MAGNETIC PHASE DIAGRAM OF A SPIN ANTIFERROMAGNETIC $S = 1/2$ LADDER WITH ALTERNATING RUNG EXCHANGE AND DIMERIZED LEGS

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We study the effect of leg dimerization on the ground-state magnetic phase diagram of a two-leg spin $S = 1/2$ ladder with alternating rung exchange. We consider two possible patterns for dimmers distribution along the legs corresponding to the checkerboard and columnar structure. We study the system in the limit of strong rung exchange and magnetic field and. map the model onto the effective spin $\tau = 1/2$ chain model and study the latter using the continuum-limit bosonization approach. We identified four quantum phase transitions and corresponding critical magnetic fields, which mark transitions from the spin gapped regimes into the gapless quantum spin-liquid regimes. In the gapped phases the magnetization curve of the system shows plateaus at magnetizations equal to zero, its saturation value $M = M_{sat}$ and at $M = 0.5M_{sat}$. We show that in the case of checkerboard structure the intra-leg dimerization has no effect on the ground state properties of the system, while the columnar pattern leads to renormalization of the critical fields, in particular to extension of the gapped phases and respectively of the magnetization plateaus.

Introduction

Low-dimensional quantum magnetism has been the subject of intense research during decades. Perpetual interest in study of these systems is determined by their rather unconventional low-energy properties (see for a review Ref. [1]). An increased current activity in this field is connected with the large number of qualitatively new and dominated by the quantum effects phenomena recently discovered in these systems [2, 3] as well as with the opened wide perspectives for use of low-dimensional magnetic materials in modern nanoscale technologies.

The spin $S = 1/2$ two-leg ladders represent one, particular subclass of low-dimensional quantum magnets which also has attracted a lot of interest for a number of reasons. On the one hand, there was remarkable progress in recent years in the fabrication of such ladder compounds [4]. On the other hand, spin-ladder models pose interesting theoretical problems since the excitation spectrum of a two-leg antiferromagnetic ladder is gapped and therefore, in the presence of a magnetic field, these systems reveal an extremely complex behavior, dominated by quantum effects. The magnetic field driven quantum phase transitions in ladder systems were intensively investigated both theoretically [5 – 15] and experimentally [16]. Usually, these most exciting properties of low dimensional quantum spin systems exhibit strongly correlated effects driving them toward regimes with no classical analog. Properties of the systems in these regimes or "quantum phases" depend in turn on the properties of their ground state and low-lying energy excitations. Therefore search for the gapped phases emerging from different sources and study of ordered phases and quantum phase transitions associated with the dynamical generation of new gaps is an important direction in theoretical studies of quantum spin systems.

A particular realization of such scenario appears in the case where the spin-exchange coupling constants are spatially modulated. The spin-Peierls effect in spin chains represent prototype example of such behavior [17]. After the seminal paper by Martin–Delgado, Shankar and Sierra [18], where extremely rich phase diagram of a ladder with dimerized legs has been shown, there is continuous interest in studies of ladders with dimerized legs [19 – 25].

Recently the new type of spin-Peirels distortion in ladder systems, connected with spontaneous dimerization of the system during the magnetization process via alternation of rung exchange (see **Fig. 1**) has been proposed [26]. It has been shown that the ladder with rung-exchange modulation exhibits the very rich ground state magnetic phase diagram and a new mechanism for magnetization plateau formation.

