Renormalization of magnetic chains in a field: Isothermal magnetocaloric effect

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(Received 17 August 2008; published 8 December 2008)

Motivated by the recently developed [T. Plackowski *et al.*, Rev. Sci. Instrum. **73**, 2755 (2002)] technique for measuring isothermal magnetocaloric coefficient (M_T), we revisit the thermodynamic properties of coupled spin chains in a field. The coupled Ising antiferromagnetic chains in two and three dimensions, quantum *XY* chain in a transverse field, and Heisenberg chain are considered. For the Ising model the shift of the critical temperature under magnetic field and dependence of M_T on interchain coupling are found. The field dependence of M_T for several models is presented. It is demonstrated that in the disordered phase 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.

DOI: 10.1103/PhysRevB.78.214411 PACS number(s): 75.10.Pq, 75.10.Jm, 75.40.Cx

I. INTRODUCTION

As recently shown, the isothermal magnetocaloric effect can be a useful tool for studying vortex melting or reversible processes in superconductors[1,2] and lines of phase transitions in magnets.[3] The technique for measuring the isothermal magnetocaloric coefficient via precise measurements of the heat flux between the sample and its surrounding was presented in Ref. 1.

Isothermal magnetocaloric coefficient can be defined as

$$M_T = -T\left(\frac{\partial S}{\partial H}\right)_T = -T\left(\frac{\partial M}{\partial T}\right)_H, \qquad (1)$$

where S and M denote the entropy and magnetization along an applied external magnetic field H, respectively. With such a definition, positive M_T means that the entropy decreases with increasing field. Plackowski *et al.*[3] studied the magnetocaloric effect in $UNi_{0.5}Sb_2$ in the vicinity of the Néel temperature (T_N) with the magnetic field applied along the easy axis and found that M_T is negative for all values of temperature and applied field. Thus, in this case, the magnetic field results in an increase in the entropy in the system. They have also noted that in the high-temperature phase the magnetocaloric coefficient is small and weakly dependent on both the field and temperature, whereas close but below the transition temperature M_T shows significant field and temperature dependencies. For temperatures $T<T_N$ at some values of the field, the magnetocaloric coefficient exhibits a maximum interpreted as a phase-transition point. This maximum is shifted toward higher fields with increasing temperature, which has allowed the authors to find the critical line (phase diagram) in the plane (external field and temperature). However, M_T can be also used as an indicator of a short-range order change in a high-temperature (disordered) phase or in materials which do not undergo any finite temperature phase transitions as, for example, one-dimensional (1D) spin systems.

As seen in Fig. 1 M_T of the exactly solvable one-dimensional Ising antiferromagnet for sufficiently low temperatures changes sign at some value of the field. At very low temperature ($t=T/J=0.2$ in Fig. 1) both M_T and two-nearest-neighbor-spin correlation function G change sign close to the critical value of the field $H/J=2$. For higher temperature the point at which the magnetocaloric coefficient changes sign is shifted toward lower field values, whereas such a point for G is shifted to higher fields. For $t\geq 2$, M_T is positive for all values of the field. It means that for the 1D Ising model with the antiferromagnetic interactions for $t<2$, the entropy first increases with increasing field and then decreases, starting with some characteristic value of the field. Of course in the case of the ferromagnetic interaction M_T is always positive (Fig. 1, right bottom plot).

In this paper the magnetocaloric coefficient is studied by using the linear perturbation renormalization-group (LPRG) transformation[4] for three spin models: (i) Ising weakly coupled antiferromagnetic chains in two and three dimensions at the presence of an external magnetic field, (ii) *XY* chain in a transverse field, and (iii) Heisenberg chain in a field. Generally, these models are described by the following Hamiltonian:

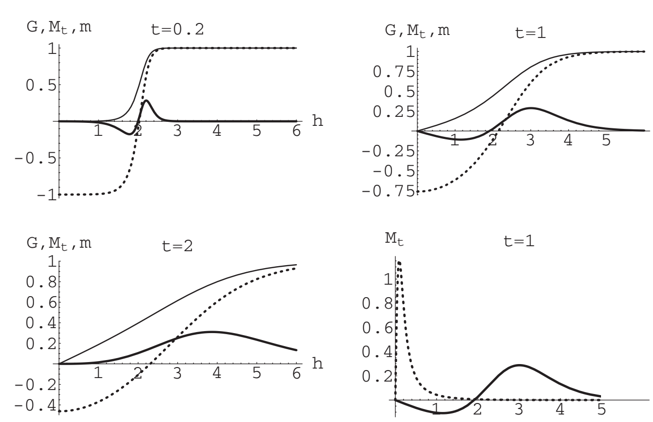

FIG. 1. Correlation function G (dashed line), magnetocaloric coefficient M_t (solid), and magnetization m (thin) as functions of field for several values of reduced temperature for 1D antiferromagnetic Ising model. The bottom right figure compares the 1D Ising model with ferromagnetic (dashed line) and antiferromagnetic (solid) interactions.

