Renormalization of ferrimagnetic alternating spin chains

2006 J. Phys.: Condens. Matter 18 11047

(http://iopscience.iop.org/0953-8984/18/48/032)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER
J. Phys.: Condens. Matter **18** (2006) 11047–11057 doi:10.1088/0953-8984/18/48/032

Renormalization of ferrimagnetic alternating spin chains

Józef Sznajd

Institute for Low Temperature and Structural Research, Polish Academy of Science, Wroclaw, Poland

Received 12 September 2006, in final form 2 November 2006
Published 17 November 2006
Online at stacks.iop.org/JPhysCM/18/11047

Abstract
The linear real space renormalization group is applied to study alternating spin $(1/2, 1)$ chains. The temperature dependences of the specific heat and spin–spin correlation functions for the quantum easy-axis mixed-spin chain are found. The role of single-ion anisotropy is discussed. The phase diagram of Ising spin chains with antiferromagnetic intrachain interactions and weak ferromagnetic interchain interactions is presented. As one expects, the weak interchain coupling leads to antiferrimagnetic long-range order in several chains. The threshold value of single-ion anisotropy below which the system does not exhibit a phase transition is found.

1. Introduction

Ferrimagnets are systems made of ions having different spins, mostly of two types, $s \neq S$. In the simplest case these spins are arranged alternately on a bipartite lattice and they are coupled by a nearest-neighbour antiferromagnetic exchange interaction. Such systems exhibit a wide variety of interesting physical phenomena, especially in one dimension, and they have been studied by several theoretical methods: quantum Monte Carlo (MC) and spin wave (SW) theory [1], density matrix renormalization group (DMRG) [2] or modified SW [3]. The growing interest in the properties of mixed-spin systems is a result of the synthesis of bimetallic magnetic chains [4]. Many of the interesting phenomena observed in these systems have been explained from theoretical studies on spin isotropic models in one dimension at very low temperature. However, experimentally, the alternating spin chains have been found to be quasi-one-dimensional materials [5], and a weak interchain coupling that can be responsible for an eventual magnetic order becomes crucial one, at sufficiently low temperature. Thus, here we focus on the role of weak interchain coupling and single-ion anisotropy. The goal of this paper is also to show that both the finite-temperature critical behaviour and the thermodynamic (nonuniversal) properties of the weakly interacting mixed-spin chains can be studied by a method based on the linear-perturbation renormalization group transformation (LPRG) [6].

0953-8984/06/4811047+11$30.00

We consider, in this paper, two kinds of spin, $s = \frac{1}{2}$ and $S = 1$, alternating on chains with intrachain antiferromagnetic exchange interaction between nearest neighbours, described by the Hamiltonian

$$\mathcal{H}_0 = \sum_{\alpha=x,y,z} K_\alpha \sum_{j=1}^{M}\sum_{i=1}^{N/2}(s^\alpha_{2i-1,j}S^\alpha_{2i,j} + S^\alpha_{2i,j}s^\alpha_{2i+1,j}) + d\sum_i (S^z_{2i,j})^2 + h\sum_{j=1}^{M}\sum_{i=1}^{N/2}(s^z_{2i-1,j} + S^z_{2i,j}), \tag{1}$$

and weak ferromagnetic interchain couplings between nearest chains given by

$$\mathcal{H}_I = \sum_{\alpha=x,y,z} K^s_\alpha \sum_{i,j} s^\alpha_{i,j}s^\alpha_{i,j+1} + \sum_{\alpha=x,y,z} K^S_\alpha \sum_{i,j} S^\alpha_{i,j}S^\alpha_{i,j+1}, \tag{2}$$

where $S^\alpha_i\,(s^\alpha_i)$ represents a spin 1 (spin 1/2), and the factor $-1/T$ has already been absorbed in the Hamiltonian ($K_\alpha = -J_\alpha/T$, $d = -D/T$, $h = -$magnetic field$/T$).

The paper is organized as follows. We start with a brief review of the LPRG scheme for a mixed-spin system in section 2. In section 3 the specific heat and the spin–spin correlation function of the alternating quantum spin chain are considered. In section 4 the LPRG technique is applied to study the character of the phase transition of weakly interacting mixed-spin Ising chains. Finally we summarize our results in section 5.

