Magnetic Phase Diagram of a Spin Antiferromagnetic $S=1/2$ Ladder with Alternating Rung Exchange

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ABSTRACT. The ground-state phase diagram of a two-leg spin ladder with alternating rung exchange $J_\perp(n) = J_\perp^0 + (-1)^n \delta J_\perp^0$ under the influence of a uniform magnetic field is studied. We have used the exact diagonalization technique. In the limit where the rung exchange is dominant, we have mapped the model onto the effective quantum sine-Gordon model with topological term and identified two quantum phase transitions at critical magnetic fields $H^-_c$ and $H^+_c$ from a gapped to the gapless regime. We have shown that for intermediate values of the magnetic field, at $H^-_c < H < H^+_c$ the magnetization curve of the system exhibits a plateau at magnetization equal to the half of the saturation value. We also present a detailed numerical analysis of the low energy excitation spectrum and the ground state magnetic phase diagram of the system using the Lanczos method of numerical diagonalizations for ladders up to $N=28$ sites. We have calculated numerically the magnetic field dependence of the low-energy excitation spectrum, the magnetization, the on-rung spin-spin correlation function. We have also calculated the width of the magnetization plateau and show that it scales as $H^{-\nu}$, where the critical exponent varies from $\nu = 0.87 \pm 0.01$. © 2008 Bull. Georg. Natl. Acad. Sci.

Key words: spin-Hamiltonian, two-leg spin ladder.

Introduction. Low-dimensional quantum magnetism has been the subject of intense research for decades. Perpetual interest in the study of these systems is determined by their rather unconventional low-energy properties (see for a review [1]). An increased current activity in this field is connected with a large number of qualitatively new and dominated by the quantum effects phenomena recently discovered in these systems [2,3] as well as with the wide perspectives opened for the 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 represents a prototype example of such behavior [17]. In a recent paper the new type of spin-Peierls phenomenon in ladder systems, connected with spontaneous dimerization of the system during the magnetization process via alternation of rung exchange (see Fig. 1) has been discussed [18]. The Hamiltonian of the corresponding model is given by

\[
\hat{H} = \sum_{n,\alpha} [J_0 \hat{S}_{n,\alpha} \cdot \hat{S}_{n+1,\alpha} - H S_n^Z] + J^\perp \sum_{n} \left[1 + (-1)^n \delta \right] \hat{S}_{n,1} \cdot \hat{S}_{n,2},
\]

where \( \hat{S}_{n,\alpha} \) is a spin \( S=1/2 \) operator of rung \( n (n=1,2,\ldots,N) \) and leg\( \alpha (\alpha=1,2) \). The intraleg and interleg couplings are antiferromagnetic, \( J_0 > 0 \), \( J^\perp = J^0_0 \left[1 \pm \delta \right] > 0 \). As it was shown in [18] the model shows rich ground state magnetic phase diagram and describes a new mechanism for magnetization plateau formation.

In [18] the model (1) has been studied analytically in the limit of strong rung exchange and magnetic field \( J^\perp, H \gg J_0, \delta J^0_0 \) using the effective field-theory approach. 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 \( \delta J^0_0 \). The continuum-limit bosonization analysis of the effective spin-chain Hamiltonian shows that the alternation of the rung-exchange leads to 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 \( \delta^\nu \), with \( \nu = 4/5 \).

In this paper we continue our studies of the model (1) using the numerical analysis based on the exact diagonalization studies of finite systems with \( N=12, \ 16, \ 20, \ 24 \) and 28 sites. We calculate the spin gap, magnetization, spin density distribution and the on-rung spin correlations as a function of applied magnetic field. We also computed the magnetization plateau scaling exponent and showed that \( \nu = 0.87 \pm 0.01 \) in the case of a ladder with isotropic antiferromagnetic legs.

**Derivation of the effective model.** In this section we briefly recall the results obtained within the analytical approach [18]. We restrict our consideration by the limit of strong rung exchange and magnetic field \( H, J^\perp, J_0, \delta J^0_0 \) and follow the route already used to study the standard ladder models in the same limit [7,8].

