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Thermodynamics, geometrical frustration and quantum fluctuations in coupled spin chains

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The linear-perturbation real space renormalization transformation (LPRG) is presented and applied to the study of quantum spin chains coupled by interchain interaction (k_1) weaker than intrachain one (k). The method is examined in two exact solvable cases: Ising chains on the square and triangular lattices and quantum XY chain. For the Ising model, in the second order in the cumulant epansion, the deviation of the critical temperature from the exact value is less than 1% for $0.5k > k_1 > 0.15k$, but even in the case of the standard Ising model ($k_1 = k$) we found the value of T_c which differs by 2% from the exact one. For the quantum XY chain the deviation of the free energy value found by using LPRG from the exact Katsura result is less than 1% for $T/J > 1$, and for rather low temperature $T/J = 0.08$ is about 6%. The LPRG is used to study the effects of interchain frustration on the phase transition in 2D Heisenberg spin chains with easy axis along the z direction. It is shown that contrary to the pure Ising model in systems with in-plane interactions (XY), the interchain frustration does not destroy the finite-temperature transition. However, such a frustration changes the character of the phase transition from Ising-like to, probably, Kosterlitz-Thouless-like. We have also applied the LPRG method to the calculation of the isothermal magnetocaloric coefficient (M_T) for several spin models in disordered phases. Is is demonstrated that in the presence of antiferromagnetic fluctuations, M_T changes sign at some value of the magnetic field. Generally, M_T is negative if magnetic field competes with a short-range order, and consequently it can be an indicator of the change in the short-range correlation.

Key words: *Heisenberg chains, renormalization group, interchain frustration, magnetocaloric effect*

PACS: *75.10.Pq, 75.10.Jm*

1. Introduction

The physics of one-dimensional (1D) spin systems has drawn considerable theoretical and experimental attention for several decades. In recent years this attention has been mainly due to the development of magnetic materials which realize close 1D models. However, the pure one-dimensional systems is a physical abstraction since in real material, spin chains are always at least weakly coupled (quasi-1D magnet). But "quasi is different" and at sufficiently low temperature even relatively small interchain interaction becomes important and it may trigger a long range ordering. Among the many quasi-1D compounds studied so far, there are for example $(C_6H_{11}NH_3)CuBr_3$ (CHAB) and $(C_6H_{11}NH_3)CuCl_3$ (CHAC) [1] which appear to be a very good approximation of a ferromagnetic $S = \frac{1}{2}$ Heisenberg 1D model. The intrachain interaction in both systems has about the same value $J/k \approx 50$, whereas the interchain coupling J_1 is smaller by almost three orders of magnitude. In a wide range of temperatures the experimental specific heat data of CHAC and CHAB can be satisfactorily described by using 1D anisotropic Heisenberg model[2]. However, at low temperature this description fails because both compounds undergo phase transitions with the three-dimensional ordering temperature $T_\mathrm{c} = 2.21$ K for CHAC and 1.5 K for CHAB. The existence of such a phase transition and long-range magnetic order at low temperature is well established in a quasi-one-dimensional Ising ferromagnet $KEr(MoO_4)_2$ [3]. In this case the estimated value of the intrachain interaction J/k is about 1, interchain interaction $J_1/k \approx 0.05$, and critical temperature $T_\mathrm{c} = 0.955$ K. The ordering process at low temperature and one dimensional feature at high T is also observed in quasi-1D oxide $Ca_3Co_2O_6$ [4] and in the $S = 1$ chain compound $LiVGe_2O_6$. In this latter case the weak ferromagnetic interchain interaction leads to the long-range antiferromagnetic order [5]. In some other quasi-1D systems – for example Yb_4As_3 [6] or UX_3 (X = S,Se,Te) [7,8] the existence of a low temperature long-range order is still an open question. So it seems to be important to have a method which allows one to control the effect of the week interchain interaction on the thermodynamic behaviour of the anisotropic quasi-one-dimensional spin systems. In order to take into account both the one-dimensional feature at high temperature and an eventual phase transition at low temperature we have used the method based on the linear perturbation renormalization-group transformation (LPRG) [9]. The LPRG method can be used to study the existence of the critical phase transition as well as some nonuniversal properties such as a location of the critical temperature or temperature dependence of the thermodynamic quantities of a broad class of weakly interacting spin chains. In section II we present the method. In section III, we apply the LPRG to find the critical temperature as a function of the interchain interaction for the Ising model on the square and triangular lattices. In section IV, the validity of the method for quantum anisotropic Heisenberg spin models is discussed. In section V, the effect of the interchain frustration on the phase transition in 2D spin systems is considered. In section VI, the LPRG is used to analyze the field dependence of the isothermal magnetocaloric coefficient.

2. LPRG

Let us consider a system made of spin chains described by the Hamiltonian:

$$\mathcal{H}(\vec{S}) = \mathcal{H}_0(\vec{S}) + \mathcal{H}_{\mathcal{I}}(\vec{\mathcal{S}}), \tag{1}$$

where $\mathcal{H}_0$ describes spin chains with intrachain interaction $J^\alpha = -k^\alpha T$ and $\mathcal{H}_{\mathcal{I}}$ interchain coupling with weaker interchain interaction $J_1^\alpha = -k_1^\alpha T$.

