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Quantum spin system with on-site exchange in a magnetic field

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We present the results of a full diagonalisation applied to a 1 D quantum spin system with on-site exchange anisotropy. The model considered is a quantum generalization of the 1 D classical Blume–Capel model. Thermodynamic properties of the system in the presence of magnetic field are examined taking into account a quantum spin ladder with a periodic boundary condition, where each rung of the ladder contains two interacting spins –1/2. This effective spin –1 system exhibits very rich thermodynamic behaviour. We present the ground state results, showing many various types of magnetic configurations and compare it with the classical case. The calculations are performed in the unified simulation environment ALPS, which offers the fulldiag application.

Key words: *quantized spin model; spin ladder*

1. Introduction

We have studued the magnetic orderings in the frustrated quantum spin –1/2 ladder with the interaction anisotropy (the AF Heisenberg generalized ladder with $J_{II} = J_{diag} = J$, $J_{\perp} = \Delta$ [1]). The scheme of the considered structure is shown in Fig. 1.

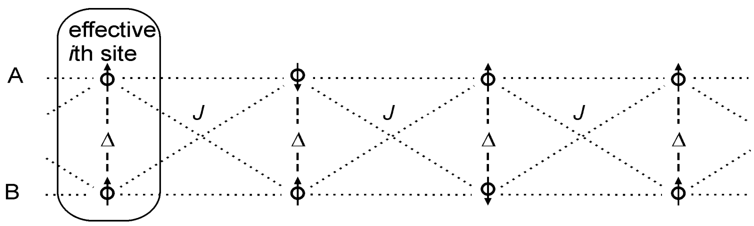

Fig. 1. The scheme of the frustrated quantum spin –1/2 ladder with the interaction anisotropy

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The exchange interactions between spins on the rung and along the main direction of the ladder are different. We examine the thermodynamic properties of the system as a function of Δ/J. The Hamiltonian of the system considered takes the form:

$$\hat{H} = J\sum_{i,\alpha,\beta}\hat{\sigma}_{i\alpha}\hat{\sigma}_{i+1\beta} + \Delta\sum_{i}\hat{\sigma}_{iA}\hat{\sigma}_{iB} \tag{1}$$

where $\hat{\sigma}_{i\alpha}$ is the quantum spin –1/2 operator on the ith rung and α-leg of the ladder. We take into account the influence of external magnetic field h on the z component of the spin and we add the Zeeman term

$$\hat{H}(h) = \hat{H} - h\sum_{i}(\hat{\sigma}^{z}_{iA} + \hat{\sigma}^{z}_{iB}) \tag{2}$$

Such a model can be treated as the effective interacting (J) chain of spin –1 on the ith site with the on-site exchange (Δ) [2] in the presence of a magnetic field (h).

We can show that the Hamiltonian (1) has a similar form as the well known Blume–Capel (BC) model [3] (we use the "classical" sign convention)

$$H_{BC} = -J\sum_{i,j}S_iS_j + D\sum_{i}S_i^2 \tag{3}$$

where S_i is the classical spin –1 Ising operator which takes the values $\{-1,0,1\}$, J is the exchange interaction and D is the single-ion anisotropy. Formally, the Hamiltonian (3) can be rewritten into the equivalent form in terms of spin –1/2. Let us express each spin S_i over the sum $\tilde{S}_i = \sigma_{iA} + \sigma_{iB}$ of two classical spins $\sigma_{i\alpha} = \pm 1/2$ on the ith site. This transformation is non-one-to-one and changes the number of eigenstates of effective spin $\tilde{S}_i = \{-1,0,0,1\}$. In our recent paper [4], we show that such a spin model with "zero"-state degeneracy can be transformed into the BC model with a temperature-dependent single ion anisotropy (at T=0 the models are identical). We rewrite the Hamiltonian (3) for $\tilde{S}_i$ in the new variable $\sigma_{i\alpha}$

$$\tilde{H} = -\tilde{J}\sum_{i,j,\alpha,\beta}\sigma_{i\alpha}\sigma_{j\beta} + 2\tilde{D}\sum_{i}\sigma_{iA}\sigma_{iB} + C \tag{4}$$

where α, β = $\{A,B\}$, $\tilde{J} = J$, $\tilde{D} = D - k_B T\ln 2$ and $C = ND/2$, which yields a similar form as in Eq. (1).

In the analysis of the system, we have implemented the unified simulation environment ALPS [5], which offers the fulldiag application [6]. Using the XML language, we have first defined a new "diagonally connected ladder" graph structure, where i = 1..., x (Fig. 2) where x is the number of rungs, $2x$ – number of vertices, 1A, 1B, $x\alpha$, $x\beta$, … – are the proper symbols of the vertex number.

dd-graph.xml

```
<LATTICES>
 <GRAPH name="generalized ladder" vertices="2x">
  <VERTEX id="1α" type="0"/>
  ...
  <VERTEX id="xα" type="0"/>
  <EDGE type="0" source="1A" target="1B"/>
  ...
  <EDGE type="0" source="xA" target="xB"/>
  <EDGE type="1" source="1α" target="2β"/>
  ...
  <EDGE type="1" source="(x-1)α" target="xβ"/>
  <EDGE type="1" source="xα" target="1β"/>
 </GRAPH>
</LATTICES>
```

Fig. 2. “Diagonally connected ladder” graph structure

On the last defined ‘EDGE’ we impose periodic boundary conditions. In the diagonalization procedure we use also the model-dspin.xml file in which the quantum interactions between local spins –1/2 are defined. After preparing the parameter.xml file, where we specify the type of the system, temperature, the value of the interactions etc., we start with the fulldiag procedure to get the eigenvalues of the system. Then we use the fulldiag-evaluate program to obtain thermodynamic properties of the system.