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\mathcal{I}}, \tag{2}$$

where $\mathcal{H}_0$ describes spin chains with intrachain interaction $J^\alpha = -K^\alpha T$ in an external magnetic field $H = hT$,

$$\mathcal{H}_0 = \sum_{\alpha=x,y,z} K^\alpha \sum_{k=1}^{L} \sum_{j=1}^{M} \sum_{i=1}^{N} S_{i,j,k}^\alpha S_{i+1,j,k}^\alpha + h \sum_{i=1}^{NML} S_{i,j,k}^z, \tag{3}$$

coupled by weaker interchain interactions ($J_1^\alpha = -K_1^\alpha T$ and $J_2^\alpha = -K_2^\alpha T$),

$$\mathcal{H}_I = \sum_{\alpha=x,y,z} K_1^\alpha \left(\sum_{i,j} S_{i,j,k}^\alpha S_{i,j+1,k}^\alpha + \sum_{i,k} S_{i,j,k}^\alpha S_{i,j,k+1}^\alpha \right) + \sum_{\alpha=x,y,z} K_2^\alpha \left(\sum_{i,j} S_{i,j,k}^\alpha S_{i+1,j+1,k}^\alpha + \sum_{i,k} S_{i,j,k}^\alpha S_{i+1,j,k+1}^\alpha \right), \tag{4}$$

where S_i^α represents a spin 1/2 and the factor $-1/T$ has already been absorbed in the Hamiltonian.

The LPRG approach starts with the exact decimation for one-dimensional Ising or approximate decimation for one-dimensional quantum spin systems.[5] Then, on the basis of it, the interchain interaction is renormalized in a perturbative way. The renormalization-group (RG) transformation for the Hamiltonian $\mathcal{H}$ is defined as usual by

$$\exp[\mathcal{H}'(\vec{\sigma})] = \mathrm{Tr}_{\vec{S}}\, P(\vec{S},\vec{\sigma}) \exp[\mathcal{H}(\vec{S})]. \tag{5}$$

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. It means that the projector of the system is defined as a product of the individual spin projectors,

$$P(\vec{S},\vec{\sigma}) = \prod_{i=0}^{N} p(\vec{S},\vec{\sigma}), \quad p_i = \frac{1}{2}\left(1 + 4 \sum_{\alpha=x,y,z} S_{mi}^\alpha \sigma_i^\alpha \right). \tag{6}$$

In this paper, the chain is divided into $(m+1)$-spin blocks and in each renormalization step, every $(m+1)$ spin survives. Transformation (5) can be written in the form

$$\mathcal{H}'(\vec{\sigma}) = \mathcal{H}_0' + \ln\langle e^{\mathcal{H}_I(\vec{S})} \rangle, \tag{7}$$

with standard cumulant expansion[6] for $\langle e^{\mathcal{H}_I(\vec{S})} \rangle$ and

$$\langle A \rangle \equiv \frac{\mathrm{Tr}_S\, A P(S,\sigma) e^{\mathcal{H}_0(S)}}{\mathrm{Tr}_S\, P(S,\sigma) e^{\mathcal{H}_0(S)}}. \tag{8}$$

The rest of the paper is organized as follows. In Sec. II transformation (5) is used to find the critical temperature and magnetocaloric coefficients as functions of interchain interactions and external magnetic field of the systems made of the weakly interacting Ising spin chains in two dimensions and three dimensions. In Sec. III the LPRG is applied to study M_T and two-point correlation function $G = \langle S_i^z S_{i+1}^z \rangle$ of the XY chain in the transverse field, and in Sec. IV the Heisenberg antiferromagnet chains in a field are considered. Concluding remarks are made in Sec. V.