The LPRG starts with the exact decimation for one-dimensional Ising or approximate decimation for one-dimensional quantum spin systems. Then, on this basis, the interchain interaction is renormalized in a perturbative way. The renormalization group transformation for the Hamiltonian $\mathcal{H}$ is defined as usually by

$$\exp[\mathcal{H}'(\vec{\sigma})] = \mathrm{Tr}_{\vec{S}} P(\vec{S}, \vec{\sigma}) \exp[\mathcal{H}(\vec{S})]. \tag{2}$$

The weight operator $P(\vec{S}, \vec{\sigma})$ which couples the original ($\vec{S}$) and effective ($\vec{\sigma}$) spins is chosen in a linear form. This means that the projector of the system is defined as a product of the individual spin projectors and for $s = \frac{1}{2}$

$$P(\vec{S}, \vec{\sigma}) = \prod_{i=0}^{N} p(\vec{S}, \vec{\sigma}), \qquad p_i = \frac{1}{2}(1 + 4 \sum_{\alpha=x,y,z} S_{mi}^\alpha \sigma_i^\alpha)\,. \tag{3}$$

With such a projector, the chain is divided into $(m+1)$-spin blocks and in each renormalization step, every $(m+1)$-th spin survives.

Now we take interchain coupling $\mathcal{H}_{\mathcal{I}}$ into account. Transformation (2) can be written in the form

$$\mathcal{H}'(\vec{\sigma}) = \mathcal{H}'_0 + \ln\langle \mathrm{e}^{\mathcal{H}_I(\vec{S})}\rangle, \tag{4}$$

with

$$\langle A \rangle \equiv \frac{Tr_S A P(S,\sigma)\mathrm{e}^{\mathcal{H}_0(S)}}{Tr_S P(S,\sigma)\mathrm{e}^{\mathcal{H}_0(S)}} \tag{5}$$

and standard cumulant expansion [10]

$$\langle \mathrm{e}^{\mathcal{H}_{\mathcal{I}}(\vec{S})}\rangle = \langle \mathcal{H}_{\mathcal{I}}(\vec{S})\rangle_0 + \frac{1}{2!}[\langle \mathcal{H}_{\mathcal{I}}(\vec{S})^2\rangle_0 - \langle \mathcal{H}_{\mathcal{I}}(\vec{S})\rangle_0^2] + \cdots\,. \tag{6}$$

The effective Hamiltonian of a single chain and all averages necessary to evaluate cumulants can be, of course, found for a relatively large spin block. However, in order to consider the chains in higher dimensions we have to confine ourselves to some reasonable size of the spin cluster and in consequence rather small block. The idea of the LPRG in 2D with $m = 3$ (four spin block) is

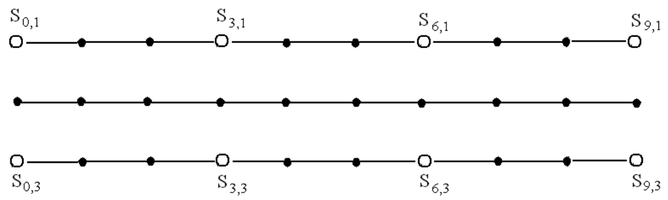

Figure 1. The cluster used to get renormalized Hamiltonian of the coupled Ising chains in 2D. Open circles denote effective spins.

presented in figure 1 The open circles represent the spins which survive in the decimation procedure. According to figure 1, in each step of the renormalization-group transformation every other row ("even" row) is removed, and from "odd" rows every third spin survives. The size of the block (value of m) as well as the size and shape of the cluster (number of rows) effect the quality of the approximation but first of all they should not violate the symmetry of the original problem. For example, blocks with odd numbers of spins (even m) are not appropriate for a description of antiferromagnetic models. It is easy to see that for such a block in the first step of the RG transformation every other spin is killed and one gets an effective ferromagnetic system.

Using the formula (3) one may get the transformation from the original set of intra- and interchain coupling parameters k_i to the set of renormalized ones k'_i. As usual, the iteration of the coupling parameters allows one to find a critical temperature, if any, while the thermodynamic properties can be evaluated from the formula for the free energy

$$f = \sum_{n=1}^{\infty} \frac{F(k_i^{(n)}, h^{(n)})}{m^n}\,, \tag{7}$$

where $F(k_i^{(n)}, h^{(n)})$ the spin-independent term created in each step of the RG transformation. $k_i^{(n)}$ and $h^{(n)}$ denote the set of effective intra- and interchain interactions and the effective field found in the n-th step of the RG transformation.