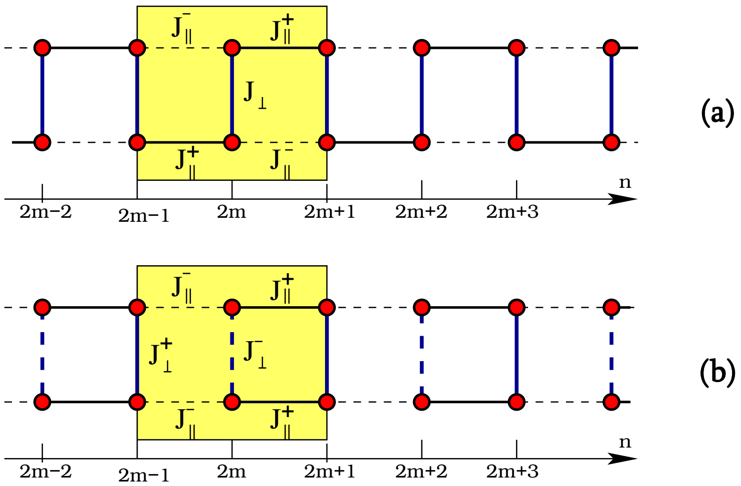

Figure 1. Schematic plot of a ladder with alternating rung exchange and "checkerboard" (a) and "columnar" (b) dimerization of legs.

In this paper we consider the effect of leg dimerization on the infrared properties of the ladder with rung alternation. In particular we consider two different types of leg dimerization, the "checkerboard" (**Fig. 1a**) given by the Hamiltonian

$$\hat{H} = \sum_{n,\alpha} J_\parallel (1 + (-1)^{n+\alpha} \delta_0) \vec{S}_{n,\alpha} \vec{S}_{n+1,\alpha} - H \sum_{n,\alpha} S_n^z + \sum_{n,\alpha} J_\perp (1 + (-1)^n \delta_1) \vec{S}_{n,1} \cdot \vec{S}_{n,2} \tag{1a}$$

and the "columnar" (see (Fig. 1.b), given by the Hamiltonian

$$\hat{H} = \sum_{n,\alpha} J_\parallel (1 + (-1)^{n} \delta_0) \vec{S}_{n,\alpha} \vec{S}_{n+1,\alpha} - H \sum_{n,\alpha} S_n^z + \sum_{n,\alpha} J_\perp (1 + (-1)^n \delta_1) \vec{S}_{n,1} \cdot \vec{S}_{n,2} \,. \tag{1b}$$

Here $\vec{S}_{n,\alpha}$ is a spin $S = 1/2$ operator of rung n ($n = 1,2,..., N$) and leg α ($\alpha = 1,2$). The intraleg and interleg spin exchange couplings are antiferromagnetic, $J_\parallel[1 \pm \delta_0] > 0$, $J_\perp^\pm = J_\perp[1 \pm \delta_1] > 0$.

Below we restrict our consideration by the limit of strong rung exchange and magnetic field $H, J_{\perp}^{\pm} >> J_{\parallel}, \delta_1 J_{\perp}, \delta_0 J_{\parallel}$ and follow the route already used to study the standard ladder models in the same limit [7, 8].

In absence of leg dimerization, at $\delta_0 = 0$ the model (1) has been studied for analytically in the limit of strong rung exchange and magnetic field $J_{\perp}^{\pm}, H >> J_{\parallel}, \delta J_{\perp}^{0}$ using the effective field-theory approach in [26]. In this limit, the model (1) is mapped onto the spin $S = 1/2$ XXZ Heisenberg chain in the presence of both longitudinal uniform and staggered magnetic fields, with the amplitude of the staggered component of the magnetic field proportional to $\delta_1 J_{\perp}$. The continuum-limit bosonization analysis of the effective spin-chain Hamiltonian show, that the alternation of the rung-exchange leads to the dynamical generation of a new energy scale in the system and to the appearance of a magnetization plateau at magnetization equal to one half of its saturation value. It was shown that the width of magnetization plateau scales as δ^{ν}, with $\nu = 8/9$. In this paper we continue our studies of the model (1) and investigate the effect of intraleg dimerization on the ground state magnetic phase diagram of the system.