2. Linear renormalization group transformation (LRG)

We define the renormalization transformation by

$$\exp[\mathcal{H}'(\vec\sigma,\vec\Gamma)] = \mathrm{Tr}_{\vec s,\vec S}P(\vec s,\vec S;\vec\sigma,\vec\Gamma)\exp[\mathcal{H}(\vec s,\vec S)], \qquad \mathcal{H} = \mathcal{H}_0 + \mathcal{H}_I. \tag{3}$$

The weight operator $P \equiv P(\vec s,\vec S;\vec\sigma,\vec\Gamma)$ which couples the original $(\vec s,\vec S)$ and effective spins $(\vec\sigma,\vec\Gamma)$ is chosen in a linear form. This means that the projector of the system is defined as a product of the individual spin projectors,

$$P = \prod_{i=0}^{N/2-1} p^s_i(\vec s,\vec\sigma)\,p^S_i(\vec S,\vec\Gamma), \tag{4}$$

where the total number of spins is N, and $p^s_i \equiv p^s_i(\vec s,\vec\sigma)$ and $p^S_i \equiv p^S_i(\vec S,\vec\Gamma)$ represent projectors for a spin $\frac{1}{2}$ and 1, respectively. The weight operator $p^s_i(\vec s,\vec\sigma)$ which couples the original to the new spins $\frac{1}{2}$ can be written in the following general (for the Ising and quantum spins) form:

$$p^s_i = \tfrac{1}{2}\left(1 + 4\sum_{\alpha=x,y,z} s^\alpha_{6i+1}\sigma^\alpha_{2i+1}\right), \tag{5}$$

and the weight operator $p^S_i(\vec S,\vec\Gamma)$ which couples the original and the new spins 1 for the Ising model is chosen as [7]

$$p^S_i = \left[1 - (S^z_{6i+4})^2 - (\Gamma^z_{2i+2})^2 + \tfrac{1}{2}S^z_{6i+4}\Gamma^z_{2i+2} + \tfrac{3}{2}\left(\sum_\alpha S^\alpha_{6i+4}\Gamma^\alpha_{2i+2}\right)^2\right], \tag{6}$$

whereas for the quantum Heisenberg model it is chosen as [7]

$$p^S_i = \prod_i\left[-1 + \sum_{\alpha=x,y,z} S^\alpha_{6i+4}\Gamma^\alpha_{2i+2} + \left(\sum_{\alpha=x,y,z} S^\alpha_{6i+4}\Gamma^\alpha_{2i+2}\right)^2\right]. \tag{7}$$

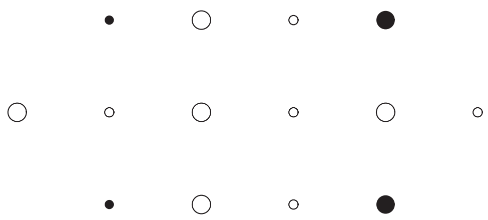

Figure 1. Renormalization scheme. Open circles denote decimated spins. Small circles and discs refer to spin $\frac{1}{2}$, and large ones to spin 1.

The transformation (3) with the projector (4) is the decimation transformation. Assuming that the spins $s = 1/2$ and $S = 1$ are at the odd and even sites, respectively, in the renormalization step only every sixth spin $(s_1, s_7, s_{13}, \ldots)$ from the $s = 1/2$-sublattice (5) and every sixth spin $(S_4, S_{10}, S_{16}, \ldots)$ from the $S = 1$-sublattice (6) or (7) are preserved and $(s_1, S_2, s_3, S_4, s_5, S_6, s_7, S_8, s_9, S_{10}, \ldots) \rightarrow (\sigma_1, \Gamma_2, \sigma_3, \Gamma_4, \ldots)$. The LPRG approach, similarly to the Suzuki–Takano (ST) one [8], starts with a decimation for a one-dimensional (1D) system. Then, on the basis of it, the interchain interaction is renormalized in a perturbative way [6]. In this paper, the chain is divided into four-spin blocks to admit periodic (antiferrimagnetic) structure with period 2, and only one block is considered. In each renormalization step, every third spin from every other row survives (figure 1).

For a single Ising chain ($K_x = K_y = 0$, $K_\alpha^s = 0$, and $K_\alpha^S = 0$) the transformation using (3)–(6) leads to the renormalized Hamiltonian $\mathcal{H}'$ in the form

$$\mathcal{H}'_0 = z_0 + K'_z \sum_i \sigma_i^z \Gamma_{i+1}^z + d' \sum_i (\Gamma_i^z)^2, \tag{8}$$

where

$$z_0 = \ln(2 + 2\,\mathrm{e}^d + \mathrm{e}^{d-K_z} + \mathrm{e}^{d+K_z}), \tag{9}$$

$$K'_z = \ln \frac{L_1}{L_2}, \qquad d' = \ln \frac{L_1 L_2\, \mathrm{e}^{d-3K_z}}{64 z_0^2}, \tag{10}$$

and

$$\begin{aligned} L_1 &= 3\,\mathrm{e}^d + 8\,\mathrm{e}^{K_z} + 8\,\mathrm{e}^{2K_z} + 15\,\mathrm{e}^{d+K_z} + 9\,\mathrm{e}^{d+2K_z} + 5\,\mathrm{e}^{d+3K_z} \\ L_2 &= 5\,\mathrm{e}^d + 8\,\mathrm{e}^{K_z} + 8\,\mathrm{e}^{2K_z} + 9\,\mathrm{e}^{d+K_z} + 15\,\mathrm{e}^{d+2K_z} + 3\,\mathrm{e}^{d+3K_z}. \end{aligned} \tag{11}$$