We start from the case \( J_0 = 0 \), where an eigenstate of \( \hat{H} \) can be 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 \( E_n = -3J_0^\perp / 4, \ E_n^0 = J_0^\perp / 4, \) and \( E_n^\pm = J_0^\perp / 4 \pm H \), respectively. When \( H \) is small, the ground state consists of a product of rung singlet states, while at \( H \approx J_0^\perp \) 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, \( \tilde{\tau}_{n} \) which act on these states as

\[
\tilde{\tau}_{n} |s_{n}^0 \rangle = -\frac{1}{2} |s_{n}^0 \rangle, \quad \tilde{\tau}_{n}^- |s_{n}^0 \rangle = |t_{n}^- \rangle, \quad \tilde{\tau}_{n}^+ |s_{n}^0 \rangle = 0;
\]

\[
\tilde{\tau}_{n}^\perp |t_{n}^0 \rangle = +\frac{1}{2} |t_{n}^0 \rangle, \quad \tilde{\tau}_{n}^- |t_{n}^0 \rangle = |s_{n}^0 \rangle, \quad \tilde{\tau}_{n}^+ |t_{n}^0 \rangle = 0,
\]

we obtain the following effective Hamiltonian of the anisotropic Heisenberg chain with anisotropy parameter \( \Delta = 1/2 \) in the uniform and staggered longitudinal magnetic fields

\[
H_{\text{eff}} = \sum_{n} \left[J_\parallel (\tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp + \tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp + \frac{1}{2} \tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp) - \right]
\]

\[
-\left[h_{\text{eff}}^0 + h_{\text{eff}}^1 \cdot (-1)^n \right] \tilde{\tau}_{n}^0,
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H_{\text{eff}} = \sum_{n} \left[J_\parallel (\tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp + \tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp + \frac{1}{2} \tilde{\tau}_{n}^\perp \cdot \tilde{\tau}_{n+1}^\perp) - \right]
\]

\[
-\left[h_{\text{eff}}^0 + h_{\text{eff}}^1 \cdot (-1)^n \right] \tilde{\tau}_{n}^0,
\]

Fig. 1. Schematic plot of a ladder with alternating rung exchange

The Hamiltonian (5) is the standard Hamiltonian for the commensurate-incommensurate [21] transition which has been intensively studied in the past using bosonization approach [22] and the Bethe ansatz technique [23]. Below we use the results obtained in [22] and [23] to describe the magnetization plateau and the transitions from a gapped (plateau) to gapless paramagnetic phases.

Let us first consider \( h_0^0 = 0 \). 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

\[ \approx h_{_0}^1 \sin(\sqrt{3}\pi\varphi). \]

From the exact solution of the SG model [24] it is known that the excitation spectrum of the model (5) is gapped and the value of the renormalized spin gap \( M_{sol} \) scales with its bare value as [25]

\[ M_{sol} \approx J_\parallel(\Delta J_\parallel / J_\parallel)^{0.8}. \]

Thus for \( h_0^0 = 0 \) the low-energy behavior of the system is determined by the strongly relevant staggered magnetic field (i.e. alternating part of the rung exchange), represented by the term

\[ \approx h_{_0}^1 \sin(\sqrt{3}\pi\varphi). \]

In the ground state the field \( \varphi \) is pinned in one of the minima of the staggered field potential \(< 0 | \sin(\sqrt{3}\pi\varphi) | 0 >= -1 \). In view of (4a) we conclude that this state corresponds to a long-range-ordered antiferromagnetic phase of the effective Heisenberg chain (2), i.e. to a phase of the initial ladder system, where odd rungs have a dominant triplet character and even rungs are predominantly singlets. At \( h_0^0 \neq 0 \) the very presence of the gradient term in the Hamiltonian (5) makes it necessary to consider the ground state of the SG model in sectors with nonzero topological charge.