3. Coupled Ising chains

3.0.1. The square lattice

In this section we will apply the LPRG to Ising chains with intrachain interaction $J = -kT$ in an external field $H = hT$ described by the Hamiltonian

$$\mathcal{H}_0 = k \sum_{j=1}^{M} \sum_{i=1}^{N} S_{i,j} S_{i+1,j} + h \sum_{i=1}^{NM} S_{i,j}\,, \tag{8}$$

coupled by weaker interchain interactions $J_1 = k_1 T$ and $J_2 = k_2 T$

$$\mathcal{H}_I = k_1 \sum_{i,j} S_{i,j} S_{i,j+1} + k_2 \sum_{i,j} S_{i,j} S_{i+1,j+1}\,, \tag{9}$$

where S_i represents the Ising spin and the factor $-1/T$ has already been absorbed in the Hamiltonian. As mentioned in the previous section, the LPRG approach starts with the decimation of one chain. For the Ising model the effective Hamiltonian $\mathcal{H}'_0$ (equation 4) and all averages to evaluate cumulants (6) can be, of course, found exactly for an arbitrary size of the spin block. In this section we will used the cluster presented in figure 1 with four spin blocks. It is easy to see that

$$\langle S_{3i,j} \rangle \equiv \frac{Tr_S S_{3i,j} P(S,\sigma) \mathrm{e}^{\mathcal{H}_0(S)}}{Tr_S P(S,\sigma) \mathrm{e}^{\mathcal{H}_0(S)}} = \sigma_{i,j} \tag{10}$$

and

$$\begin{aligned}\langle S_{3i+1,j}\rangle &= w_0 + w_1\sigma_{i,j} + w_2\sigma_{i+1,j} + w_{12}\sigma_{i,j}\sigma_{i+1,j}\,,\\ \langle S_{3i+2,j}\rangle &= w_0 + w_2\sigma_{i,j} + w_1\sigma_{i+1,j} + w_{12}\sigma_{i,j}\sigma_{i+1,j}\,,\end{aligned}\tag{11}$$

where i numbers the spins in the chain, j numbers rows, and w_i are the exactly known functions of the intrachain interaction k and external field h

$$\begin{aligned}w_0 &= \frac{1}{2R}(\mathrm{e}^{4h}-1)(\mathrm{e}^{4h}+2\mathrm{e}^{8h}+7\mathrm{e}^{4(h+k)}+2\mathrm{e}^{8(h+k)}+\mathrm{e}^{4(h+3k)}\\ &\quad+4\mathrm{e}^{2h+4k}+4\mathrm{e}^{6h+4k}+4\mathrm{e}^{2h+8k}+3\mathrm{e}^{4h+8k}+4\mathrm{e}^{6h+8k}),\\ w_1 &= \frac{1}{2R}\mathrm{e}^{2h}(1+\mathrm{e}^{2h})^2(\mathrm{e}^{4k}-1)(3\mathrm{e}^{2h}+2\mathrm{e}^{4k}+2\mathrm{e}^{4(h+k)}+\mathrm{e}^{2h+8k}),\\ w_2 &= \frac{1}{2R}\mathrm{e}^{4h}(\mathrm{e}^{4k}-1)^2(1+4\mathrm{e}^{2h}+\mathrm{e}^{4h}+\mathrm{e}^{4k}+\mathrm{e}^{4(h+k)}),\\ w_{12} &= \frac{1}{2R}\mathrm{e}^{4h}(\mathrm{e}^{4k}-1)(\mathrm{e}^{4k}-1)^3,\end{aligned}\tag{12}$$

where

$$R = (2\mathrm{e}^{2h}+\mathrm{e}^{4h}+\mathrm{e}^{4k})(1+2\mathrm{e}^{2h}+\mathrm{e}^{4(h+k)})(\mathrm{e}^{2h}+\mathrm{e}^{4k}+\mathrm{e}^{4(h+k)}+\mathrm{e}^{2h+4k}.\tag{13}$$

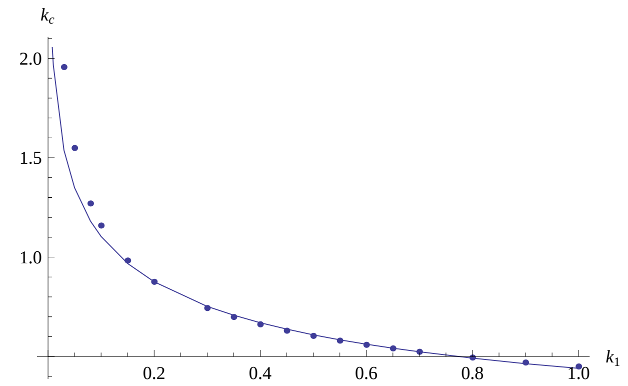

Figure 2. Critical inverse temperature (k_c) of the Ising model as a function of interchain interaction (k_1): dots – LPRG, thin line – exact result.