By using the transformation (9)–(11) the free energy per spin can be calculated from the formula

$$f = \sum_{n=1}^{\infty} \frac{\ln z_0(K_z^{(n)}, d^{(n)})}{3^n}, \tag{12}$$

which reproduces exactly the rigorous result for the alternating spins (1/2, 1) Ising model free energy

$$f_{\text{exact}} = -\tfrac{1}{2} T \ln\{2(\mathrm{e}^{D/T}[1 + \cosh(J_z/T)] + 1)\}. \tag{13}$$

In figure 2 the specific heat c of the alternate-spin Ising chain as a function of the reduced temperature (T/J) for several values of d is presented. For $-1 < d < d_g$, where $d_g \approx -0.7683$, a double-peak specific heat structure is observed as a result of a competition between the antiferromagnetic ordering interaction K_z and condensation of the spins $S = 1$ at the state $S = 0$ caused by the single-ion term d.

In the presence of the external magnetic field the LRG transformation generates new odd terms. Instead of the one external field h one has to take into account two of them, conjugate

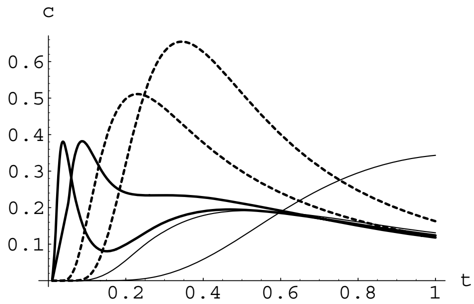

Figure 2. Temperature dependence of the alternate-spin Ising chain specific heat for $d = 0$ and -0.5 (dashed lines) $d = -0.77$ and $-0, 9$ (solid lines), and $d = -1$ and -3 (thin lines).

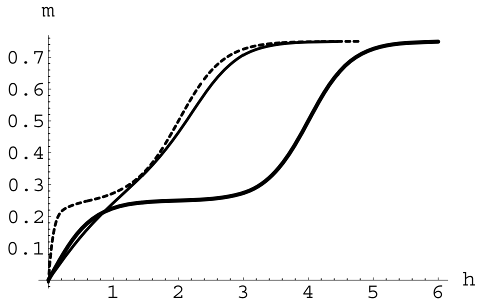

Figure 3. Magnetization as a function of field for $t = 1/3$, and $d = 0$ (dashed line) $d = -1$ (thin line), and $d = -3$ (solid line).

to spins $s = 1/2$ (h^s) and $S = 1$ (h^S), respectively, and additionally the third-order term h^m comes into play:

$$h^m \sum_i s_i^z (S_{i+1}^z)^2. \tag{14}$$

Also, in this case the analytical formulae for the renormalized couplings K_z', d', $(h^s)'$, $(h^S)'$, and $(h^m)'$ and spin-independent term z_0 (9) can be found quite easily, although they are, of course, much more complicated. Using these formulae we may calculate numerically the field dependence of the free energy and then other thermodynamic quantities. The magnetization per spin m and specific heat for the alternating-spin Ising model as functions of the external magnetic field h for the original values of parameters $h^s = h^S = h$ and $h^m = 0$ are presented in figures 3, 5, and 6. Figure 3 shows the field dependence of the magnetization at the reduced temperature $t = \frac{1}{3}$ for several values of d. The trace of the zero-field magnetic plateau at $m = 0.25$ $[(S - s)/2]$ and the saturation for the high field at $m = 0.75$ $[(S + s)/2]$ are visible. The trace of the plateau disappears for $d = -1$ where the antiferromagnetic interaction K_z and single-ion term d balance each other. In figure 4 the sublattice magnetizations $m_{\frac{1}{2}}$ and m_1 as functions of the magnetic field for $t = \frac{1}{3}$ and $d = -1$ are presented. In figures 5 and 6 the field dependences of the magnetization and specific heat for $d = 0$ and $d = -3$, respectively, are shown. In both cases the specific heat exhibits three-peak structure connected with remagnetization processes.

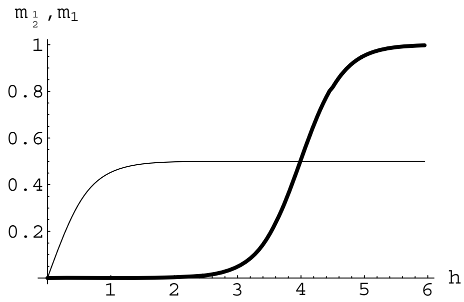

Figure 4. Sublattice $s = 1/2$ (thin line) and $S = 1$ (bold line) magnetizations per sublattice spin as functions of field for $t = 1/3$ and $d = -3$.

