Frustrated ferrimagnetic ladder in a magnetic field

N. B. Ivanov[1] and J. Richter[2]

[1] *Max-Planck Institut für Physik Komplexer Systeme, Nöthnitzer Strasse 38, D-39016 Dresden, Germany**

[2] *Institut für Theoretische Physik, Universität Magdeburg, PF 4120, D-39016 Magdeburg, Germany*

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We study the magnetic phase diagram of two coupled mixed-spin $(1, \frac{1}{2})$ Heisenberg chains as a function of the frustration parameter related to diagonal exchange couplings. The analysis is performed by using spin-wave series and exact numerical diagonalization techniques. The obtained phase diagram – containing the Luttinger liquid phase, a plateau magnetic phase with the magnetization per rung $M = 1/2$, and the fully polarized phase – is closely related to the generic $(J/U, \mu/U)$ phase diagram of the one-dimensional boson Hubbard model.

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Some special classes of quantum spin ladders composed of different types of spins or/and regular mixtures of ferromagnetic and antiferromagnetic exchange bonds exhibit a number of novel quantum spin phases and unusual thermodynamic properties.[1,2] Moreover, such systems are appropriate for studying magnetic quantum critical points in one spatial dimension (1D), since many of them sustain magnetically-ordered ground states. Possible realizations of such ladder structures can be based, for instance, on the synthesized quasi-1D bimetallic molecular magnets.[3,4]

In a recent paper we have considered the role of geometric frustration in a system of two coupled mixed-spin $(1, \frac{1}{2})$ Heisenberg chains.[5] It has been argued that a relatively moderate strength of the magnetic frustration produced by the nearest-neighbor diagonal bonds was able to destroy the ferrimagnetic phase and to stabilize the Luttinger liquid phase. The quantum phase transition between these two phases is smooth and is realized through an intermediate canted spin phase. This latter phase is characterized by a net ferromagnetic moment per rung, $0 < M < 0.5$, and power-law transverse spin-spin correlations. In this Brief Report we show that the magnetic phase diagram of the discussed model as a function of the frustration parameter is closely related to the $(J/U, \mu/U)$ phase diagram of the boson Hubbard model in periodic 1D potentials,[6] where μ, J, and U are, respectively, the chemical potential, the hopping strength constant, and the on-site repulsion potential.

The relevant spin Hamiltonian reads

$$\mathcal{H} = \sum_{n=1}^{L} \left[J_1 \left(\mathbf{s}_{1n} \cdot \mathbf{s}_{2n+1} + \mathbf{s}_{2n} \cdot \mathbf{s}_{1n+1} \right) + J_\perp \mathbf{s}_{1n} \cdot \mathbf{s}_{2n} + J_2 \left(\mathbf{s}_{1n} \cdot \mathbf{s}_{1n+1} + \mathbf{s}_{2n} \cdot \mathbf{s}_{2n+1} \right) - g\mu_B H (s_{1n}^z + s_{2n}^z) \right] , \tag{1}$$

where L, g, μ_B, and H are, respectively, the number of rungs, the gyromagnetic ratio, the Bohr magneton, and the external magnetic field applied in z direction. The spin operators $\mathbf{s}_{1n}$ and $\mathbf{s}_{2n}$ (characterized by the quantum spin numbers $s_1 > s_2$ and the rung index n) are alternatively distributed on the ladder sites. The parameters J_1, $J_\perp$, and J_2 are positive coupling constants of the nearest-neighbor horizontal, vertical, and diagonal exchange bonds, respectively (see Fig. 1 in Ref. 5). We set the energy and length scales by $J_1 \equiv 1$ and $a_0 = 1$, where a_0 is the lattice spacing. For simplicity, in the following we consider the case $J_\perp = 1$ and set $h = g\mu_B H$.