We are looking for the renormalized interactions between two effective spins:

$$k'\sigma_{1,1}\sigma_{2,1}\,,\qquad k_1'\sigma_{1,1}\sigma_{1,3}\,,\qquad k_2'\sigma_{1,1}\sigma_{2,3}\,,\tag{14}$$

and as seen from equation (10) contributions to interaction (14) come only from the original spins $S_{1,j},\ldots,S_{8,j}$. The other spins from odd rows, for example $S_{0,1}$ and $S_{9,1}$ in figure 1, do not contribute to interaction (9) because they involve other effective spins, $\sigma_{0,1}$ and $\sigma_{3,1}$, respectively. Thus, in order to have all contributions to bilinear interactions (14) in the LPRG transformation with four-spin block one has to consider eight spins from “odd” rows and ten from “even” row, i. e., the cluster $(8-10-8)$. In zero field $w_0=0$, $w_{12}=0$ (12) and the averages of the spins from decimated “odd” rows reduce to

$$\langle S_{3i}\rangle = \sigma_i\,,\qquad \langle S_{3i+1}\rangle = w_1\sigma_i + w_2\sigma_{i+1}\,,\qquad \langle S_{3i}S_{3i+1}\rangle = w_1 + w_2\sigma_i\sigma_{i+1}\,,\tag{15}$$

whereas from the removed (“even”) rows yield

$$\langle S_i\rangle = 0,\qquad \langle S_iS_{i+n}\rangle = \tanh^n(K).\tag{16}$$

Now we are able to numerically evaluate the renormalization transformation (4) which in the second order in the cumulant expansion has a form of the three recursion relations for three parameters, intrachain interaction k and two interchain interactions k_1 and k_2. As usually, in order to determine the critical temperature one has to find a critical surface which separates in the parameter space the regions of attraction of the two stable fixed points: zero temperature $k_i = \infty$ and infinite temperature $k_i = 0$. Figure 2 shows the critical inverse temperature as a function of the interchain interaction k_1 ($k_2 = 0$) for Ising model on the square lattice in the absence of the applied field. For the standard Ising model ($k_1 = k, k_2 = 0$) we have found the critical inverse temperature $k_c = 0.45$ [12] which differs about 2% from the exact result 0.4407. For the interchain interaction $0.5k < k_1 < 0.15k$ the deviation from the exact values is even less than 1%. For smaller values of k_1 the error becomes larger because then the phase transition is shifted to the very low temperature where the LPRG fails.

3.0.2. The triangular lattice

In this subsection we shall apply LPRG to the study of magnetic chains which form the triangular lattice with intrachain interaction k and interchain interaction k_1. For $k_1 = k$ one has the standard Ising model. If one is interested in studying a ferromagnetic model, then the choice of the three spin block and a cluster presented in figure 3 which we denote $(5-7-5)$, is appropriate. Such a choice preserves a one-sublattice structure of the system and, to the third order in the cumulant expansion, only the nearest neighbor interaction should be considered. This means that in this case, the LPRG transformation does not generate any additional interaction up to the third order. Using the same formulae for the spin averages as in the previous subsection it is easy to find the critical temperature of the ferromagnetic Ising model on the triangular lattice. For the standard Ising model $k_1 = k$ we have found $k_c = 0.268$ which should be compared with the exact value $k_c = 0.274$.

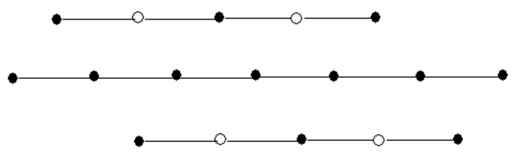

Figure 3. The cluster used to get renormalized Hamiltonian of the coupled Ising chains on triangular lattice for one-sublattice case. Open circles denote effective spins.

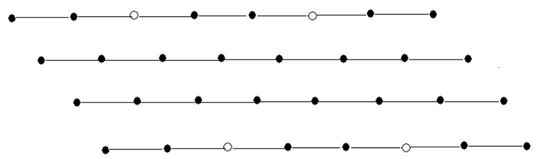

Figure 4. The cluster used to get renormalized Hamiltonian of the coupled Ising chains on triangular lattice for three-sublattice case. Open circles denote effective spins.

As mentioned in the section 2, the LPRG transformation should preserve the symmetry of the original system. So, if one is interested in multi-sublattice model, then the cluster presented in figure 3 cannot be used. It is easy to see that the four spin block and the cluster showed in figure 4 $(8-8-8-8)$ suits for the three-sublattice model. In this case the lowest nontrivial order of the expansion is the third order and for the ferromagnetic case $k_1 = k > 0$ we have found the critical inverse temperature $k_c = 0.309$. This result is worse than that found by using the cluster $(5-7-5)$ which is clear because for the cluster $(8-8-8-8)$, the lowest order contribution to the effective Hamiltonian is proportional to k_1^3 whereas for the cluster $(5-7-5)$ to k_1^2. The approximation could be, of course, improved by taking into account higher orders in the cumulant expansion though the higher-order calculations become labor and time consuming. However, the division of the triangular lattice into three sublattices allows us to consider an antiferromagnetic model. In this latter case, the system is frustrated and the LPRG transformation exhibits only one fixed point describing the system at $T = \infty$. This means, of course, that such a system does not undergo a finite temperature phase transition, as expected.