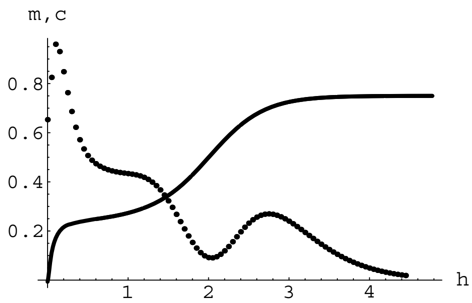

Figure 5. Magnetization (solid line) and specific heat (dotted) as functions of field for $t = 1/3$, and $d = 0$.

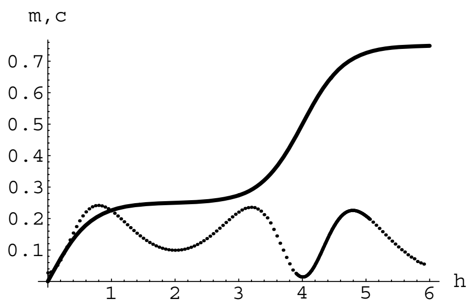

Figure 6. Magnetization (solid line) and specific heat (dotted) as functions of field for $t = 1/3$, and $d = -3$.

3. Alternating-spin XXZ chain

In this section, we consider a 1D quantum spin system defined by the Hamiltonian (1) with $K_x = K_y$, and $h = 0$ (XXZ model). For a quantum system, because of the non-commutativity of several terms of the Hamiltonian (1), the renormalization transformation (3), (4), (5), (7) cannot be carried out exactly even for a 1D lattice and in zero magnetic field. The decimation procedure takes the quantum effect into account within a single cluster [8], in our case four spins, and neglects the effect of non-commutativity of several clusters. This means that the

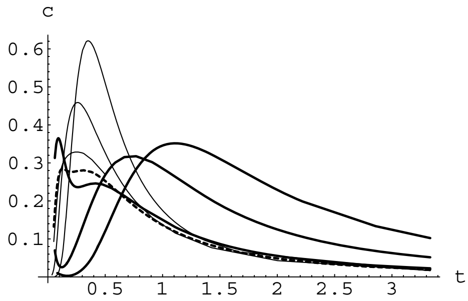

Figure 7. Specific heat of the alternate uniaxial $K_x/K_z = 0.2$ model for $d = 0$, 0.5, and 0.7 (thin lines), and $d = -0.8$ (dashed line), and $d = -1$, -2, and -3 (solid lines) from left to the right.

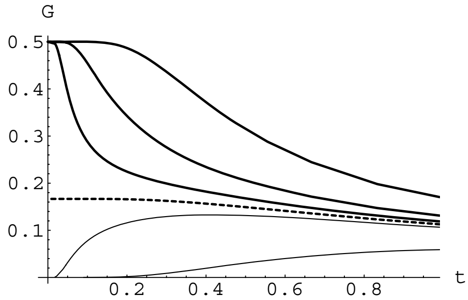

Figure 8. Temperature dependence of the Ising model correlation for $d = 0$, -1, and -3 from top to the bottom.

LRG procedure may deteriorate at low temperature. However, for sufficiently high temperature it should lead to reasonable results.

Applying the transformation (3), (4), (5), (7) to the 1D XXZ model Hamiltonian one obtains the transformed Hamiltonian $\mathcal{H}'$ in the same form as the original one with new parameters K_x', K_z', d', and the constant term z_0 independent of σ_α and Γ_α (see the appendix). Using the recursion formulae (A.5) one can find the free energy and specific heat of the 1D XXZ model with single-ion anisotropy. In figure 7 the temperature dependence of the specific heat of the uniaxial ($K_x/K_z = 0.2$) model for several values of the single-ion anisotropy is presented. As is seen, similarly as for the Ising model the second maximum of the specific heat at $d \approx -0.8$ appears. However, in this case, due to transverse fluctuations this maximum does not vanish for $d \leqslant -1$ as in the Ising model case.

