$T = 0$ phase diagram of 1D extended anisotropic spin-$\frac{1}{2}$ Heisenberg model

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Abstract. For the 1D spin-1/2 Heisenberg model with ferromagnetic nearest-neighbor interaction and antiferromagnetic next-nearest neighbor we present the phase diagram at $T = 0$ as obtained by DMRG analysis. The interplay of interactions generates two massless and two massive phases in the range of parameters considered. We discuss the properties of the correlations in these phases.

1. Introduction
The interplay of frustration, symmetry and low-dimensionality is one of the central issues of spin physics. In this context, much attention has been dedicated to the AF-AF one-dimensional Heisenberg model. On the other hand, the opposite situation, when a ferromagnetic nearest-neighbor (NN) interaction is frustrated by an AF next-nearest-neighbor (NNN) one, is less studied. The interest to the properties of such ferromagnetic systems has become recently much more practical since the discovery of materials containing edge-sharing CuO$_2$ chains (e.g. Rb$_2$Cu$_2$Mo$_3$O$_{12}$ as in Ref. [1], NaCu$_2$O$_2$ as in Ref. [2] or LiCuVO$_4$ as in Ref. [3]). While the ferromagnetic character of the NN interaction in such materials seems to be widely accepted, its spatial isotropy, or the precise form of the NNN term are still under investigation. We believe, therefore, that the study of the phase diagram of the ferromagnetic frustrated 1D spin models could shed some light on the physics of such materials.

In order to investigate the interplay between frustration and anisotropy, in this article, we consider an extended anisotropic spin-$\frac{1}{2}$ Heisenberg model:

$$H = -J_z \sum_i S_z^i S_z^{i+1} + J_\perp \sum_i (S_x^i S_x^{i+1} + S_y^i S_y^{i+1}) + J' \sum_i S_i S_{i+2}. \quad (1)$$

Here we choose ferromagnetic NN interaction in $z$–channel ($J_z > 0$), antiferromagnetic NN in-plane one ($J_\perp > 0$) and antiferromagnetic isotropic coupling between next-nearest neighbors ($J' > 0$). It is worth noting that the Hamiltonian (1) with $J_\perp > 0$ can be easily mapped onto the one with $J_\perp < 0$. Indeed, an inversion of the in-plane components of the spins on, for instance, the even-numbered sites changes the sign in front of $J_\perp$ in (1). Under such transformation, an in-plane correlation function $\langle S_\alpha^i S_\alpha^{i+n} \rangle$, where $\alpha = x, y$, acquires the prefactor $(-1)^n$. We choose AF sign of $J_\perp > 0$ to be compatible with our previous work [8], although in the edge-sharing CuO$_2$ materials $J_\perp$ should be negative. The model (1) can be mapped to a two-leg zig-zag...
ladder. From this point of view, the interaction parametrized by $J'$ becomes the intra-chain one, while the former NN terms realize the inter-chain couplings.

It is worth noting that, despite the non-integrability of (1), there exist two isolated points in the model parameter space where analytic expressions for the ground state energies and wave functions are known. These are the points ($J_z = -1$, $J_\perp = J_z$, $J' = J_z/2$) as proven in Ref. [4] (Majumdar-Ghosh point) and ($J_z = 1$, $J_\perp = J_z$, $J' = -J_z/4$) as found in Ref. [5].

2. Results
We obtain the ground state properties of the Hamiltonian (1) numerically by means of the Density Matrix Renormalization Group (DMRG) [6, 7] technique on a chain with $L = 100$ sites, subject to open boundary conditions. At every DMRG step, we truncate the Hilbert space of the system so to leave at most 200 lowest eigenstates of the density matrix. The real-space spin-spin correlation functions are calculated by means of the finite-system algorithm.

In Fig. 1, we present the phase diagram of the model (1) in the ($J'$, $J_\perp$) plane, taking $J_z$ as energy unit. The ferromagnetic phase has been previously located in Ref. [8]. The two massive phases (M-I, M-II) [9] exhibit qualitatively different correlations and the transition line between them goes from the point ($J' = J_z/4$, $J_\perp = J_z$) to the point ($J' = 0.41J_z$, $J_\perp = 0.5J_z$), as shown in Fig. 1. The massless phase XXZ is located between the vertical axis $J' = 0$ and the phase M-II, while the massless phase XXZ-II is placed between the phase M-II and the horizontal axis $J_\perp = 0$.

The transition lines are determined by the behavior of the correlation functions. In massless phases the correlation functions are linear in the log-log scale (power-law decay), while for massive phases they are linear in the semi-log scale (exponential decay).

When the NNN interaction $J'$ is weak and $J_\perp > J_z$, the system enters the XXZ-model regime. Spin-spin correlations are much stronger in the $XY$ plane. In the upper two panels of Fig. 2, we plot the typical behavior of the correlations in this case. The in-plane correlations are commensurate of Ne’el type and show power-law decay. The out-of-plane correlations show a non-alternating behavior that goes asymptotically as $-1/d^2$, where $d$ is the separation between two sites. In addition, they show an alternating component probably owing to a sub-leading term proportional to $(-1)^d d^\mu$ with $\mu < -2$.