The effective chemical potential \( \approx h_{_0}^0 \partial_+ \varphi \) tends to change the number of particles in the ground state, i.e. to create finite and uniform density of solitons; however, this implies that the vacuum distribution of the field \( \varphi \) will be shifted with respect to the corresponding minima. This competition between contributions of the smooth and staggered components of the magnetic field is resolved as a continuous phase transition from a gapped state at \( h_0^0 < M_{sol} \) to a gapless (paramagnetic) phase at \( h_0^0 > M_{sol} \) [20]. The condition \( h_0^0 = M_{sol} \) gives two additional critical values of the magnetic field

\[ H_c^± = J_\perp^0 + J_\parallel^0 \left(J_\parallel^0 / J_\parallel \right)^{4/5}. \]

As usual in the case of C-IC transition, the magnetic susceptibility of the system shows a square-root
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divergence at the transition points: $\chi(H) \approx (H^-_c - H)\, H^-_c$ for $H < H^-_c$ and $\chi(H) \approx (H - H^+_c)\, H^+_c$ for $H > H^+_c$. Thus from analytical studies we obtain the following magnetic phase diagram for a ladder with alternating rung exchange. For $H < H_{c1}$, the system is in a rung-singlet phase with zero magnetization and vanishing magnetic susceptibility. For $H > H_{c1}$ some of the singlet rungs melt and the magnetization increase as $\sqrt{H_H - H_{c1}}$. 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 $H < H_{c1}$ this linear dependence changes again into a square-root behavior $M \approx 0.5 M_{sat} - \sqrt{H_{c1} - H}$. For fields in the interval between $H_{c1} < H < H_{c2}$ the magnetization is constant $M = 0.5 M_{sat}$. At $H > H_{c2}$ the magnetization increases as $M \approx 0.5 M_{sat} + \sqrt{H_{c1} - H}$, then passes again through a linear regime until, in the vicinity of the saturation field $H_{c2}$, it becomes $M \approx M_{sat} - \sqrt{H_{c2} - H}$ (see Fig. 2).

The width of the magnetization plateau is given by $H_{c2} - H_{c1} = 2C_0 J_{||}(\Delta J_{||}/J_{||})^{1/5}$.

Numerical Results. Below in this paper we check predictions based on the analytical treatment using the exact diagonalization approach for finite ladders with the number of sites $N=2L=12,16,20,24,28$. We apply the Lanczos method and calculate numerically the magnetic field dependence of the low-energy excitation spectrum, magnetization and the on-rung spin-spin correlation function.

1. The Energy Gap. First, we have computed the three lowest energy eigenvalues of $L=6, 8, 10$ ladders with $J_{||}=1.0$, $J_{||}^0 = 5.5$ and $\Delta J_{||}^0 = 1.0$. In Fig. 3, we have plotted results of these calculations. We determine the excitation gap in the system as the difference between the first excited state and the ground state. As is clearly seen from Fig. 3 at zero magnetic field the excitation spectrum of the system is gapped. For $H \neq 0$ the energy gap decreases linearly with $H$ and vanishes at $H = H_{c1}$. The spectrum remains gapless for $H_{c1} < H < H_{c1}^-$ and once again becomes gapped for $H_{c1} < H < H_{c1}^+$. At $H = H_{c1}^+$ the spectrum becomes gapless and remains gapless up to $H = H_{c2}$, where the gap opens once again and for a sufficiently large field becomes proportional to $H$. Using the results for finite ladders we obtain the following extrapolated to the limit $L \rightarrow \infty$ values of critical fields: $H_{c1} = 4.48 \pm 0.01$, $H_{c1}^- = 5.32 \pm 0.01$, $H_{c1}^+ = 6.87 \pm 0.01$ and $H_{c2} = 7.76 \pm 0.01$. It is straightforward to check that the exact values of the critical fields obtained from numerical studies of the finite ladders are very close to their values estimated analytically.