To check the short-range structure of our system and an eventual ground-state long-range order we can find the temperature dependence of the two-spin longitudinal G^L and transverse G^T correlation functions defined as

$$G^{L(T)} = -\langle s_i^{z(x)} S_{i+1}^{z(x)} \rangle. \tag{15}$$

To compare, in figure 8 the two-spin correlation function (G) for the Ising model is presented. Of course, in the latter case for $d > -1$, G tends to $1/2$ as $T \to 0$ which means (anti)ferrimagnetic ground-state long-range order. For $d = -1$, $G \to 1/6$, and for $d < -1$, $G \to 0$ for $T \to 0$, with all spins 1 at the state $S = 0$. In figure 9 both longitudinal (solid lines) and transversal (dashed and thin lines) correlation functions of the uniaxial model for $d = 0, -1, -2$, and -3 are presented. As one expects, there is no fully saturated ferrimagnetic ground state even for $d = 0$ ($G^L < 0.5$). Instead, the finite transverse fluctuations (bottom

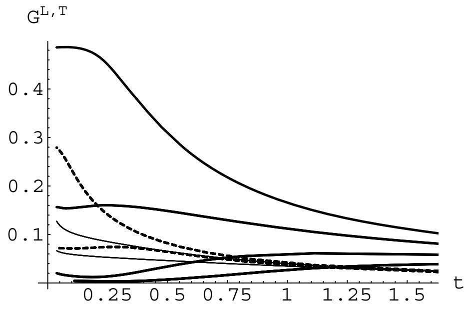

Figure 9. Temperature dependence of the XXZ model correlation for $d = 0, -1, -2$ and -3; solid lines from top to the bottom denote longitudinal correlation, and dashed lines denote transverse correlation for $d = 0, -1$ (top), and thin lines for $d = -2$ (top), -3, respectively.

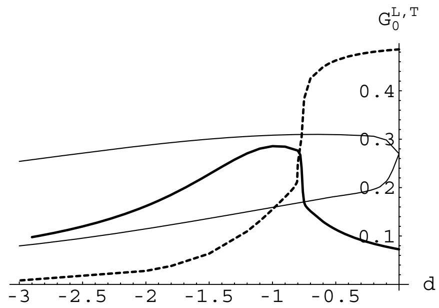

Figure 10. Zero-temperature correlation as function of d for the uniaxial model $K_x/K_z = 0.2$—longitudinal (dashed line) and transverse (solid line) and for Heisenberg model—thin lines (the bottom line refers to G_0^L).

dashed line in figure 9) are observed, and $G^T \approx 0.0725$ for $T \to 0$ at $d = 0$. G^L decreases with decreasing d, and for $d = -1$ goes to 0.154 55 which is slightly less than Ising value $1/6$, but also for $d < -1$ due to the quantum fluctuations it has finite values. The transverse correlation first increases with decreasing d, reaches a maximum at $d = -1$ and then decreases.

It should be emphasized once more that the procedure in which we confine ourselves to the relatively small cluster and neglect the effect of non-commutativity of several clusters can fail at very low temperature and particularly at a ground state. However, it seems that the zero-temperature values of the correlation functions can be reasonable extrapolated from higher temperatures (compare figure 9) at least for easy-axis systems. The results of such an extrapolation for the uniaxial model with $K_x/K_z = 0.2$ and Heisenberg model with isotropic exchange interaction ($K_x = K_z$) are presented in figure 10. As is seen, there is a sharp change in the correlation functions behaviour of the uniaxial model about $d \simeq -0.8$ where single-ion anisotropy balances the exchange anisotropy. For $d < -0.8$ one gets a planar (easy-plane) model with no long-range order at $T = 0$ (critical state). The same is of course the case for the isotropic exchange model with any negative single-ion anisotropy.

4. Weakly coupled Ising chains

We now consider an infinite number of mixed-spin Ising chains at finite temperature, where the chains are coupled by weak interchain interactions K_z^s and K_z^S (2). For the LPRG procedure we use the cluster (4–6–4) presented in figure 1, with four spins $(s_1^z, S_2^z, s_3^z, S_4^z)$, six spins and again four spins for the first, second, and third row, respectively. The spins from odd rows are decimated; this means

$$(s_1^z, S_2^z, s_3^z, S_4^z) \to (\sigma_1^z, \Gamma_2^z),$$

and spins from even rows are removed (a trace is carried out). In addition, for simplification we confine ourselves to only two-spin bilinear interactions, thereby neglecting three- and four-spin interactions which are generated by the RG for the (4–6–4) cluster. Thus, in the second-order cumulant expansion only one new interaction comes into play:

$$K_z^m \sum_{\langle ij \rangle} s_{i,j}^z S_{i+1,j+1}^z, \tag{16}$$

where i refers to rows and j refers to columns.

As usual, the transformation (3) can be written in the form

$$\mathcal{H}'(\sigma, \Gamma) = \mathcal{H}'_0 + \ln \langle \mathrm{e}^{\mathcal{H}_I(s,S)} \rangle, \tag{17}$$

with standard cumulant expansion [9] for $\langle \exp[\mathcal{H}_I(s, S)] \rangle$, $\mathcal{H}'_0$ for a decimated row is presented in equation (8), and

$$\langle A \rangle \equiv \frac{\mathrm{Tr}_{s,S} A P(s, S; \sigma, \Gamma)\, \mathrm{e}^{\mathcal{H}_0(s,S)}}{\mathrm{Tr}_{s,S} P(s, S; \sigma, \Gamma)\, \mathrm{e}^{\mathcal{H}_0(s,S)}}. \tag{18}$$

For the cluster shown in figure 1, the interchain Hamiltonian $\mathcal{H}_I$ contains the interaction between the first and second rows $\mathcal{H}_{12}$ and between second and third rows $\mathcal{H}_{23}$.