4. The anisotropic Heisenberg model

The LPRG can also be used to study quantum systems described by the Hamiltonian

$$\begin{aligned}\mathcal{H} \;=\; & \sum_{\alpha=x,y,z} K_0^\alpha \sum_{k=1}^{L}\sum_{j=1}^{M}\sum_{i=1}^{N} S_{i,j,k}^\alpha S_{i+1,j,k}^\alpha + h\sum_{i=1}^{NML} S_{i,j,k}^z + \sum_{\alpha=x,y,z} K_1^\alpha (\sum_{i,j} S_{i,j,k}^\alpha S_{i,j+1,k}^\alpha \\ & + \sum_{i,k} S_{i,j,k}^\alpha S_{i,j,k+1}^\alpha) + \sum_{\alpha=x,y,z} K_2^\alpha (\sum_{i,j} S_{i,j,k}^\alpha S_{i+1,j+1,k}^\alpha + \sum_{i,k} S_{i,j,k}^\alpha S_{i+1,j,k+1}^\alpha), \qquad (17)\end{aligned}$$

where S_i^α represents a spin 1/2. However, in this case because of the noncommutativity of several terms of the Hamiltonian (17) the decimation transformation cannot be carried out exactly and we apply the approximate decimation proposed by Suzuki and Takano [11]. The Suzuki-Takano procedure takes quantum effect into account within a single block and neglects the effect of non-commutativity of several blocks. Thus, contrary to the Ising case, the results even for a one chain depend on the division of the chain into blocks, i.e. on the size of the block. Of course, also the expressions for the averages of the spins are now more complicated than in the Ising case (15) and, for example

$$\langle S_{3i}^x \rangle = r_{1x}\sigma_i^x + r_{2x}\sigma_{i+1}^x \,, \qquad \langle S_{3i+1}^x \rangle = r_{3x}\sigma_i^x + r_{4x}\sigma_{i+1}^x \qquad (18)$$

and

$$\langle S_{3i}^x S_{3i+1}^x \rangle = r_{5x} + r_{6x}\sigma_i^x\sigma_{i+1}^x + r_{7x}\sigma_i^y\sigma_{i+1}^y + r_{8x}\sigma_i^z\sigma_{i+1}^z \,, \qquad (19)$$

where coefficients r_{ix} are functions of the intrachain interactions K_0^α.

In figure 5 the results of the LRG [12] for the zero field XY chain free energy obtained by using 4-, 6-, and 8-spin blocks are compared with the exact results found by Katsura [13]. As one expects for high temperatures, all three approximations are in quite good agreement with the exact result. For low temperatures there is a considerable deviation from the exact result especially for the smallest block. However, even for rather low reduced temperature $t = 0.08$ the deviation of the free energy from the exact values for the 8-spin block is about 6%, and for $t = 1$ it is about 1%. So, for a sufficiently high temperature LRG should lead to reasonable results also for the quantum models.

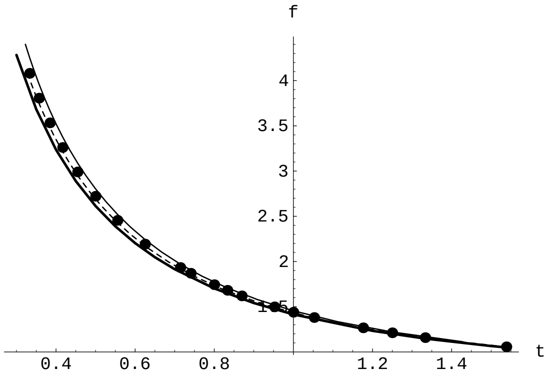

Figure 5. (Figure 7 from [12]) Temperature dependence of the one-dimensional XY model free energy found by using the 4-spin (thin line), 6-spin (dotted line), and 8-spin (dashed line) blocks. The solid line denotes the exact result found by Katsura[13].

5. Geometrical frustration and quantum fluctuations

In the system made of the spin chains or layers, an interchain (interlayers) frustration can cause the spatial dimensionality of the system to be reduced [14]. The idea is that the frustration leads to a cancellation of the coupling along one of the spatial dimensions, so that two-dimensional units (layers) are effectively decoupled. However, as shown by Maltseva and Coleman [15] the quantum or thermal fluctuations are expected to restore the interlayer coupling. So, it is still under discussion if the fully frustrated nD interactions between $(n-1)D$ objects effectively vanish and in what conditions. In many cases it is rather difficult to distinguish between the $3D$ and $2D$ critical singularities whereas the difference between $2D$ and $1D$ behavior is of course dramatic. So, it seems to be reasonable to consider the effect of the frustration on the phase transition in the systems of chains coupled by frustrated interchain interaction in 2D.

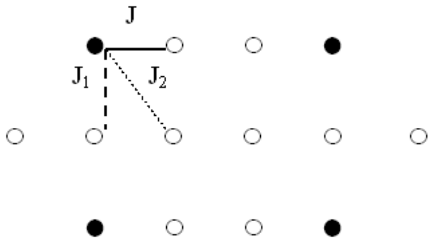

Figure 6. The cluster $(4-6-4)$ used to get renormalized Hamiltonian. Open circles denote decimated spins.

