On the Exact Solution of the Mixed-Spin Ising Chain with Axial and Rhombic Zero-Field Splitting Parameters

M. Dančo and J. Strečka

Department of Theoretical Physics and Astrophysics, Faculty of Science, P.J. Šafárik University
Park Angelinum 9, 040 01 Košice, Slovak Republic

Ground-state phase diagram of the mixed spin-1/2 and spin-1 Ising chain with axial and rhombic zero-field splitting parameters is exactly calculated within the framework of the transfer-matrix method. It is shown that the rhombic zero-field splitting parameter prefers the magnetically ordered phase instead of the disordered phase.

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1. Introduction

Exactly solved one-dimensional quantum spin models traditionally belong to the most fascinating research areas as they provide valuable insight into otherwise hardly understandable aspects of cooperative and quantum phenomena [1]. In this work, we will exactly treat the mixed spin-1/2 and spin-1 Ising chain with axial and rhombic zero-field splitting parameters.

2. Model and its exact solution

Consider the Ising model for a chain consisting of the alternating spin-1/2 and spin-1 atoms, which accounts also for axial and rhombic zero-field splitting (ZFS) parameters. The total Hamiltonian of this spin system can be written as a sum of two terms \( H = H_{\text{ex}} + H_{zfs}^{(1)} \). The former term accounts for the Ising-type exchange interaction between the nearest-neighbor spins

\[
H_{\text{ex}} = -J \sum_{k=1}^{N} \hat{S}_k^z (\sigma_k^+ + \sigma_{k+1}^-),
\]

and the latter term accounts for the axial (\( D \)) and rhombic (\( E \)) ZFS parameters acting on the spin-1 atoms only

\[
H_{zfs}^{(1)} = -D \sum_{k=1}^{N} (\hat{S}_k^x)^2 - E \sum_{k=1}^{N} [(\hat{S}_k^x)^2 - (\hat{S}_k^y)^2].
\]

Above, \( \sigma_k^\alpha \) and \( \hat{S}_k^\alpha \) (\( \alpha = x, y, z \)) denote standard spatial components of the spin-1/2 and spin-1 operators, respectively, \( N \) denotes a total number of spin-1/2 (spin-1) atoms and the periodic boundary condition \( \sigma_{N+1} = \sigma_1 \) is imposed for further convenience. It is worthwhile to remark that there is one-to-one correspondence between the Hamiltonian \( H_{zfs}^{(1)} \) given by Eq. (2) and the Hamiltonian with three different parameters \( D^x, D^y \) and \( D^z \)

\[
H_{zfs}^{(2)} = -D^x \sum_{k=1}^{N} (\hat{S}_k^x)^2 - D^y \sum_{k=1}^{N} (\hat{S}_k^y)^2 - D^z \sum_{k=1}^{N} (\hat{S}_k^z)^2.
\]

The equivalence between \( H_{zfs}^{(1)} \) and \( H_{zfs}^{(2)} \) can easily be verified by establishing a rigorous mapping correspondence between the relevant interaction terms appearing in the Hamiltonians (2) and (3). The total angular momentum of the spin-1 atoms is integral of motion \( \hat{S}_k^2 = (\hat{S}_k^x)^2 + (\hat{S}_k^y)^2 + (\hat{S}_k^z)^2 = 2 \) and hence, one of three parameters \( D^x, D^y \) and \( D^z \) must depend on the other two. Consequently, the Hamiltonians \( H_{zfs}^{(1)} \) and \( H_{zfs}^{(2)} \) differ one from the other just by some constant factor \( H_{zfs}^{(1)} = H_{zfs}^{(2)} + C \), whereas the relevant interaction terms \( C \), \( D \) and \( E \) are connected to the ones \( D^x, D^y \) and \( D^z \) through the mapping relations

\[
C = D^x + D^y, \quad D = D^x - D^y - D^z, \quad E = \frac{D^z}{2}.
\]

The model under investigation thus turns out to be equivalent to the one recently studied by Wu et al. [2] using the approach based on the Jordan–Wigner transformation.

Here, the investigated model system will be exactly treated within the framework of transfer-matrix method [3]. First, it is useful to rewrite the total Hamiltonian as a sum of site Hamiltonians \( \hat{H} = \sum_k \hat{H}_k \), whereas each site Hamiltonian \( \hat{H}_k \) involves all the interaction terms associated with the spin-1 atom from the \( k \)-th lattice site

\[
\hat{H}_k = -J \hat{S}_k^z (\sigma_k^+ + \sigma_{k+1}^-) - D(\hat{S}_k^x)^2 - E[(\hat{S}_k^x)^2 - (\hat{S}_k^y)^2].
\]