To evaluate the transformation (17) one has to know the averages of several spins and spin products from decimated (odd) and removed (even) rows. The latter ones are of course numbers. For example, to find contributions to $\mathcal{H}'(\sigma, \Gamma)$ from $\langle \mathcal{H}_{12}^2 \rangle$, the averages $\langle S_i^2 \rangle$ and the averages of the two-spin products are needed. All of them have a form

$$a_0 + a_1 \sigma_1 \Gamma_2 + a_2 \Gamma_2^2. \tag{19}$$

where a_i are functions of the intrachain parameters. Hereafter for convenience we will omit the superscript z. In order to find the contributions from $\langle \mathcal{H}_{12} \mathcal{H}_{23} \rangle$, one has to know the averages of several spins $\langle s_i \rangle$ and $\langle S_i \rangle$ which generally have a form

$$c_1 \sigma_1 + c_2 \Gamma_2 + c_3 \sigma_1 \Gamma_2 + c_4 \Gamma_2^2, \tag{20}$$

where c_i are also functions of the intrachain parameters. However, because we are interested only in two-spin interactions it is sufficient to consider in the latter case only linear terms in the effective spins.

Now we are able to evaluate numerically the renormalization transformation (17) from the original set of five parameters $(K_z, d, K_z^s, K_z^S, K_z^m)$ to the set of renormalized ones. Choosing as original values $K_z^m = 0$ and $K_z^s = K_z^S = q K_z$ with $q \leqslant 0.8$, we find for $d > -1.26$ two fixed points which describe the behaviour of the system at $T = 0$ and ∞, and also the critical surface at the space of five parameters. The critical lines in the plane $(t_c = 1/K_z^c, q)$ for several values of the single-ion anisotropy are presented in figure 11. As is seen, a change in the critical line behaviour is observed at $d = -1$. For $d < -1$ the critical line does not reach the point $q = 0$. For $d < d_{\mathrm{g}}(q)$, where $d_{\mathrm{g}}(0.8) < -1.26$ there is only one fixed point describing the system at $T = \infty$. This means that a system with $q \leqslant 0.8$ and $d < -1.26$ does not undergo a finite-temperature phase transition. It is well known that such a limit value of d below which there is no phase transition for pure $S = 1$ (Blume–Capel, BC) model [10] is observed, and it has also been found by using the LPRG [7]. However, in contradistinction to the pure BC model in the mixed-spin case we have not found any tricritical point and in consequence a

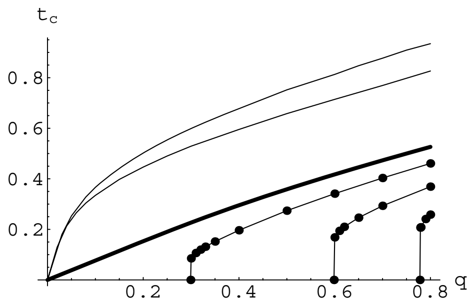

Figure 11. Critical temperature of coupled ferrimagnetic Ising chains as a function of interchain interaction q for $d = 1, 0, -1$ (solid line), $-1.1, -1.2, -1.26$ from left to the right, respectively.

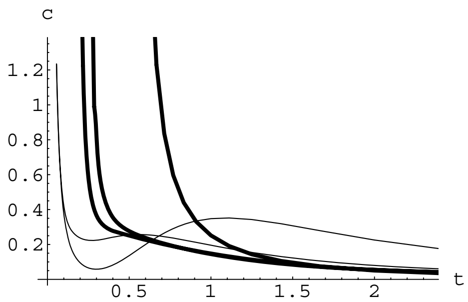

Figure 12. Temperature dependence of the specific heat for the ferrimagnetic Ising chains coupled by interchain ferromagnetic interaction $\delta = K_2/K_1 = 0.3$ for $d = 0, -1, -1.05$ (solid lines) and $d = -1.5$ and -3 (thin lines) from right to the left, respectively.

region of d for which the system undergoes a discontinuous (first-order) phase transition. Such a point was found by means of the LPRG [7] for the pure $S = 1$ system. Figure 12 shows the temperature dependence of the specific heat for several values of d for which the system exhibits a phase transition to the ordered ferrimagnetic state (solid lines) and for which there is no phase transition (thin lines).