Derivation of the effective model

We start from the case $J_{\parallel} = 0$, where an eigenstate of $\hat{H}$ can written as a product of on-rung states. At each rung two spins form either a singlet state $|s_n^0\rangle$ or one of the triplet states: $|t_n^0\rangle$,$|t_n^+\rangle$ and$|t_n^-\rangle$ with energies $E_S = -3J_{\perp}^n/4$, $E_t^0 = J_{\perp}^n/4$, and $E_t^{\pm} = J_{\perp}^n/4 \pm H$, respectively, where $J_{\perp}^n$ denotes the spin exchange on the nth rung. When H is small, the ground state consists of a product of rung singlet states, while at $H \approx J_{\perp}^n$ the $|t_n^-\rangle$ becomes almost degenerate with $|s_n^0\rangle$, while other states have much higher energy. Integrating out the high energy states and introducing the effective pseudo-spin $\tau = 1/2$ operators, $\vec{\tau}_n$ which act on these states as

$$\tau_n^z |s_n^0\rangle = -\frac{1}{2}|s_n^0\rangle, \qquad \tau_n^+ |s_n^0\rangle = |t_n^+\rangle, \qquad \tau_n^- |s_n^0\rangle = 0,$$

$$\tau_n^z |t_n^+\rangle = +\frac{1}{2}|t_n^-\rangle, \qquad \tau_n^- |t_n^+\rangle = |s_n^0\rangle, \qquad \tau_n^+ |t_n^+\rangle = 0.$$

In the case of "checkerboard" type dimerization of legs, contributions to the effective Hamiltonian from two legs with opposite dimerization compensate each. As the result the obtained effective Hamiltonian

$$H_{eff} = \sum_n \{J_{\parallel}(\tau_n^x \cdot \tau_{n+1}^x + \tau_n^y \cdot \tau_{n+1}^y + \tfrac{1}{2}\tau_n^z \cdot \tau_{n+1}^z) - [h_0 + (-1)^n \cdot h_1] \cdot \tau_n^z\}, \tag{2}$$

where

$$h_0 = H - J_{\perp} - J_{\parallel}/2 \qquad \text{and} \qquad h_1 = \delta_1 J_{\perp}, \tag{3}$$

is the Hamiltonian of the Heisenberg chain with anisotropy parameter $\gamma = 1/2$ in the uniform and staggered magnetic fields, studied in [26]. Therefore, in the limit of strong on-rung coupling the effect of "checkerboard" dimerization of legs on the ground state magnetic properties of the system *is absent*.

In the marked contrast with the "checkerboard" case, in the case of "columnar" dimerization of legs, the effective Hamiltonian explicitly shows dependence on the leg dimerization parameter δ_0 and is given by

$$H_{eff} = \sum_n \{J_{\parallel}[1+(-1)^n \delta_0](\tau_n^x \cdot \tau_{n+1}^x + \tau_n^y \cdot \tau_{n+1}^y + \tfrac{1}{2}\tau_n^z \cdot \tau_{n+1}^z) - [h_0 + (-1)^n \cdot h_1] \cdot \tau_n^z\}, \qquad (4)$$

with h_0 and h_1 given by Eq. (3). Thus the effective Hamiltonian describes a *dimerized* anisotropic XXZ Heisenbeg chain with the anisotropy parameter $\gamma = 1/2$ in the uniform and staggered magnetic fields.

At $\delta_0 = \delta_1 = 0$, the effective Hamiltonian reduces to the XXZ Heisenberg chain in an uniform longitudinal magnetic field. The magnetization curve of this model has only saturation plateau corresponding to the fully polarized chain. At $H = 0$ and $J_{\perp}^0 >> J_{\parallel}$, spins coupled by strong rung exchange form singlet pairs and the nonmagnetic and gapped ground state of the ladder system is well described by superposition of on-rung singlets. In terms of effective τ-spin model, the ground state corresponds to the ferromagnetic order with magnetization per site $m = -1/2$. In the opposite limit of very strong magnetic field $H >> J_{\perp}^0$, fully polarized state of the ladder with magnetization per rung $M = 1$, is represented in terms of effective τ-spin chain as the fully polarized state with magnetization per site $m = 1/2$. This gives the following relation between the magnetization per rung of the ladder system and the magnetization per site of the effective chain $M = m + 1/2$.