Fig. 2. Schematic drawing of the magnetization (in units of $M_{sat}$) of a two-leg isotropic ladder with alternating rung exchange as a function of the external magnetic field.

Fig. 3. Excitation gap as a function of the magnetic field for $J_{||}=1.0$, $J_{||}^0 = 5$, $J_{||}^0 = 6$ and different ladder lengths. The inserts show enlarged version in the vicinity of transition points.
2. Magnetization curve. To study the magnetic order of the ground state of the system, we start with the magnetization process. We have implemented the Lanczos algorithm on the finite ladders (L=6, 8, 10, 12, 14) to calculate the lowest energy state. The magnetization along the field axis is defined as

$$M^z = \frac{1}{L} \sum_{n=1}^{L} \langle 0 | (S_{n1}^z + S_{n2}^z) | 0 \rangle$$

where the notation $\langle 0 | ... | 0 \rangle$ represent the ground state expectation value. In Fig. 4, we have plotted the magnetization $M^z$ as a function of the external magnetic field $H$, for $J_{||} = 1$, and for rung exchanges $J_{\perp} = 5$, $J^+_{\perp} = 6$ and different ladder lengths L=6, 8, 10, 12.

As we observe, the numerical data clearly shows the existence of three plateaus in the magnetization curve, at $M^z = 0$, $M^z = 0.25$ and $M^z = 0.5$.

3. Intra-rung correlations. An additional insight into the nature of different phases can be obtained by studying the on-rung correlations. We define the on-rung spin correlation function for even and odd sites, as

$$d^e_r = \frac{2}{L} \sum_{m=1}^{L/2} \langle 0 | \tilde{S}_{1,2m} \tilde{S}_{2,2m} | 0 \rangle$$

$$d^o_r = \frac{2}{L} \sum_{m=1}^{L/2} \langle 0 | \tilde{S}_{1,2m+1} \tilde{S}_{2,2m+1} | 0 \rangle$$

taking the sum over even or odd sites, respectively. In Fig.5 we have plotted the $d^e_r$ and $d^o_r$ as a function of the magnetic field $H$, for $J_{||} = 1$, and for rung exchanges $J_{\perp} = 5$, $J^+_{\perp} = 6$ for a ladder of length $L=10$. As is seen from this figure, at $H_1 < H < H_{c2}$ spins on all rungs are in a singlet state $d^e_r = d^o_r \approx -0.75$, while at $H > H_{c2}$ the on-rung correlation function is equal on even and odd rungs and is slightly less than the saturation value $d^e_r = d^o_r \approx 0.25$. Deviation from the saturation values -0.75 and 0.25 reflects the weak effects of quantum fluctuations.

On the other hand, for intermediate values of the magnetic field, at $H_1 < H < H_{c2}$ the data presented in Fig.5 provides us with an unique possibility to trace the mechanism of singlet-pair melting with increasing magnetic field. At $H$ slightly above $H_1$ the on-rung singlets start to melt in all rungs simultaneously and almost with the same intensity. With further increase of $H$, melting of weak rungs gets more intensive; however, at $H = H_c$ the process of melting stops. As it is seen in Fig.5, weak rungs are polarized; however, their polarization is far from the saturation value $d^o_r \approx 0.1$, while the strong rungs still manifest strong on-site singlet features with $d^e_r \approx -0.62$. At $H > H^+_{c}$ strong rungs start to melt intensively while the polarization of weak rungs increases slowly. Finally at $H = H^+_{c}$ both, even and odd rungs...
odd rung subsystems reach an identical, almost fully polarized state. Note that the fluctuations in on-rung correlations, increase precisely in $H \leq H_c^-$ and decrease in $H \geq H_c^+$ which reflects the enhanced role of quantum fluctuations in the vicinity of quantum critical points.