We have applied the LPRG [16] to consider the system of chains described by the Hamiltonian (17) with uniaxial ferromagnetic intrachain interaction $K_0^z > K_0^x = K_0^y = K_0^{\perp}$ coupled by weaker interchain interactions $K_1^z, K_2^z < K_0^z$ and $K_1^{\perp}, K_2^{\perp} < K_0^{\perp}$ $(K_i^{\alpha} = -J_i^{\alpha}/T)$ (figure 6). For

$$\phi^{\alpha} = K_2^{\alpha}/K_1^{\alpha} = -0.5, \tag{20}$$

the interchain interaction is fully frustrated. For a nonfrustrated case $\phi^{\alpha} \neq -0.5$, the Hamiltonian (17) describes the standard Ising-like phase transition from the paramagnetic phase to the phase with the magnetization along the z direction $(K_i^z > K_i^{\perp})$. Let us start with the pure Ising interactions $K_0^z = 1, K_1^z = 0.4, K_2^z = -0.2$, and $K_i^{\perp} = 0$. In this case the system is fully frustrated $(\phi^z = -0.5)$, the interchain interaction is canceled and the chains are effectively decoupled. Consequently, similarly as for the triangular lattice, the transformation exhibits only one fixed point describing the system at $(T = \infty)$ with all K_i^z approaching zero (figure 7). This means, of course, that the system has no long range order at any finite temperature.

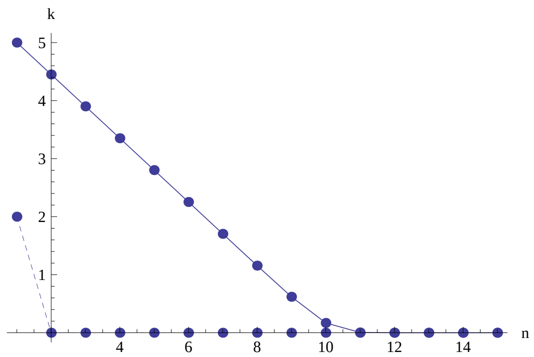

Figure 7. The iteration of the coupling parameters K_0^z (solid line) and K_1^z (dashed) for original values $J^z = 1, J_1^z = 0.4, J_2^z = -0.2, J^x = 0.0$ and $J_i^x = 0.0$ at $t = 0.2$.

Let us now introduce a small fully frustrated perpendicular interaction, $J^x = J_1^x = 0.2, J_2^x = -0.1$ and evaluate numerically the renormalization transformation. After each step of the iteration, we get new values of the effective interaction constants which is shown in figure 8. As seen, for the reduced temperature $t = 0.926$ the parameters tend to zero (infinite temperature fixed point) and for $t = 0.91$ to infinity (zero temperature fixed point). This means that there is a point of singularity – critical point, between these two temperatures. Unfortunately, by using the LPRG method we are able only to say that the frustration does not destroy a phase transition in the considered system, but we are not able to define the nature of the low temperature – "ordered" phase. However, taking into account that the effective interchain Ising interaction K_1^z vanishes (figure 8), it is natural to assume the existence of the XY type order and the Kosterlitz-Thouless (KT) type finite temperature phase transition in the model under consideration.

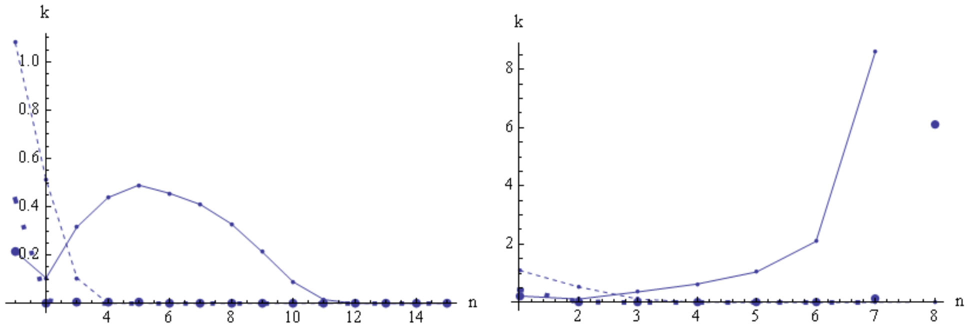

Figure 8. The iteration of the coupling parameters K_0^x (dots), K_1^x (thin line), K_0^z (dashed), and K_1^z (quadrates) for original values $J^z = 1, J_1^z = 0.4, J_2^z = -0.2, J^x = 0.2, J_1^x = 0.2$, and $J_2^x = -0.1$ at $t = 0.926$ (left plot) and $t = 0.91$ (right plot).

6. The isothermal magnetocaloric effect

Motivated by the recently developed [17] technique for measuring isothermal magnetocaloric coefficient

$$M_{\mathrm{T}} = -T\left(\frac{\partial S}{\partial H}\right)_T = -T\left(\frac{\partial M}{\partial T}\right)_H, \tag{21}$$

we have applied the LPRG method to the study of thermodynamic properties of the coupled spin chains in a field [12]. For the Ising model, the appropriate averages of the spins from "odd" rows are defined in equations (10) and (11) whereas in the presence of the external field the exact formulae for the spin from "even" rows are

$$\langle s_i^z\rangle = \frac{\sinh h}{\sqrt{\cosh^2 h + \mathrm{e}^{-4k} - 1}}, \qquad \langle s_i^z s_{i+n}^z\rangle = \frac{1}{A^2}\left[\frac{4(B-A)}{B+A}\mathrm{e}^{2h} + \mathrm{e}^{4k}(\mathrm{e}^{2h}-1)^2\right], \tag{22}$$

where

$$A = \sqrt{4\mathrm{e}^{2h} + \mathrm{e}^{4k} + \mathrm{e}^{4(h+k)} - 2\mathrm{e}^{2h+4k}}, \qquad B = \mathrm{e}^{2k} + \mathrm{e}^{2(h+k)}. \tag{23}$$