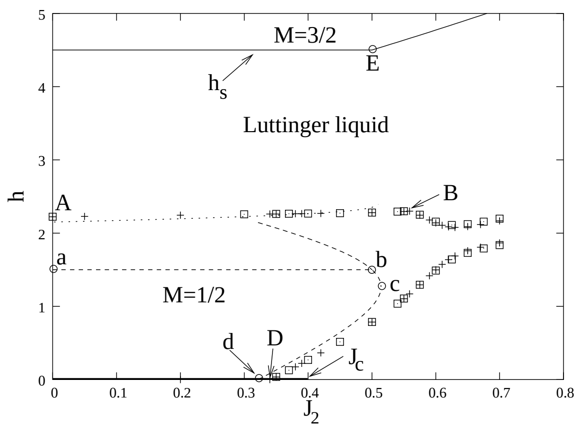

FIG. 1: Phase diagram of the model (1) in the (J_2, h) plane. The phase boundary $h_s = h_s(J_2)$ of the fully polarized phase $(M = 3/2)$ is exact. The dashed curve *abcd* marks the area occupied by the $M = 1/2$ plateau phase, as obtained in a linear spin-wave approximation. The boundary position of this phase, as obtained from the exact numerical diagonalization of periodic clusters, is traced by squares ($L = 10$) and crosses ($L = 12$). The dotted curve shows the phase boundary where $\Delta_0^{(-)}(h) = 0$ [see Eq. (4)], as obtained from the first-order spin-wave theory. The dashed curve starting from the point b and going upwards left as well as the piece bc represent in a linear spin-wave approximation the boundary where $\Delta_\pi^{(-)}(h) = 0$. The canted spin phase exists for $h = 0$ in the interval $0.342 < J_2 < J_c$, where $J_c = 0.399$ is the phase transition point from the canted phase to the Luttinger liquid phase. The rest of the area is occupied by the Luttinger liquid phase.

The magnetic phase diagram of the model (1) in the (J_2, h) plane is presented in Fig. 1. The diagram contains the Luttinger liquid phase, the plateau magnetic phase with a quantized magnetic moment per rung $M = 1/2$ and the fully polarized phase with $M = 3/2$. In addition, there is a canted magnetic phase which exists only at zero magnetic field (in the interval $0.342 < J_2 < J_c = 0.399$) and for $h > 0$ merges into the Luttinger liquid phase. Some properties of the latter phase at $h = 0$ have already been studied in Ref. 5, by using a conformal-field-theory analysis of the numerical exact-diagonalization (ED) data for the ground-state energy and the energies of some low-lying excited states in finite periodic systems. As is well-known, the external magnetic field varies the parameters of the Luttinger liquid phase without changing its basic properties up to a saturation field (h_s), where the system becomes fully polarized.[7]

In this connection, let us firstly consider the critical field h_s defining the phase boundary of the fully polarized $M = 3/2$ phase. The boundary $h_s = h_s(J_2)$ can be obtained by examining the instabilities of the one-magnon excitations above the ferromagnetic vacuum. We assume, as generally accepted, that the multimagnon excitations become unstable at a weaker magnetic field as compared to the one-magnon excitations. As a matter of fact, the latter assumption is confirmed by our ED data, which exactly reproduce the analytical result for h_s presented below. A straightforward calculation results in the following exact expression for the one-magnon dispersion relations in the fully polarized phase

$$\omega^{(1,2)}(k) = h - \frac{9}{4} - 3J_2\sin^2\left(\frac{k}{2}\right) \pm \frac{1}{2}\sqrt{\left[\frac{3}{2} - 2J_2\sin^2\left(\frac{k}{2}\right)\right]^2 + 2\left[3 - 4\sin^2\left(\frac{k}{2}\right)\right]^2}\,, \tag{2}$$

where the wave vector k runs in the lattice Brillouin zone $-\pi \leq k < \pi$. Equation (2) describes two folding ferromagnetic (FM) branches of one-magnon excitations. The phase boundary $h_s = h_s(J_2)$ is defined by the expressions

$$\begin{aligned} h_s &= \frac{9}{2}, \quad 0 \leq J_2 \leq 0.5 \\ &= \frac{9}{4} + 3J_2 + \frac{1}{2}\left[\left(\frac{3}{2} - 2J_2\right)^2 + 2\right]^{\frac{1}{2}}, J_2 \geq 0.5, \end{aligned}$$

where the first and second lines correspond, respectively, to instabilities of $\omega^{(2)}(k)$ at the wave vectors $k = 0$ and π. For $h < h_s(J_2)$, the modes around $k = 0$ and π become unstable and destroy the fully polarized state. As discussed in the following text, the point E in Fig. 1 is a crossover point at which both minima in $\omega^{(2)}(k)$ reach the ground state.