To complete our description of the phase at magnetization plateau with $M = 0.5M_{sat}$ we have calculated the rung-spin distribution in the ground state

$$M^z(n) = \frac{1}{2} < 0 | S_{n1}^z + S_{n2}^z ) | 0 > \quad (8)$$

In Fig. 6 we have plotted the spin distribution in the ground state of a ladder with rung-exchange parameters $J_1 = 1.0$, $J_2 = 5$, $J_4 = 6$ as a function of the rung number “n” for magnetization corresponding to plateau $M = 0.5M_{sat}$.

Scaling properties of the magnetization plateau. To find an accurate estimate on the critical exponent characterizing the width of the magnetization plateau on the parameter $\delta$ we have computed the critical fields $H^\pm_c$ for finite ladder systems with $J_1^0 = 10$, $L = 6, 8, 10, 12, 14$ and for different values of the parameter $\delta$ and extrapolate their values corresponding to the thermodynamic limit $L \to \infty$. To calculate the critical exponent $\nu$, we have plotted in Fig. 7, the log-log plot of the plateau width versus $\delta$. We found that the best fit to our data (using the equation $H^\pm_c = (\delta J_1^0)^\nu$) yields $\nu = 0.87 \pm 0.01$.

**Conclusion.** We have studied the ground state magnetic phase diagram of a spin $S=1/2$ two-leg ladder with alternating rung-exchange using the Lanczos method of numerical diagonalizations. We have shown that the rung-exchange alternation leads to generation of a gap in the excitation spectrum of the system at magnetization equal to the half of its saturation value. As a result of this additional energy scale formation the magnetization curve of the system $M(H)$ exhibits a plateau at $M = 0.5M_{sat}$. The width of this plateau, is proportional to the rung-exchange alternation $\delta J_1^0$ and scales as $\delta^\nu$, where $\nu = 0.87 \pm 0.01$. The obtained numerical results are in an excellent agreement with estimations obtained within the analytical studies.

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ინტეგრირებით $S=1/2$ "ჰოლოების ბოლოს" მუდმივი დარღვევით „საფარულს“ განუსაზღვრელ პიროთორბულების
აღწერილობას.

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მახასიათებლად ინტეგრირით არამკვიდრი ჯერკების მოპოვებისათვის შემთხვევითად „ბოლოს“ სივრცეების ქვეპირთ სივრცე $S=1/2$ ინტეგრირებით ხარჯის მოდულარობის მცველი მაგნიტური ფაზურის საფარულის აღწერილობას შემთხვევით. ხარჯით (N=8, 12, 16, 20, 22 და 28 ჯერკების შემთხვევა) სივრცე სივრცეების ზედა მაგნიტურობის ქვეპირთ ინტეგრირით არამკვიდრი ჯერკების მოპოვებისათვის შემთხვევითად ხარჯის აღწერილობის მაგნიტური ფაზურის საფარულის აღწერილობა, დიამეტრიულების, ხარჯით სივრცეების ზედა მაგნიტური ფაზური (ჯერკების განვითარება) გამოყენებით და საფარულის განვითარება სივრცე-ჰოლოების კოორდინატების დასავლეთობით ხარჯ მაგნიტური ფაზურის ხალხალი. ხარჯით, რომ „საფარულის“ განვითარების აღწერილობა განსაზღვრის ხარჯის აღწერილობის საფარულის დონის კარგად და ამის შებძენა 3 წ. ძალაში დახმარების პროცესი წარმოადგენს ხარჯით მაგნიტური ფაზის იმ ქვეპირთ აღწერილობისათვის, რომლისაც სივრცეების ღიანგრძლივობათა სახით საჯარო ქვეპირთ აღწერილობის ხარჯას. სივრცეების ღიანგრძლივობის შემთხვევაში პიროთორბულები და საფარულის განვითარების კოორდინატების დასავლეთობა ხარჯ მაგნიტური ფაზას. სივრცეების ღიანგრძლივობის აღწერილობის ღიანგრძლივობა, და საწარმო, რომ ჰოლოების სივრცე განვითარებით აღწერილობაში ფართის საფარულის ხარჯით $\nu = 0.87 \pm 0.01$.

REFERENCES

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