The performed mapping allows to estimate the critical field H_{on} corresponding to the transition from a gapped rung-singlet phase to a gapless paramagnetic phase, the saturation field H_{sat} corresponding to the transition onto the fully polarized phase as well as the critical fields $H_c^{\pm}$ which mark borders of the magnetization plateaus at $M = 0.5M_{sat}$. The direct way to express H_{on} and H_{sat} in terms of ladder parameters is to perform the Jordan–Wigner transformation which maps the problem onto a system of interacting spinless fermions [27]:

$$\hat{H}_{sf}^i = \tfrac{1}{2} J_{\parallel} \sum_n (1+(-1)^n \delta_0)[(a_n^+ a_{n+1} + h.c.) + \rho_n \cdot \rho_{n+1}] - \sum_n [\mu_0 + (-1)^n \mu_1]\rho_n, \qquad (5)$$

where $\rho_n = a_n^+ a_n$, $\mu_0 = \tfrac{1}{2} J_{\parallel} + h_0$, $\mu_1 = h_1$.

The critical magnetic fields

The lowest onset (H_{on}) and highest saturation (H_{sat}) critical field corresponds to that value of the chemical potential μ_0 for which the band of fermions (or holes, after the corresponding particle-hole transformation) starts to fill up. In this limit we can neglect the interaction term in (5) and obtain that $H_{on} = J_{\parallel} - \sqrt{J_{\parallel}^2 + (2\delta_0 J_{\parallel})^2 + (\delta_1 J_{\perp})^2}$ and $H_{sat} = J_{\perp} + J_{\parallel} + \sqrt{J_{\parallel}^2 + (2\delta_0 J_{\parallel})^2 + (\delta_1 J_{\perp})^2}$.

To determine the critical fields $H_c^{\pm}$ we use the continuum-limit bosonization approach. Using the standard bosonized expressions for the spin operators [28]

$$\tau_n^z = \frac{1}{\sqrt{\pi}} \partial_x \phi(x) + (-1)^n \frac{A}{\pi} \sin\sqrt{4\pi}\phi(x), \qquad (6a)$$

$$\tau_n^+ = e^{-i\sqrt{\pi/K}\theta}\left[B_0(-1)^n + \frac{B_1}{\pi} \cdot \sin\sqrt{4\pi}\phi(x)\right], \qquad (6b)$$

Where $\phi(x)$ and $\theta(x)$ are dual bosonic fields $\partial_x \phi = \partial_t \theta$, which satisfy the commutation relation $[\phi(x);\theta(x')] = -i\vartheta_{step}(x - x')$ and A and B are non-universal real constants of the order of unity [29], we obtain the bosonized expressions for the smooth and staggered parts of the relevant spin operators

$$(\tau_n^x \cdot \tau_{n+1}^x + \tau_n^y \cdot \tau_{n+1}^y) \approx \tfrac{1}{2}(\partial_x \phi)^2 + \tfrac{1}{2}(\partial_x \theta)^2 , \quad (7a)$$

$$(-1)^n (\tau_n^x \cdot \tau_{n+1}^x + \tau_n^y \cdot \tau_{n+1}^y) \approx d_{xy} \cos\sqrt{4\pi K}\phi(x) , \quad (7b)$$

$$\gamma \tau_n^z \cdot \tau_{n+1}^z \approx \frac{4\gamma}{\pi}(\delta_x \phi)^2 , \quad (7c)$$

$$(-1)^n \tau_n^z \cdot \tau_{n+1}^z \approx d_z \cos\sqrt{4\pi}\phi(x) . \quad (7d)$$

Using (7a – d), after rescaling the field we get the following bosonized Hamiltonian

$$H_{KG} = \int dx \left[\frac{v}{2}[(\partial_x \phi)^2 + (\partial_x \theta)^2] - \frac{\Delta_0}{\pi a_0}\sin(\sqrt{4\pi K}\phi + \varphi_0) - h_0 \sqrt{\frac{K}{\pi}}\partial_x \varphi \right], \quad (8a)$$

where

$$\Delta_0 = \delta_1 J_\perp \sqrt{1 + \tan^2 \varphi_0} \quad (8b)$$

and

$$\tan \varphi_0 = \arctan\left(\frac{2J_\parallel \delta_0 (d_{xy} + d_z)}{J_\perp \delta_1} \right). \quad (9)$$