On the other hand, when $J'$ is strong enough and $J_\perp$ is weak, the correlations of (1) can once again be reduced to those of $XXZ$ model, at least qualitatively. This time, however, such correlations establish along the legs of the ladder. This analogy becomes more and more precise.

**Figure 1.** The phase diagram of the model (1) as obtained from the DMRG data for 100 sites.
Figure 2. Examples of correlation pictures in the various phases of the phase diagram in Fig. 1. Upper left and right panels show the out-of-plane and in-plane form-factors, respectively, for the phase $XXZ$ at the point $(J' = 0.1, J_\perp = J_z, J_z = 0.193)$ in log–log scale.

Middle left and right panels: $XXZ-\Pi$ phase at the point $J' = 0.8, J_\perp = 0.5, J_z = 0.8$ in log–log scale. The in-plane spin form-factor multiplied by the exponential prefactor $e^{d/\xi}$ are shown on the bottom right panel. Lines are guides to the eye.
as $J′ \to \infty$. Because of this new mapping of the model, inter- and intra-chain correlations become, in general, different. At the point $(J′ = 0.8J_z, J_\perp = 0.5J_z)$ (middle right panel of Fig. 2), in the in-plane channel there is a considerable difference in the exponents of inter- and intra-chain correlations, while in the out-of-plane channel (middle left panel of Fig. 2) both inter- and intra-chain exponents are essentially the same.

When both $J′$ and $J_\perp$ are of the same order, we find two massive phases in the phase diagram of (1). The first massive phase M-I is adjacent to the ferromagnetic phase and shows finite magnetization in the vicinity of the transition line (at least on a 100 site cluster), which gradually goes to zero at $J′ \approx 0.35J_z$. In this phase, the in-plane channel is characterized by an exponential decay on a background of anomalously large finite-size effects (for distances $d \geq 16$). Contrarily, the out-of-plane channel presents an exponential decay with different correlation lengths for inter- and intra-chain distances.

In the M-II phase, when both $J′$ and $J_\perp$ become strong enough compared to $J_z$, the correlations change qualitatively. Now, the out-of-plane correlations exhibit an exponential decay regardless whether the two sites belong to the same or different legs (see the left bottom panel in Fig. 2), while in the in-plane channel the correlation picture becomes highly non-trivial. Namely, the in-plane correlation function shows an exponential decay with a correlation length $\xi_\perp$ ($\xi_\perp = 14$ for $J′ = 0.6J_z$ and $J_\perp = 1.4J_z$). Once multiplied by $e^{d/\xi_\perp}$, as shown in the right bottom panel of Fig. 2, the correlation function presents incommensurate oscillations as a function of $d$ with a periodicity vector $q$ ($q = 0.29$ for $J′ = 0.6J_z$ and $J_\perp = 1.4J_z$) and a phase depending on mod($d,4$). Such multiplicity of four can be easily understood if one remembers that the even distances of 1D chain correspond to the distances along the legs of the zig-zag ladder (intra-chain distances), while the odd ones connect the sites on different legs (inter-chain). Moreover, inter- and intra-chain distances can be defined by classifying the whole set of distances $d \equiv |i−j|$ between any two sites $i$ and $j$ on a 1D cluster into four sequences:

- $d_0(l) = 4l + 0$ intra – chain even
- $d_1(l) = 4l + 1$ inter – chain odd
- $d_2(l) = 4l + 2$ intra – chain odd
- $d_3(l) = 4l + 3$ inter – chain even,

here $l = 0, \ldots, 24$ for a 100 site cluster. All four sequences appear to be modulated by the same harmonic term, but with different phases. Peculiarly, the phase shift between $d_0(l)$ and $d_2(l)$ and between $d_1(l)$ and $d_3(l)$ equals to $\pi$. Finally, the phases of $d_0(l)$ and $d_1(l)$ differ by $\pi/2$.

3. Conclusions
Summarizing, we have explored the phase diagram of a 1D extended anisotropic spin-$\frac{1}{2}$ model (1) with ferromagnetic NN coupling and antiferromagnetic NNN one in the range $(0 < J′ < J_z, 0 < J_\perp < 2.5J_z)$. In addition to the ferromagnetic phase, we identified two XXZ-like phases: one when $J′$ is small and another when $J′$ is large compared to the other couplings ($J_z, J_\perp$). In the latter case, the XXZ-like correlations develop along the legs of the ladder. In between these two massless phases, we also identified two massive ones. Such massive phases develop at the boundaries of the massless ones when one of the inter-chain couplings becomes small enough. A more detailed article with technical details is in preparation and will be published elsewhere.

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