Due to a validity of commutation relation between different site Hamiltonians, the partition function can be partially factorized into the product

\[
Z = \sum_{\{\sigma_k\}} \prod_{k=1}^{N} \text{Tr}_{S_k} \exp(-\beta \hat{H}_k),
\]

where \( \beta = 1/k_B T \), \( k_B \) is Boltzmann’s constant, \( T \) is the absolute temperature, \( \text{Tr}_{S_k} \) means a trace over spin degrees of freedom of the \( k \)-th spin-1 atom and \( \sum_{\{\sigma_k\}} \) de-
notes a summation over all possible configurations of the spin-1/2 atoms. After tracing out spin degrees of freedom of the spin-1 atom, the relevant expression on right hand side of Eq. (6) will depend just on its two nearest-neighbor spins $\sigma_k$ and $\sigma_{k+1}$. Moreover, this expression can be subsequently used in order to define the transfer matrix

$$T(\sigma_k, \sigma_{k+1}) = \text{Tr}_{S_k} \exp(-\beta \mathcal{H}_k) = 1 + 2\exp(\beta D) \cos(\sqrt{J^2 + (\sigma_k^z + \sigma_{k+1}^z)^2} + E^2).$$  \hspace{1cm} (7)

The rest of our exact calculations can be accomplished using the standard procedure developed within the transfer-matrix approach [3]. This rigorous technique allows one to express the partition function in terms of respective eigenvalues of the transfer matrix

$$Z = \sum_{\{\sigma_k\}} \prod_{k=1}^{N} T(\sigma_k^z, \sigma_{k+1}^z) = \text{Tr}T^N = \lambda_+^N + \lambda_-^N. \hspace{1cm} (8)$$

In the thermodynamic limit $N \to \infty$, the free energy per unit cell can be expressed solely in terms of the largest eigenvalue of the transfer matrix

$$f = -k_B T \lim_{N \to \infty} \frac{1}{N} \ln Z = -k_B T \ln (T_{11} + T_{12}), \hspace{1cm} (9)$$

where $T_{11} = T(\pm 1/2, \pm 1/2)$ and $T_{12} = T(\pm 1/2, \mp 1/2)$ were used to denote two different matrix elements of the transfer matrix defined through Eq. (7).

3. Results and discussion

Now, let us take a closer look at the ground-state behavior of the investigated model system. For simplicity, our subsequent analysis will be restricted only to the particular case with the ferromagnetic interaction $J > 0$, since the relevant change in sign of the parameter $J$ causes just a rather trivial reversal of all the spin-1/2 atoms.

In the zero temperature limit, the first-order phase transition line given by the condition $D = -\sqrt{J^2 + E^2}$ separates the ferromagnetically ordered phase (OP) from the disordered phase (DP). The relevant spin order appearing in the OP and DP can be unambiguously defined through the eigenvectors

$$|\text{OP}\rangle = \otimes_k |1/2\>_k \left[ \cos \left(\frac{\varphi}{2}\right) |+1\>_k + \sin \left(\frac{\varphi}{2}\right) |-1\>_k \right],$$

$$|\text{DP}\rangle = \otimes_k |\pm 1/2\>_k |0\>_k,$$  \hspace{1cm} (10)

where the product runs over all lattice sites, the former (latter) ket vectors specify the state of the spin-1/2 (spin-1) atoms and the mixing angle $\varphi$ is given by $\varphi = \arctan(E/J)$. In the DP, all the spin-1 atoms tend toward their “non-magnetic” spin state $|0\rangle$ on behalf of a sufficiently strong (negative) axial ZFS parameter and hence, each spin-1/2 atom may completely independently choose any of two available spin states $|\pm 1/2\rangle$. However, the more striking spin order emerges in the OP, where the magnetic behavior of the spin-1 atoms is governed by a quantum entanglement of two magnetic spin states $|+1\rangle$ and $|-1\rangle$ and all the spin-1/2 atoms reside their “up” spin state $|1/2\rangle$. In this respect, the rhombic ZFS parameter gradually destroys a perfect ferromagnetic order between the spin-1/2 and spin-1 atoms, which appears in an absence of the rhombic term.

Fig. 1. Ground-state phase diagram in two different planes: (a) $E/J - D/J$ plane; (b) $2J/D_x - D_z/J$ plane for $D_y = 0$.

For better illustration, Fig. 1a depicts the ground-state phase diagram in the $E/J - D/J$ plane. The most surprising finding stemming from Fig. 1a is that the phase boundary between OP and DP shifts toward more negative values of the axial ZFS parameter when increasing a strength of the rhombic ZFS parameter. Accordingly, it turns out that the quantum entanglement between the spin states $|+1\rangle$ and $|-1\rangle$, which is caused solely by the rhombic ZFS parameter, energetically stabilizes the OP before the DP. For comparison, Fig. 1b illustrates the ground-state phase diagram in the $2J/D_x - D_z/J$ plane when using Eq. (3) in order to define the ZFS Hamiltonian. Let us note that this phase diagram is in accord with the recent results of Wu et al. [2], but this phase diagram is apparently less convenient for interpreting the phase boundary between OP and DP as the parameter $D_z$ changes according Eq. (4) both axial as well as rhombic ZFS parameters.

In conclusion, it is worthy to notice that the rigorous procedure developed on the grounds of the transfer-matrix method can readily be adapted to treat the investigated model system even in a presence of non-zero external magnetic field, which will be examined in detail in our forthcoming work.

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References