The parameter $K(\gamma,\eta)$ is the spin stiffness parameter for spin chain with anisotropy γ and magnetization $\lambda = m / m_{sat}$. At zero magnetization the spin stiffness parameter can be exactly evaluated from Bethe ansatz $K(\gamma,0) = \pi / 2(1 - \arccos\gamma)$ [29] and thus, in the considered case of a ladder with isotropic antiferromagnetic legs $K(1/2,0) = 0.75$. At the transition line into the ferromagnetic phase, the spin stiffness parameter takes the universal value $K(\gamma,1) = 1$ [6]. Therefore at $J_\parallel > 0$ and for finite magnetization $0 < m < m_{sat}$ the function $K(\gamma,\lambda)$ monotonically increases with increasing m and reaches its maximum value at saturation magnetization $K(1,\gamma) = 1$. To evaluate the numerical value of the parameter $K(\gamma,\lambda)$ in this paper we use the following ansatz [30]

$$K(\gamma,\lambda) = \lambda + (1-\lambda)K(0,\gamma) . \quad (10)$$

The coefficients d_z and d_{xy} are functions of the parameter K and can be calculated numerically [31].

The Hamiltonian (5) is the standard Hamiltonian for the commensurate–incommensurate [32] transition which has been intensively studied in the past using bosonization approach [33] and the Bethe ansatz technique [34]. We use the results obtained in Refs. [33, 34] to describe magnetization plateau and the transitions from a gapped (plateau) to gapless paramagnetic phases.

Let us first consider $h_0 = 0$. In this case the continuum theory of the initial ladder model in the magnetic field $H = J_\perp + J_\parallel / 2$ is given by the quantum sine-Gordon (SG) model with a massive term $\approx \Delta_0 \sin(\sqrt{4\pi K}\phi)$. From the exact solution of the SG model [35] it is known that the excitation spectrum of the model (7) is gapped and the value of the renormalized spin gap M_{sol} scales with its bare value as [36] $M_{sol} \approx J_\parallel (\Delta_0 / J_\parallel)^{1/(2-K)}$. Thus for $h_0 = 0$ the low-energy behavior of the system is determined by the composite effect of the rung and leg modulation represented in the effective continuum limit theory by the term $\Delta_0 \sin(\sqrt{4\pi K}\phi)$.

In the ground state the field φ is pinned in one of the minima of the potential $V(\phi) \approx -\Delta_0 \sin(\sqrt{4\pi K}\phi - \varphi_0)$ given by the condition $< 0 | \sin(\sqrt{4\pi K}\phi - \varphi_0) | 0 > = 1$. Using Eqs. (6a – d) we obtain that in the ordered state, the ground-state average value of the on-site magnetization $< \tau_n^z > \approx (-1)^n \cos\varphi_0$ and of the on-link dimerization operator $< \vec{\tau}_n \cdot \vec{\tau}_{n+1} > \approx (-1)^n (d_{xy} + d_z) \sin\varphi_0$. Thus in the case of “columnar” type of leg dimerization, the state corresponding to the magnetization plateau at gnetization equal to half of the saturation value, rather unconventional gapped and long-range ordered (LRO) phase with coexisting of Néel antiferromagnetic and Peierls type dimerized order is realized. The ratio of amplitudes of these coexisting ordered state is determined by the parameter φ_0, which interpolates between the values $\varphi_0 = 0$ at $\delta_1 = 0$ where the LRO Néel antiferromagnetic is realized, to $\varphi_0 = \pi/2$ at $\delta_1 >> \delta_0$ where only the Peierls dimerized phase is present in the ground state. In terms of the initial ladder system this corresponds to the phase, where spins on weak odd rungs with have a dominant triplet character and spins on strong even rungs are predominantly coupled into singlets.