Using the recursion relations for the parameters k_i, h and formula (7) one can find the thermodynamic quantities as functions of temperature or field. Figure 9 shows the field dependence of the magnetocaloric coefficient of the antiferromagnetic Ising chains coupled by weak interchain interaction $|k_1/k| = 0.3$ for several values of inverse temperature $k = -1/t$. The left plot represents the system with $k_1 > 0$ (ferromagnetic interchain interaction) and right $k_1 < 0$ (antiferromagnetic). For the highest temperature $k = -0.3$ the magnetocaloric coefficient is positive for all values of field. For $k < -0.3$ there is a range of the field for which M_{T} is negative and the point of the sign changing is shifted towards the smaller fields for decreasing temperature. The solid lines denote the curves for the temperature t $= 1/0.8$, lower than zero field critical temperature of the system $t_{\mathrm{c}} = -1/k_{\mathrm{c}} = 1/0.744$. In this case ($k = -0.8$) M_{T} diverges at $h_{\mathrm{c}} = 0.769$ for $k_1 = 0.3$ and $h_{\mathrm{c}} = 0.716$ for $k_1 = -0.3$. However, in this latter case, the LPRG transformation with three-row cluster (figure 1) does not preserve the symmetry of the original problem.

Figure 10 shows the field dependence of M_{T} for one-dimensional Heisenberg ferromagnet ($K > 0$) and antiferromagnet ($K < 0$) at several temperatures. In the ferromagnetic case M_{T} is positive

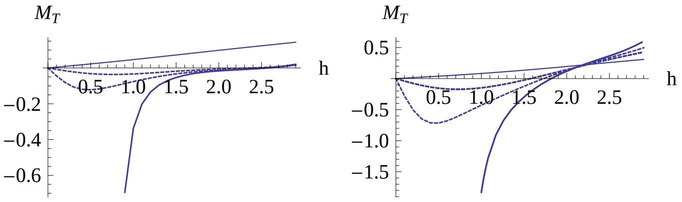

Figure 9. Field dependence of the 2D antiferromagnetic Ising coupled chains magnetocaloric coefficient with $k_1/k = -0.3$ (left plot) and $k_1/k = 0.3$ (right plot) for $k = -0.8$ (solid line), $-0.7, -0.6$ (dashed lines,), and -0.3 (thin line).

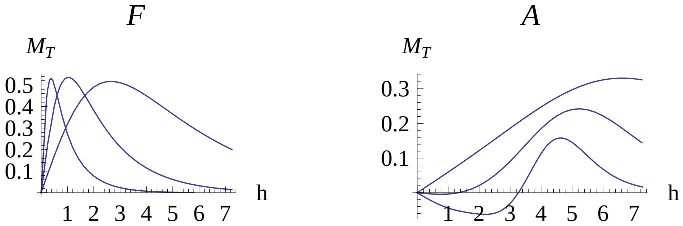

Figure 10. Field dependence of the magnetocaloric coefficient for one-dimensional Heiseneberg ferromagnet (F) for inverse temperature $1/t = 0.2, 0.4, 0.8$ from right to the left and antiferromagnet (A) for inverse temperature $1/t = 0.2, 0.4, 0.8$ from top to the bottom, respectively.

for all values of field whereas in the antiferromagnetic case for sufficiently low temperature there is a field value at which M_{T} changes the sign. In figure 11 the temperature dependences of M_{T} and correlation function $G = \langle S_i^z S_{i+1}^z \rangle$ for Heisenberg model are shown. As seen for sufficiently large fields, both quantities are positive for all values of t. For smaller fields, both quantities change sign but at different temperatures.

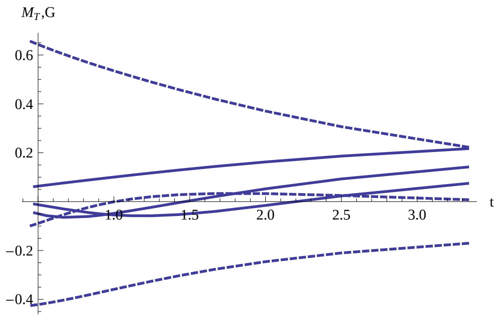

Figure 11. Temperature dependence of the magnetocaloric coefficient (solid lines) and two point correlation function (dashed lines) for one-dimensional Heiseneberg antiferromagnet for the field $h = 4, 3$, and 2 from top to the bottom, respectively.

