state [19–21]. Finally in the third case, \(m_{j-3,0}(96) \approx -m_{j-1,0}(96)\) and \(m_{j,0}(96) \approx 0,\) which show that the ground state is the F-SD state.

Both of the phase transition between the AFstN and Haldane states and that between the Haldane and F-SD states are of the 2D Ising type, since the \(\mathbb{Z}_2\) symmetry is broken in the AFstN and F-SD states while it is not broken in the Haldane state. It is well known that the phenomenological renormalization group (PRG) method [22] is a useful one to determine the phase boundary line for this phase transition. The PRG equations for the (AFstN,Haldane)-transition and for the (Haldane,F-SD)-transition are, respectively, given by

\[
L \Delta_{00}(L) = (L + 2) \Delta_{00}(L + 2), \quad L \Delta_{00}(L) = (L + 4) \Delta_{00}(L + 4).
\]

This is because the periods along each leg are 2 and 4 in the AFstN and F-SD states, respectively. Solving numerically these PRG equations for a given value of \(\gamma\) (or \(J'_{\text{ring}}\)), we have computed the finite-size (AFstN,Haldane)-transition point \(J'_{\text{ring},c}^{(\text{AFstN,H})}(L) = \gamma_{c}^{(\text{AFstN,H})}(L)\) for \(L=6, 8, 10, 12,\) and the finite-size (Haldane,F-SD)-transition point \(J'_{\text{ring},c}^{(\text{H,F-SD})}(L) = \gamma_{c}^{(\text{H,F-SD})}(L)\) for \(L=4, 8, 12.\) We have extrapolated these finite-size data to the thermodynamic \((L \to \infty)\) limit by fitting them for the former and for the latter to quadratic functions of \((L + 1)^{-2}\) and of \((L + 2)^{-2}\), respectively. Some examples of the results are \(J'_{\text{ring},c}^{(\text{AFstN,H})}(\infty) = 0.225 \pm 0.001\) and \(J'_{\text{ring},c}^{(\text{H,F-SD})}(\infty) = 0.428 \pm 0.001\) for \(\gamma = 0.6,\) and also \(\gamma_{c}^{(\text{AFstN,H})}(\infty) = 0.942 \pm 0.002\) for \(J'_{\text{ring}} = -1.0.\) It is noted that the above value of \(\gamma_{c}^{(\text{AFstN,H})}(\infty)\) for \(J'_{\text{ring}} = -1.0\) is in fairly good agreement with the corresponding value \(\approx 0.9\) obtained by mapping the present Hamiltonian (1) onto the effective Hamiltonian (2) for the \(S=1\) chain (see subsection 2.1). We have carried out the same procedure for various values of \(\gamma\) and \(J'_{\text{ring}}\) to obtain the 2D Ising phase boundary lines shown by the solid lines in Fig. 2.

The Lifshitz line which separates the commensurate and incommensurate regions can be estimated by examining the Fourier transform of the site magnetization \(m_{j,L}(L)\) [23, 24]. When we adopt open boundary conditions, the present \(S=1/2\) rung-alternating ladder system has no inversion symmetry with respect to its center position, that is, \(m_{j,L}(L) \neq m_{L+1-j,L}(L).\) Therefore, it is important, especially in the region of the Haldane phase, to discuss two kinds of the Fourier transforms, \(S_{q}^{c}(L; \text{left})\) and \(S_{q}^{c}(L; \text{right})\), defined by

\[
S_{q}^{c}(L; \text{left}) = \frac{1}{\sqrt{L/2}} \sum_{j=1}^{L/2} \exp(ijq) m_{j,L}(L), \quad S_{q}^{c}(L; \text{right}) = \frac{1}{\sqrt{L/2}} \sum_{j=1}^{L/2} \exp(ijq) m_{L+1-j,L}(L)
\]

with \(m_{j,L}(L) = m_{j,a}(L) + m_{j,b}(L),\) in order to avoid the mismatch of the edge states of both edges. In the above equations \(q\) is the wave number.

In Fig. 5 the \(q\)-dependences of the squared modulus of \(S_{q}^{c}(192; \text{left})\), which have been calculated by using the DMRG results for \(m_{j,L}(192)\) for the finite-size system with \(2L=384\) spins, are shown for the cases of \(J'_{\text{ring}}=0.1, 0.3, 0.37\) and 0.5. It is noted that the \(q\)-dependences of \(|S_{q}^{c}(192; \text{right})|^{2}\) show almost the same behavior. Thus, the values of \(q_{0}^{c}(192; \text{left})\)
Figure 5. Squared modulus of the Fourier transform of the site magnetization, $|S_q^x(192; \text{left})|^2$, plotted versus $q/\pi$ with $\gamma$ fixed at $\gamma = 0.6$. The solid, dashed, dot-dashed and dotted lines show, respectively, the result for $J'_\text{rung}=0.1$ (divided by 3), that for $J'_\text{rung}=0.3$ (multiplied by 460), that for $J'_\text{rung}=0.37$ (multiplied by 900) and that for $J'_\text{rung}=0.5$.

and $q_0^x(192;\text{right})$ of $q$ which give, respectively, the maximum values of $|S_q^x(192;\text{left})|^2$ and $|S_q^x(192;\text{right})|^2$ are almost equal to each other. Figure 6 depicts the plots of $q_0^x(192;\text{left})$ and $q_0^x(192;\text{right})$ versus $J'_\text{rung}$ for $\gamma = 0.6$. From this figure we clearly see that, there are two Lifshitz points $J_{\text{rung,Lifshitz}}^{(1)}(192)$ and $J_{\text{rung,Lifshitz}}^{(2)}(192)$, and in the region of $J_{\text{rung,Lifshitz}}^{(1)}(192)\leq J'_\text{rung} \leq J_{\text{rung,Lifshitz}}^{(2)}(192)$, the system has the incommensurate character in the sense that both of $q_0^x(192;\text{left})$ and $q_0^x(192;\text{right})$ are larger than $\pi/2$ and smaller than $\pi$, where $J_{\text{rung,Lifshitz}}^{(1)}(192)=0.251 \pm 0.001$ and $J_{\text{rung,Lifshitz}}^{(2)}(192)=0.415 \pm 0.001$. These values of the Lifshitz points yield good approximations for the corresponding $L\rightarrow \infty$ ones, since our calculations show that the finite-size values for $L=192$, $96$ and $72$ agree with each other within numerical errors. We have performed the same procedure for various values of $\gamma$, and obtained the Lifshitz lines shown by the dotted lines in Fig. 2. It is noted that, in the region between these two Lifshitz lines, the ground state of the present system has an incommensurate character.

4. Summary
We have numerically determined, with the help of some physical considerations, the ground-state phase diagram of an anisotropic rung-alternating $S=1/2$ ladder, which is described by the Hamiltonian (1), in the case where $J_{xy}=0.2$, $J_{xy}=-1$, $|J'_\text{rung}| \leq 1$ and $0 \leq \gamma < 1$. The obtained phase diagram on the $\gamma$ versus $J'_\text{rung}$ plane is shown in Fig. 2. We hope that the present research stimulates future experimental studies on related subjects, which include the synthesis of spin ladder systems with alternating rung interactions.

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