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Spin-1/2 XXZ Diamond Chain within the Jordan–Wigner Fermionization Approach

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The spin-1/2 XXZ diamond chain is considered within the Jordan–Wigner fermionization. The fermionized Hamiltonian contains the interacting terms which are treated within the Hartree–Fock approximation. We obtain the ground-state magnetization curve of the model for some particular cases and compare the results with the exact diagonalization data for finite chains of 30 spins and known exact results. We also analyze the validity of the suggested approximation.

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1. Introduction

The spin-1/2 XXZ diamond chain as a quantum frustrated system is an interesting topic for the theoretical research, since it exhibits many phenomena related to interplay of quantum fluctuations and competing interactions. The exact results for this model are available only for limited cases [1, 2], and the earlier studies used mainly the numerical methods [3–5]. We suggest an analytical method based on the fermionization of the initial spin-1/2 model. The present work is an extension of our previous study of the XX diamond chain [6] using the Jordan–Wigner transformation and the Hartree–Fock approximation.

The goal of the paper is to explain the properties of the frustrated model on the fermionic language for a more general XXZ model. We accompany our approximate calculations by the results of the exact diagonalization and also compare them with the particular cases where the exact results are available [1, 2].

2. Model and method

We consider the quantum spin-1/2 XXZ model on the generally distorted diamond chain (see Fig. 1 in Ref. [6]) with the following Hamiltonian:

$$H = \sum_{l=1}^{N} \Bigg\{ \sum_{\alpha=x,y,z} \Big[J_1^{\alpha}(s_{1,l}^{\alpha}s_{2,l}^{\alpha} + s_{3,l}^{\alpha}s_{1,l+1}^{\alpha}) + J_2^{\alpha}s_{2,l}^{\alpha}s_{3,l}^{\alpha} + J_3^{\alpha}(s_{1,l}^{\alpha}s_{3,l}^{\alpha} + s_{2,l}^{\alpha}s_{1,l+1}^{\alpha}) \Big] - h\sum_{p=1}^{3} s_{p,l}^{z} \Bigg\}. \quad (1)$$

Here, $s_{p,l}^{\alpha}$ ($\alpha = x, y, z$) are the Pauli spin-1/2 operators with the first index corresponding to a sublattice and the second index to a cell, $J_p^x = J_p^y = J_p > 0$, $J_p^z = \Delta J_p > 0$, Δ is the interaction anisotropy, and h is the external magnetic field (we set $g\mu_{\mathrm{B}} = 1$). Using the spin raising and lowering operators $s_{p,l}^{\pm} = s_{p,l}^{x} \pm \mathrm{i}\, s_{p,l}^{y}$ one can rewrite the xy-part of the Hamiltonian as a quadratic form of the mentioned operators. The zz interaction, due to the relation $s_{p,l}^{z} = s_{p,l}^{+}s_{p,l}^{-} - 1/2$, leads to the product of four spin-lowering and raising operators.

Following the procedure described in Ref. [6], we specify the Jordan–Wigner transformation in the form: $c_{1,l} = \prod_{p=1}^{3}\prod_{i=1}^{l-1} P_{q,i}s_{1,l}^{-}$, $c_{2,l} = \prod_{p=1}^{3}\prod_{i=1}^{l-1} P_{q,i}P_{1,l}s_{1,l}^{-}$, $c_{3,l} = \prod_{p=1}^{3}\prod_{i=1}^{l-1} P_{q,i}P_{1,l}P_{2,l}s_{1,l}^{-}$, where $P_{q,l} = (-2s_{q,l}^{z}) = \exp(\mathrm{i}\pi c_{q,l}^{+}c_{q,l})$ is the Jordan–Wigner factor. Here new operators $c_{p,l}$ satisfy the Fermi commutation relations. The fermionic expression for the z-component of the spin operator can be easily obtained as $s_{q,l}^{z} = c_{q,l}^{+}c_{q,l} - 1/2$. Therefore, the zz-part of the Hamiltonian contains the four-fermion term. The xy-part of the Hamiltonian in terms of new Fermi operators is as follows:

$$H_{xx} = \frac{1}{2}\sum_{l=1}^{N} \Bigg\{ \Big[J_1(c_{1,l}^{+}c_{2,l} + c_{3,l}^{+}c_{1,l+1}) + J_2c_{2,l}^{+}c_{3,l} + J_3(c_{1,l}^{+}P_{2,l}c_{3,l} + c_{2,l}^{+}P_{3,l}c_{1,l+1}) + \mathrm{H.c.} \Big] \Bigg\}. \quad (2)$$

Let us note that the transformed Hamiltonian contains the fermion interaction for terms proportional to the J_3 coupling which is usually assumed to be smaller than J_2. We should also note the relation between the spins-1/2 and spinless fermions: the spin-down (-up) state corresponds to the empty (filled) fermionic state; the action of the fermion creation and annihilation operators is analogous to the action of spin raising and lowering operators in spin language. The resulting Hamiltonian represents the interacting Fermi gas. To proceed we use the Hartree–Fock approximation where all interacting terms are factorized preserving all pair correlations between nearest neighbors of type $\langle c_{p,l}^{+}c_{q,m}\rangle$. Thus, the Hamiltonian becomes a quadratic form in terms of the Fermi operators. It can be diagonalized using the Fourier and Bogolyubov transformation, and the thermodynamics and fermionic correlation functions are easily found. However, it depends parametrically on the unknown contractions $\langle c_{p,l}^{+}c_{q,m}\rangle$ which have to be found self-consistently.