Now we address the $M = 1/2$ plateau phase. The presence of quantum fluctuations in the ferrimagnetic state does not allow exact considerations, so that we shall rely on a qualitative analysis based on the spin-wave theory (SWT) supplemented by numerical ED data for finite periodic systems containing up to $L = 12$ rungs. In a linear SWT approximation, the magnon excitations above the classical ferrimagnetic ground state are described by the following dispersion relations:

$$\omega^{(\pm)}(k) = \pm h \mp \left[\frac{3}{4} + J_2\sin^2\left(\frac{k}{2}\right)\right] + \frac{1}{2}\sqrt{9\left[\frac{3}{2} - 2J_2\sin^2\left(\frac{k}{2}\right)\right]^2 - 2\left[3 - 4\sin^2\left(\frac{k}{2}\right)\right]^2}\,. \tag{3}$$

In the last equation, $\omega^{(+)}(k)$ is a FM branch, whereas $\omega^{(-)}(k)$ describes antiferromagnetic (AFM) one-magnon excitations. In the whole region occupied by the $M = 1/2$ phase, the dispersion relations (3) exhibit minima at the center ($k = 0$) as well as at the boundary ($k = \pi$) of the Brillouin zone. Close to these wave vectors the magnon energies take the generic form

$$\omega_{k_0}^{(\pm)}(k) = \Delta_{k_0}^{(\pm)}(h) + \frac{(k-k_0)^2}{2m_{k_0}^{(\pm)}}\,, k_0 = 0, \pi\,. \tag{4}$$

Here $\Delta_{k_0}^{(\pm)}(h)$ and $m_{k_0}^{(\pm)}$ are, respectively, the magnon gaps and effective masses. Since $\omega_0^{(+)}(k)$ is a Goldstone mode, we have $\Delta_0^{(+)}(0) = 0$.

The magnon modes in Eq. (4) become gapless on different parts of the phase boundary marked by the points a, b, c, and d; $\omega_0^{(-)}(k)$, $\omega_\pi^{(-)}(k)$, and $\omega_\pi^{(+)}(k)$ are gapless, respectively, on the pieces ab, bc, and cd. At the special point b (analogous to the point E), both AFM modes $\omega_0^{(-)}(k)$ and $\omega_\pi^{(-)}(k)$ are gapless. Similar special points have been found in other 1D spin models with folding excitation spectra.[8] In the case when the related magnon masses in (4) diverge, such points produce cusps in the magnetization curves. Otherwise, as in our case, these are crossover points marking the boundary between regions with different low-lying excitations which belong to a single excitation branch. On the other hand, at the special point c with coordinates $(J_2^*, h^*) = (0.75 - \sqrt{2}/6, 1.5 - \sqrt{2}/6)$, two different types of modes – the FM mode $\omega_\pi^{(+)}(k)$ and the AFM mode $\omega_\pi^{(-)}(k)$ – reach the ground state. The point c belongs to the special line $h = 0.75 + J_2$ on which the energies of both magnon modes coincide: $\omega_\pi^{(+)}(k) = \omega_\pi^{(-)}(k)$. Using the picture of "particle-hole" excitations defined by $\omega_{ph}(k) = \omega^{(+)}(k) + \omega^{(-)}(k)$, we find that close enough to (J_2^*, h^*) the dispersion relation $\omega_{ph}(k)$ takes the relativistic form

$$\omega_{ph}(k) = \sqrt{\Delta_{ph}^2 + v_{ph}^2\,(k-\pi)^2}\,. \tag{5}$$

While the velocity v_{ph} remains finite at (J_2^*, h^*), the excitation gap vanishes as $\Delta_{ph} \propto (J_2^* - J_2)^{1/2}$. Clearly, the discussed structure of the low-lying excitations in a vicinity of (J_2^*, h^*) remembers the known structure of low-lying excitations close to the commensurate Mott-insulator-superfluid transition.[6]