To conclude we have shown that a simple perturbation method, LPRG, can be used to study the location of the transition temperature and the temperature or field dependence of the thermodynamic quantities of a broad class of classical and quantum systems made of weakly interacting spin chains. It has been demonstrated that even in the lowest approximation, the LPRG results are in quite good agreement with the exact ones. The conclusions to be drawn from this work are as follows. If, in the fully frustrated magnet with easy axis along “z” direction, small XY interactions are present, the finite-temperature phase transition survives even though the XY interchain interactions are also fully frustrated. However, in this case, there is not long range order along z direction any more. So, it seems that such an interaction should change the character of the phase transition from Ising-like to KT-like. It has also been shown that by using the measurements of the magnetocaloric coefficient as a function of magnetic field one can detect a change in the short-range correlation character, which is pronounced in the change of sign of M_{T}, for example, as shown above by the existence of the antiferromagnetic correlations. Generally, M_{T} is negative if there is a competition between an external field and exchange interaction.

References

1. Kopinga K., Tinus A.M.C., de Jonge W.J.M., Phys. Rev. B, 1982, **25**, 4485–4690.
2. Campana L.S., Caramico D'Auria A., Esposito U., Kamieniarz G., Phys. Rev. B, 1990, **10**, 6733–6740.
3. Orendacova A., Orendac M., Bondarenko V., Feher A., Anders A.G., J. Phys.: Condens. Matter, 1998, **10**, 1125–130.
4. Hardy V., Lambert S., Lees M.R., McK. Paul D., Phys. Rev. B, 2003, **68**, 014424-1–014424-7.
5. Lumsden M.D., Granroth G.E., Mandrus D., Nagler S.E., Thompson J.R., Castellan J.P., Gaulin B.D., Phys. Rev. B, 2000, **62**, R9244.
6. Köppen M., Lang M., Helfrich R., Steglich F., Thalmaier P., Schmidt B., Wand B., Pankert D., Benner H., Aoki H., Ochiai A., Phys. Rev. Lett., 1999, **82**, 4548.
7. Noel H., J. Less-Common Met., 1986, **121**, 265.
8. Suski W., Bull. Acad. Pol. Sci., Ser. Sci., Math., Astron. Phys., 1976, **24**, 75.
9. Sznajd J., Phys. Rev. B, 2001, **63**, 184404-1–184404-7.
10. Th. Niemeijer, Van Leeuwen J.M.J., Physica (Amsterdam), 1974, **71**, 17–40.
11. Suzuki M., Takano H., Phys. Lett. A, 1979, **69**, 426.
12. Sznajd J., Phys. Rev. B, 2008, **78**, 214411-1–214411-7.
13. Katsura S., Phys. Rev., 1962, **127**, 1508.
14. Stockert O., von Lohneysen H., Rosch A., Pyka N., Loewenhaupt M., Phys. Rev. Lett., 1998, **80**, 5627.
15. Maltseva M., Coleman P., Phys. Rev. B, 2005, **72**, 174415.
16. Sznajd J., Phys. Rev. B, 2007, **76**, 092405-1–092405-4.
17. Plackowski T., Wang Y.X., Junod A., Review of Scientific Instruments, 2002, **73**, 2755.

Термодинаміка, геометрична фрустрація та квантові флуктуації в зв'язаних спінових ланцюжках

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Сформульовано лінійно-пертурбативне ренормалізаційне перетворення у дійсному просторі (ЛПРП), що використовується для вивчення квантових спінових ланцюжків, зв'язаних міжланцюжковою взаємодією (k_1), яка є слабшою за взаємодію (k) між спінами у ланцюжку. Метод протестовано для двох точно розв'язуваних моделей: Ізингівських ланцюжків на квадратній та трикутній ґратках і квантових XY ланцюжків. Для моделі Ізинга у другому порядку кумулянтного розкладу показано, що відхилення критичної температури від точного значення є меншим 1% для $0.5k > k_1 > 0.15k$; однак навіть у випадку стандартної моделі Ізинга $(k_1 = k)$ отримано значення T_c, що відрізняється від точного на 2%. Для квантового XY ланцюжка відхилення вільної енергії, що знайдена методом ЛПРП, від точного результату Кацура не перевищує 1% для $T/J > 1$, а для доволі низької температури $T/J = 0.08$ складає біля 6%. Метод ЛПРП використовується для вивчення впливу міжланцюжкової фрустрації на фазовий перехід у двовимірних Гайзенбергівських спінових ланцюжках з віссю легкого намагнічення вздовж напрямку z. Показано, що на відміну від чисто Ізингівської моделі, у системах із планарною XY взаємодією міжланцюжкова фрустрація не порушує фазовий перехід при скінчених температурах. Однак, така фрустрація змінює характер фазових переходів від ізингівського типу до, імовірно, переходів типу Костерліца-Таулса. Ми використали також метод ЛПРП для розрахунку ізотермічного магнетокалоричного коефіцієнта (M_T) кількох спінових моделей у невпорядкованих фазах. Показано, що за наявності антиферомагнітних флуктуацій, M_T змінює свій знак при певному значенні магнітного поля. Загалом M_T – від'ємна величина, якщо магнітне поле конкурує з близьким порядком, і тому це може служити індикатором зміни короткосяжних кореляцій.

Ключові слова: *Ланцюжки Гайзенберга, ренормалізаційна група, міжланцюжкова фрустрація, магнетокалоричний ефект*

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