5. Conclusion

We have applied the real-space RG method to study ferrimagnetic chains made of alternating spins $(1/2, 1)$. We have focused our attention on the role of the weak interchain coupling which, from the experimental point of view, is present in all, so-called, quasi-one-dimensional systems [11], single-ion anisotropy [12], and validity of the LRG as a method for the description of mixed-spin systems.

As we discussed in our previous papers [6, 7], the LPRG is reliable at high temperature. The method starts with a decimation for a chain which can be done exactly for the Ising model, and then the interchain interaction is renormalized in a perturbative way. So, for the models of the Ising type, the control parameter plays, to some extent, the role of the interchain interaction. The application of the LPRG to quantum systems needs some additional approximations because of the non-commutativity of the several terms of the Hamiltonian. However, it was shown [6] for example that for the $s = 1/2XY$ chain the free energy found by using LRG at $K = J/T \approx 1$ differs by less than 1% from the exact value. Unfortunately, an exact treatment

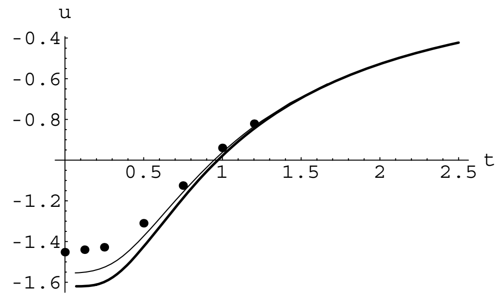

Figure 13. Temperature dependence of the internal energy of the Heisenberg model (per spin pair) found from the LRG with a four-spin cluster (solid line), a six-spin cluster (thin line), and from the EFS (points), respectively.

is not available for the model considered in this paper. Thus, to check the validity of the results we compare the internal energy per spin pair (1/2, 1) for the mixed-spin Heisenberg model found by the LRG with four- and six-spin clusters and from the exact results computed for finite rings (EFS) [13]. As is seen from figure 13, the results are very close to each other for high temperature and can be improved by increasing the size of the cluster used. We have not found any results for the anisotropic models which could be compared with ours. However, one would expect that the LPRG should work better for the models with uniaxial (Ising-type) symmetry considered in this paper.

First we have defined the RG transformation with the projector which couples the original spins $s = 1/2$ and $S = 1$ and effective spins $\sigma = 1/2$ and $\Gamma = 1$. Such a transformation reproduces exactly the rigorous results for the 1D mixed-spin Ising model. The field dependences of the magnetization with a 'plateau' and specific heat with three-peak structure, for several values of the single-ion anisotropy, have been presented.

For the quantum alternating-spin easy-axis chain the specific heat as a function of temperature, similarly as for the Ising model, shows a two-peak structure starting from $d \approx -0.8$. However, in this case we are not able to decide for which value of d the second maximum disappears because, as we have already mentioned, for a quantum model our method is less reliable at very low temperature. We have also calculated the temperature dependence of the nearest-neighbour spin–spin correlation function for several values of the single-ion anisotropy. For the Ising model such a function exhibits a jump from $G = \frac{1}{2}$ to 0 at $d = -1$ and $T = 0$. This indicates the ground-state phase transition from the fully saturated ferrimagnetic phase to the disordered phase with all spins $S = 1$ at the state 0. For the quantum easy-axis chain with $K_x/K_z = 0.2$, sharp changes in both the longitudinal and transverse correlation functions are observed at $d \approx -0.8$. This indicates the zero-temperature phase transition from a non-saturated ferrimagnetic state to the critical state of the 1D quantum planar model.

Finally, the phase diagram of the mixed-spin $(\frac{1}{2}, 1)$ chains with antiferromagnetic intrachain interaction coupled by weak ferromagnetic interchain interactions has been found. The weak interchain interaction leads to antiferrimagnetic long-range order in several chains provided $d > d_g(q)$ and the temperature is sufficiently low. Similarly as for the pure $S = 1$ BC model, for the mixed-spin model there is also a threshold value of the single-ion anisotropy $d = d_g(q)$ below which there is no phase transition. However, in contradistinction to the BC model, the mixed-spin model does not undergo a first-order phase transition for any value of d. The temperature dependence of the specific heat of the model with $K_2^s = K_2^S = 0.3$ for several values of d has been presented. For $d > d_g(q = 0.3) \approx -1.05$ the specific heat is singular at the phase transition temperature and for $d < d_g(0.3)$ an upturn of the specific heat is observed.