In fact, the outlined peculiarities of the (J_2, h) phase diagram – basically deduced from the linear SWT approximation – share a number of common features with the $(J/U, \mu/U)$ phase diagram of the boson Hubbard model on 1D periodic lattices. Before discussing this issue, let us present our quantitative estimates for the boundary positions based on higher-order spin-wave series and numerical ED data. Unfortunately, already the first-order corrections in the SWT series exhibit divergences of the form $\delta^{-1/2}$, δ being the distance in the parametric (J_2, h) space from the point (J_2^*, h^*). Thus, reliable quantitative results can be achieved only for large enough δ. As an example, we show in Fig. 1 the first-order SWT result for the critical field h_c defined through the relation $\Delta_0^{(-)}(h_c) = 0$. In spite of the relatively large correction of the boundary position, we observe a good agreement with the ED data. In fact, one may expect further improvement of the theoretical result in a second-order SWT approximation.[9] Relatively large finite-size effects in the ED data can be indicated only in the vicinity of the tip of the region occupied by the $M = 1/2$ phase. It is remarkable that the peculiarities of the phase boundary – found in the framework of the linear SWT approximation – are reproduced by the ED data. In particular, the cusp at the point B – signaling a change in the type of low-lying excitations – can easily be indicated by the ED data. This is important because the ED data (due to finite-size effects) do not fix the position of the tip.

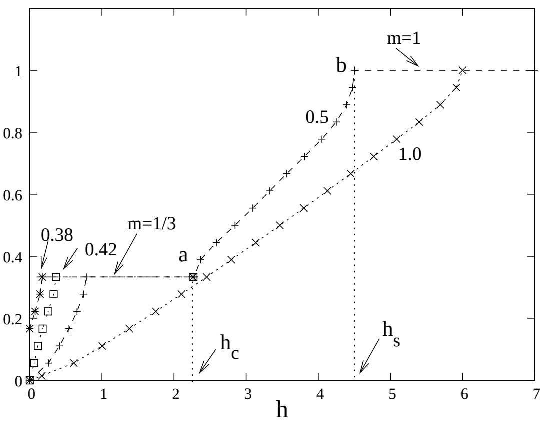

FIG. 2: Magnetization curves of the model (1) for different values of the frustration parameter J_2 ($= 0.38, 0.42, 0.5$, and 1). $m = M/M_s$ is the reduced magnetization, M being the magnetic moment per rung, and $M_s = 3/2$. The symbols mark the midpoints of the magnetization steps, as obtained from the ED data for $L = 12$. For clarity, we do not show the data points for $J_2 = 0.38$ and 0.42 in the interval $h_c < h < h_s$ since they closely follow the presented data for $J_2 = 0.5$.

To compare with the phase diagram of the boson Hubbard model, recall that the magnetic field h plays the role of a chemical potential and the magnetization M is an analogue of the conserved density of particles ρ. As is well-known, the Luttinger liquid phase is an analogue of the superfluid phase in the boson model, and the plateau phases can be viewed as Mott-insulator phases,[10] characterized by an integer ρ, a finite gap for particle-hole excitations, and zero compressibility, $\kappa = \partial\rho/\partial\mu = 0$. Examples of magnetization curves $m(h)$ for different parameters J_2 are presented in Fig. 2. These are analogues of the $\rho(\mu)$ curves for the 1D boson Hubbard model.[11] Note that in the case $J_2 = 1$ the curve $m(h)$ describes the reduced magnetization of the spin-$\frac{3}{2}$ antiferromagnetic Heisenberg chain.[12] The magnetization curves also indicate a divergence of the zero-field magnetic susceptibility $\chi = \chi(J_2)$ as J_2 approaches the isolated critical point J_c ($J_2 \to J_c \pm 0$), in accord with the generic Luttinger liquid relation[7] $\chi(h, J_2) = K(h, J_2)/[\pi v_s(h, J_2)]$ and the observation that the spin-wave velocity $v_s(0, J_2) \to 0$ as $J_2 \to J_c \pm 0$.[5] Here $K(h, J_2)$ is the Luttinger liquid parameter at finite h and J_2. Up to now, only a few studies analyzing such ferromagnetic quantum critical points in 1D have been published.[13–15] In particular, as recently shown in Ref. 15, the Berry term plays an important role in the critical theory, so that in the isotropic limit one can expect different critical behavior near J_c, as compared to the behavior established in the Ising limit.[14] The magnetization curves also indicate that the canted magnetic phase is characterized by a finite susceptibility $\chi(0, J_2)$, as can be expected since this state may be viewed as a kind of ferromagnetic Luttinger liquid phase.[16]