3. Results

Solving the self-consistent equation we found that the dimer–monomer ground state for the symmetric diamond chain [1] is recovered. Indeed, if $J_2 \geq 2J_1$ and the external field $0 < h < J_1\Delta + J_2(1+\Delta)/2$, we obtain the following solutions for the elementary contractions: $\langle c^+_{1,l}c_{1,l}\rangle = 1$, $\langle c^+_{2,l}c_{2,l}\rangle = \langle c^+_{3,l}c_{3,l}\rangle = 1/2$, $\langle c^+_{1,l}c_{2,l}\rangle = \langle c^+_{1,l}c_{3,l}\rangle = 0$, $\langle c^+_{2,l}c_{3,l}\rangle = -1/2$. The ground state of the corresponding fermion model is as follows: $|\mathrm{GS}\rangle = \prod_l c^+_{1,l}(c^+_{2,l} - c^+_{3,l})/\sqrt{2}|0\rangle$ where $|0\rangle$ denotes the empty state. Using the relation between fermionic and spin states one can see that it corresponds to the dimer–monomer state in spin language (see also Ref. [6]).

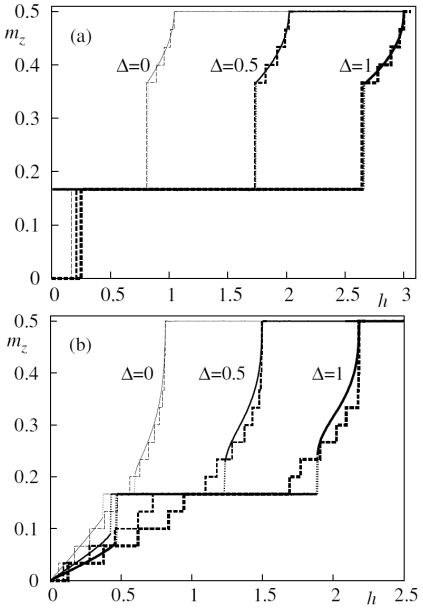

Fig. 1. The ground state magnetization versus external field for (a) $J_1 = J_3 = 1$, $J_2 = 1.75$; (b) $J_1 = 1$, $J_2 = 1.25$, $J_3 = 0.45$. Step-like dashed lines represent the exact diagonalization data for 30 spins, solid lines correspond to the approximated results, dotted lines indicate the magnetization jumps.

The results for the symmetric diamond chain below the dimer–monomer limit is shown in Fig. 1a. We observe an excellent agreement with the exact diagonalization data except for small fields where our mean-field-type approximation produces the non-zero magnetization. As an example of the distorted chain, we have chosen the parameter set used previously for azurite [7]. In Fig. 1b we obtain a good agreement with the XX limit. Particularly, the magnetization curve shows the 1/3-plateau and zero-magnetization in zero field. However, for the isotropic Heisenberg interaction the discrepancy between the approximate and exact results raises up quickly below the upper critical field. The exact diagonalization data for $\Delta = 1$ seem to show a cusp in the magnetization curve at 2/3 of the saturation magnetization. It might be the sign that the magnetic cell is doubled for this model. As it was discussed in [6], to describe this kind of behavior, it is necessary to consider also non-uniform elementary contractions. Another drawback of the Hartree–Fock approximation is the artificial jumps of the magnetization.

We have also examined our method by comparison with the exact results for the Ising–Heisenberg diamond chain obtained by means of decoration–iteration procedure [2]. It is the special case of the anisotropic diamond chain where the spins on the vertical bond are coupled by the Heisenberg interaction whereas all other couplings are of the Ising type. The model (1) corresponds to the model considered in [2], if we put $J_1^{x,y} = J_3^{x,y} = 0$, $J_2^{x,y} = \Delta J_2$, $J_1^z = J_3^z = J_1$, $J_2^z = J_2$. Depending on the ratio between the interaction couplings, anisotropy and external field the system may stay in different phases: $|\mathrm{FRI}\rangle = \prod_l |\downarrow_{1,l}\rangle|\uparrow_{2,l}\ \uparrow_{3,l}\rangle$, $|\mathrm{FRU}\rangle = \prod_l |\uparrow_{1,l}\rangle(|\uparrow_{2,l}\downarrow_{3,l}\rangle - |\downarrow_{2,l}\uparrow_{3,l}\rangle)/\sqrt{2}$, $|\mathrm{SPP}\rangle = \prod_l |\uparrow_{1,l}\rangle|\uparrow_{2,l}\ \uparrow_{3,l}\rangle$. Within our Hartree–Fock approach it is possible to recover the ground state phase diagram and all phase boundaries. The mentioned states in the fermion representation have the form: $|\mathrm{FRI}\rangle = \prod_l c^+_{2,l}c^+_{3,l}|0\rangle$, $|\mathrm{FRU}\rangle = \prod_l c^+_{1,l}(c^+_{2,l} - c^+_{3,l})/\sqrt{2}|0\rangle$, $|\mathrm{SPP}\rangle = \prod_l c^+_{1,l}c^+_{2,l}c^+_{3,l}|0\rangle$.

4. Conclusions

To conclude, we have considered the approach based on the Jordan–Wigner fermionization and subsequent Hartree–Fock approximation for the spin-1/2 anisotropic diamond chain. We have revealed that such an approach recovers the exact results for the phases characterized by short-range correlations as, for instance, the dimer–monomer phase. It also provides a good description of the ground state magnetization for the symmetric diamond chain. However, for the distorted diamond chain the inclusion of the zz interactions between spins may lead to the qualitative change of the magnetization curve which cannot be explained within the current approximate method.

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