2. Results

We present the exact results of 12 quantum spins on the ladder with antiferromagnetic (AF) exchange interaction ($\Delta > 0$, $J = 1$). For the family of Δ/J values we obtained the following thermodynamic characteristics: magnetization, specific heat, susceptibility, entropy and energy as functions of the magnetic field. In Figure 4, exemplary results for $\Delta = 1.8$ are presented. The diagrams are symmetrical due to the spin degeneracy in the absence of magnetic field. Figure 4 presents possible magnetic orderings in the ground state in the plane $h\Delta$ for the quantum case (Fig. 4a) and in hD for the classical case (Fig. 4b) (the results have been extrapolated from very low temperatures). In the quantum case, we observe some states with magnetization analogous as in the classical case. The classical disordered phase ($M = 0$) corresponds to the dimer phase D2 of singlets along the rungs, while the Ising spin –1 AF1 phase (–1,1) is replaced by the dimer phase D1 (equivalent to the Haldane phase of the $S = 1$ chain) [3, 7]. For $|M| = 0.5$ we observe equivalent magnetic order in the classical, as well as in the quantum case. For $|h| > h_c$ there is paramagnetic state (the saturated ferromagnetic) in both situations.

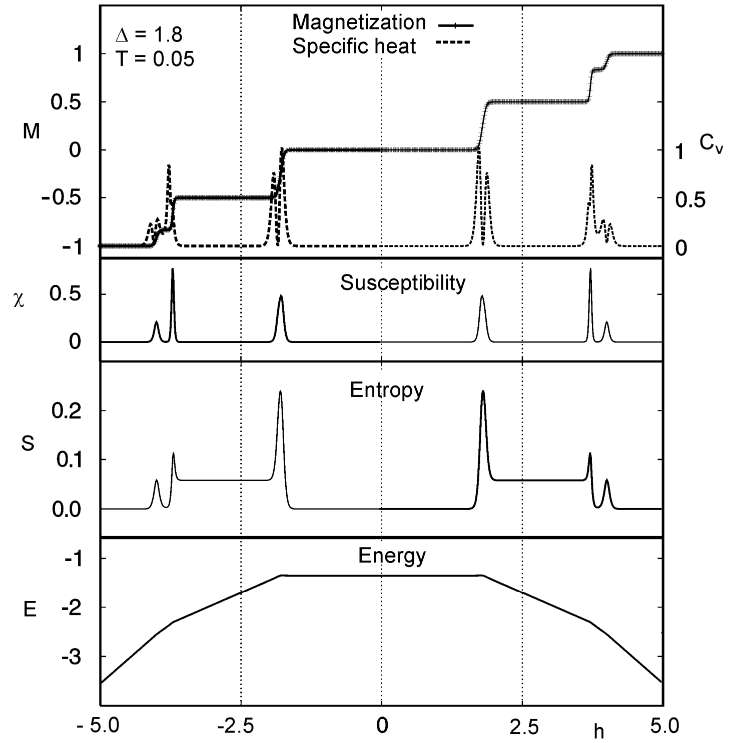

Fig. 3. The thermodynamic characteristics of the system as a function of external magnetic field h for Δ = 1.8 and T = 0.05

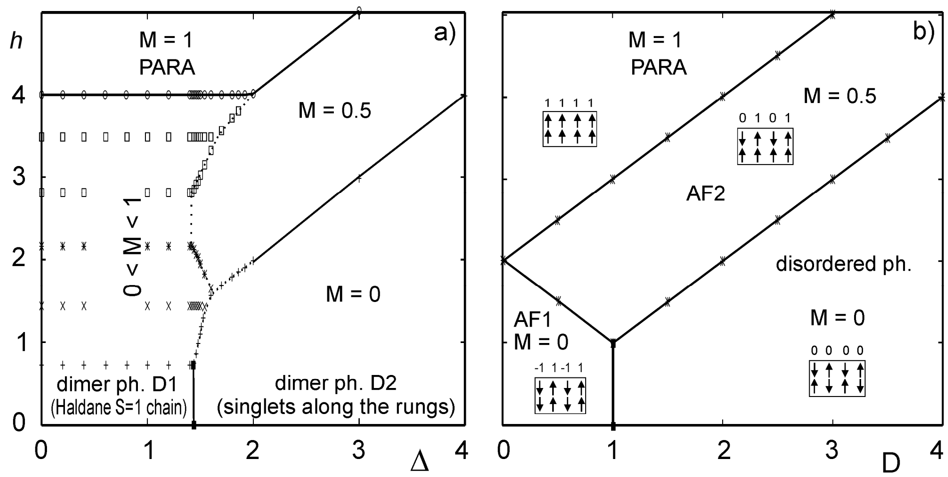

Fig. 4. The magnetic orderings in the ground state in the presence of magnetic field for the antiferromagnetic ladder described by the quantum model (a) and by the classical one (b)

Though the detailed structure of phase diagrams of the classical BC model (Fig. 4b) must be different from that presented for the quantum system (Fig. 4a), the mulitiphase composition for large Δ and h of both models is similar.

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