At $h_{eff}^0 \neq 0$ the very presence of the gradient term in the Hamiltonian (12) makes it necessary to consider the ground state of the SG model in sectors with nonzero topological charge. The effective chemical potential $\approx h_0 \partial_x \phi$ tends to change the number of particles in the ground state i.e. to create a finite and uniform density solitons. However this implies that the vacuum distribution of the field φ will be shifted with respect of the corresponding minima. This competition between contributions of the smooth and staggered components of magnetic field is resolved as a continuous phase transition from a gapped state at $h_0 < M_{sol}$ to a gapless (paramagnetic) phase at $h_0 > M_{sol}$ [32]. The condition $h_{eff}^0 = M_{sol}$ gives two additional critical values of the magnetic field $H_{c1}^{\pm} = J_{\perp}^0 + \frac{1}{2} J_{\parallel} \pm J_{\parallel} (\Delta_0 / J_{\parallel})^{1/(2-K)}$. Correspondingly the width of each magnetization plateaus is given by $H_{c1}^{+} - H_{c1}^{-} = 2C_0 J_{\parallel} (\Delta_0 / J_{\parallel})^{1/(2-K)}$. Using Eq. (10) we obtain $K(0.5, 0.5) \cong 0.875$ what gives that the width of the magnetization plateau scales as $\delta^{8/9}$.

As usual in the case of C – IC transition, the magnetic susceptibility of the system shows a square-root divergence at the transition points: $\chi(H) \approx (H_c^- - H)^{-1/2}$ for $H < H_c^-$ and $\chi(H) \approx (H - H_c^+)^{-1/2}$ for $H > H_c^+$. Thus from analytical studies we obtain the following magnetic phase diagram for a ladder with alternating rung exchange. For $H < H_{on}$, the system is in a rung-singlet phase with zero magnetization and vanishing magnetic susceptibility. For $H > H_{on}$ some of singlet rungs melt and the magnetization increase as $\sqrt{H - H_{on}}$. With further increase of the magnetic field the system gradually crosses to a regime with linearly increasing magnetization. However, in the vicinity of the magnetization plateau, for $H < H_c^-$ this linear dependence changes again into a square-root behavior $M \approx 0.5 M_{sat} - \sqrt{H_c^- - H}$. For fields in the interval between $H_c^- < H < H_c^+$ the magnetization is constant $M = 0.5 M_{sat}$. At $H > H_c^+$ the magnetization increases as $M \approx 0.5 M_{sat} + \sqrt{H - H_c^+}$, then passes again through a linear regime until, in the vicinity of the saturation field H_{sat}, it becomes $M \approx M_{sat} - \sqrt{H_{sat} - H}$. The width of the magnetization plateau is given by $H_{c2}^- - H_{c1}^+ = 2C_0 J_{\parallel} (\Delta_0 / J_{\parallel})^{8/9}$.

Conclusion

We have studied the ground state magnetic phase diagram of a spin $S=1/2$ two-leg ladder with alternating rung-exchange and dimerized legs in the limit of strong rung exchange and magnetic field. We have considered two possible leg dimerization patterns – checkerboard and columnar. We have shown, that in the case of checkerboard pattern, dimerization of the legs does not effect the ground state phase diagram, while in the case of columnar pattern dimerization of legs leads to renormalization of the critical fields, in particular to extension of the gapped phases and respectively of the magnetization plateaus. We have also shown, that columnar leg dimerization leads to appearance of composite order in the ground state in the gapped phase corresponding to the plateau at magnetization $M=0.5M_{sat}$. In particular, in this phase the system is characterized by the coexistence of long-range-ordered Néel antiferromagnetic state with the "rung-rung" dimer phase. The former state corresponds to the magnetic order where all spins on weak (odd) rungs are aligned along the field and form a $S_z=1$ triplet state, while spins on strong (even) rungs form a singlet pairs. The latter, "rung-rung" dimer order corresponds to the phase, where these on-rung triplet and singlet states, coupled via the strong intraleg exchanges (even links) form an entangled (singlet) state. In the composite phase, which is realized along the magnetization plateau at magnetization equal to the half of the saturation value, both these phases are present and their weight is controlled by the mixing angle φ_0. In absence of the leg dimerization ($\varphi_0=0$) only the Néel antiferromagnetic phase is present, while in absence of the rung-exchange modulation ($\varphi_0=\pi/2$) only the "rung-rung" dimmer phase is realized.

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