Discussed instabilities at h_c and h_s share the same physics as those at the lower (h_{c1}) and upper (h_{c2}) critical fields in Haldane-gap chains in a magnetic field.[17] In particular, the instability at h_c may be viewed as a condensation of dilute gas of magnon excitations, as in the case of Haldane-gap chains slightly above the lower critical field h_{c1}.[18–20] At the critical field h_c, the gap of the AFM mode $\omega_0^{(-)}(k)$ vanishes and, as a result, a macroscopic amount of AFM magnons condense onto the ground state. The collapse of quasiparticles is prevented by the repulsive on-site quasiparticle interaction. For $h > h_c$, the magnetization M continuously exceeds the quantized value 1/2. The instabilities related to the FM modes, as in the case of a Haldane chain at the upper critical field h_{c2}, are expected to share the same critical properties.[7,21] In fact, discussed transitions are of a commensurate-incommensurate type,[22] like the insulator-superfluid transition in the 1D boson Hubbard model for non-integer ρ. Since magnons behave as a dilute gas of hard-core bosons, in a first approximation the specific form of the interaction is irrelevant.[20,23] This results, in particular, in the universal behavior of the Haldane chain magnetization[19,24] $M = [2\Delta_H(h - h_{c1})]^{1/2}/(\pi v_s)$, where Δ_H is the Haldane gap and v_s (≈ 2.49) is the spin-wave velocity. Similar universal expressions can be obtained close to the phase boundaries of the (J_2, h) diagram of our model. Using the equivalence of 1D hard-core bosons and free spinless fermions, this implies, in particular, the Luttinger liquid parameter $K = 1$ on the entire boundary of the $M = 1/2$ phase as well as on the $h_s(J_2)$ boundary, excluding the special point at the tip of the region occupied by the $M = 1/2$ phase. Respectively, the spin-spin correlation exponents take the values $\eta_z = 2$ and $\eta_x = \frac{1}{2}$, and the magnetization exponent $\beta = 1/2$. Based on the established picture of the low-lying excitations close to the point (J_2^*, h^*) and using the analogy with the boson phase diagram, it is plausible to assume that the latter critical point describes a Berezinskii-Kosterlitz-Thouless (BKT) type transition. Although our ED data do not fix the position of the tip, it is easy to indicate the typical pointed-type shape of the boundary[25] resulting from the specific BKT particle-hole excitation gap Δ_{ph} close to this transition: $\Delta_{ph} \sim \exp\left(const/\sqrt{J_2^* - J_2}\right)$. As might be expected, the SWT does not reproduce the correct behavior of the gap Δ_{ph} close to this special point.

In conclusion, we have demonstrated that a generic mixed-spin ladder exhibits a magnetic phase diagram which is closely related to the one of the boson Hubbard model in one spatial dimension. Similar magnetic phase diagrams may be expected for arbitrary quantum spin numbers s_1 and s_2, provided that $s_1 \neq s_2$ and $s_1 + s_2$ =half-integer.

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[*] Permanent address: Institute of Solid State Physics, Bulgarian Academy of Sciences, Tsarigradsko chaussee 72, 1784 Sofia, Bulgaria

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