Appendix. Recursion relations

Applying the transformation (3), (4), (5), (7) to the four-spin cluster $(\vec{s}_1, \vec{S}_2, \vec{s}_3, \vec{S}_4)_\alpha$ of the 1D XXZ model with the projector (4) for the αth cluster

$$P_\alpha = p_\alpha^s(\vec{s}_1, \vec{\sigma}_1) p_\alpha^S(\vec{S}_4, \vec{\Gamma}_2), \tag{A.1}$$

we get the renormalized Hamiltonian as

$$\mathcal{H}'_\alpha = \ln[f_0 + f_{k_z}\sigma_1^z\Gamma_2^z + f_{k_x}(\sigma_1^x\Gamma_2^x + \sigma_1^y\Gamma_2^y) + f_d(\Gamma_2^z)^2], \tag{A.2}$$

where

$$\begin{aligned} f_0 &= \tfrac{1}{12}\mathrm{Tr}_{\vec{s}_1,\vec{S}_4}[2(S_4^x)^2 - 1]\,\mathrm{e}^{\mathcal{H}}, \qquad & f_{k_x} &= \tfrac{1}{6}\mathrm{Tr}_{\vec{s}_1,\vec{S}_4} s_1^x S_4^x\,\mathrm{e}^{\mathcal{H}}, \\ f_d &= \tfrac{1}{12}\mathrm{Tr}_{\vec{s}_1,\vec{S}_4}[(S_4^z)^2 - (S_4^x)^2]\,\mathrm{e}^{\mathcal{H}}, \qquad & f_{k_z} &= \tfrac{1}{6}\mathrm{Tr}_{\vec{s}_1,\vec{S}_4} s_1^z S_4^z\,\mathrm{e}^{\mathcal{H}}. \end{aligned} \tag{A.3}$$

This allows us to find the renormalized Hamiltonian in the same form as the original one:

$$\mathcal{H}'_\alpha = z_0 + K'_z\sigma_1^z\Gamma_2^z + K'_x(\sigma_1^x\Gamma_2^x + \sigma_1^y\Gamma_2^y) + d'(\Gamma_2^z)^2, \tag{A.4}$$

with

$$\begin{aligned} z_0 &= \frac{1}{2q}[(q + 2f_d - f_{k_z})\ln\lambda_1 + (q - 2f_d + f_{k_z})\ln\lambda_2], \\ K'_z &= \frac{2f_{k_x}}{q}\ln\frac{\lambda_2}{\lambda_1}, \\ K'_x &= \frac{1}{2q}[2q\ln\lambda_3 - (q - 2f_d + f_{k_z})\ln\lambda_1 - (q + 2f_d - f_{k_z})\ln\lambda_2], \\ d' &= \frac{1}{2q}[2q\ln\lambda_3 - (q + 6f_d - 3f_{k_z})\ln\lambda_1 - (q - 6f_d + 3f_{k_z})\ln\lambda_2], \end{aligned} \tag{A.5}$$

and

$$\begin{aligned} \lambda_1 &= \tfrac{1}{4}(4f_0 + 2f_d - f_{k_z} - q), \qquad & \lambda_2 &= \tfrac{1}{4}(4f_0 + 2f_d - f_{k_z} + q), \\ \lambda_3 &= f_0 + f_d + \tfrac{1}{2}f_{k_z}, \qquad & q &= \sqrt{8f_{k_x}^2 + (f_{k_z} - 2f_d)^2}. \end{aligned} \tag{A.6}$$

References

[1] Brehmer S, Mikeska H-J and Yamamoto S 1997 *J. Phys.: Condens. Matter* **9** 3921
[2] Pati S K, Ramasesha S and Sen D 1997 *Phys. Rev.* B **55** 8894
[3] Yamamoto S and Hori H 2005 *Phys. Rev.* B **72** 054423
[4] Khan O, Pei Y and Journaux Y 1992 *Inorganic Materials* ed D W Bruce and D O'Hare (New York: Wiley) p 95
[5] Gleizes A and Verdegauer M 1981 *J. Am. Chem. Soc.* **103** 7373
Gleizes A and Verdegauer M 1984 *J. Am. Chem. Soc.* **106** 3727
Coronado E, Drillon M, Nugteren P R, de Jongh L J, Beltran D and Georges R 1989 *J. Am. Chem. Soc.* **111** 3874
Zhou P, Morin B G and Epstein A J 1993 *J. Appl. Phys.* **73** 6569
[6] Sznajd J 2001 *Phys. Rev.* B **63** 184404
[7] Sznajd J 2002 *Phys. Rev.* B **66** 104420
[8] Suzuki M and Takano H 1979 *Phys. Lett.* A **69** 426
[9] Niemeijer Th and Van Leeuwen J M J 1974 *Physica* **17** 17
[10] Blume M 1966 *Phys. Rev.* **141** 517
Capel H W 1966 *Physica* **32** 966
[11] Trumper A E and Gazza C 2001 *Phys. Rev.* B **64** 134408
[12] Park J-H, Culp J T, Hall D W, Talham D R and Meisel M W 2003 *Physica* B **329–333** 1152
[13] Drillon M, Coronado E, Georges R, Gianduzzo J C and Curely J 1989 *Phys. Rev.* **40** 10992