II. WEAKLY INTERACTING ISING CHAINS

The 1D Ising model is described by Hamiltonian (3) with $K^x = 0$, $K^y = 0$, and $K^z = k$, where $k = J^z/T = t^{-1}$ denotes the reduced inverse temperature (in numerical calculation we will always assume $J = \max\{J^\alpha\} = 1$). The effective Hamiltonian of such a chain $\mathcal{H}_0'$ and all averages necessary to evaluate cumulants can be, of course, found exactly for an arbitrary size of the spin block. However, in order to consider the Ising chains in higher dimensions we have to confine ourselves to some reasonable size of the spin cluster and in consequence rather small block. In our previous paper[7] we used the four-spin block which is the smallest nontrivial block appropriate to analyze an antiferromagnetic chain. The idea of the LPRG in two dimensions is presented in Fig. 2. The open circles represent the spins which survive in the decimation procedure. In each step of the renormalization-group transformation every other row ("even" row) is removed, and from "odd" rows every third spin survives. As usual, we are looking for the renormalized interactions

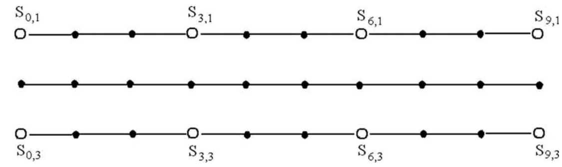

FIG. 2. The cluster used to get renormalized Hamiltonian of the coupled Ising chains in two dimensions. Open circles denote effective spins.

$$h'\sigma_{i,j}, \quad k'\sigma_{1,1}\sigma_{2,1}, \quad k_1'\sigma_{1,1}\sigma_{1,3}, \quad k_2'\sigma_{1,1}\sigma_{2,3}. \tag{9}$$

It is easy to find that

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

and

$$\langle S_{3i+1,j} \rangle = w_0 + w_1 \sigma_{i,j} + w_2 \sigma_{i+1,j} + w_{12} \sigma_{i,j} \sigma_{i+1,j},$$

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

where i is the number of the spins in the chain, j is the number of rows, and w_i are exactly known functions of the intrachain interaction k and external field h (see the Appendix). In the lowest nontrivial order of the cumulant expansion which in our case is the second order, one should consider the contributions to the effective Hamiltonian from

$$\langle H_I(S) \rangle + \frac{1}{2}\{\langle [H_I(S)]^2 \rangle - \langle H_I(S) \rangle^2\}, \tag{12}$$

where

$$[H_I(S)]^2 = \sum_i [(V_{j,j+1})^2 + 2V_{j,j+1}V_{j+1,j+2}], \tag{13}$$

and $V_{j,j+1}$ describes the interaction between j and $j+1$ rows. The first term in Eq. (13) contributes, of course, only to the intrachain interaction $h'\sigma_{i,j}$ and $k'\sigma_{i,j}\sigma_{i+1,j}$, and second to the interchain interaction $k_1'\sigma_{i,j}\sigma_{i,j+2}$ and $k_1'\sigma_{i,j}\sigma_{i+1,j+2}$. As seen from Eq. (10) contributions to interaction (9) 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 Fig. 2, do not contribute to interaction (9) because they involve other effective spins,

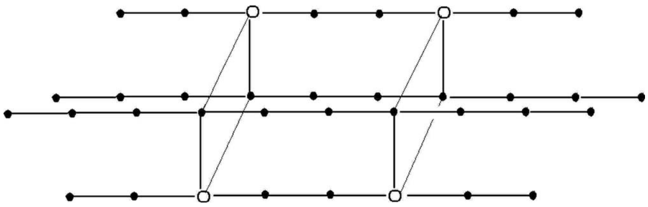

FIG. 3. The cluster used to renormalize coupled Ising chains in three dimensions. Open circles denote effective spins.

$\sigma_{0,1}$ and $\sigma_{3,1}$, respectively. So, similarly as in Ref. 6 in order to consider the interchain interactions we can use the cluster (8-10-8). However, the contributions to the effective intrachain interactions in row j ($h'\sigma_{i,j}$ and $k'\sigma_{i,j}\sigma_{i+1,j}$) come not only from the coupling $V_{j,j+1}$ but also from $V_{j-1,j}$, which we have not considered in our previous paper. Taking into account these additional contributions slightly improves the results. For example, for the standard Ising model on the square lattice ($k_1=k$ and $k_2=0$), we have found here the critical inverse temperature $k_c=0.45$ and previously[4] $k_c=0.41$ which should be compared with the exact result $k_c=0.4407$. Figure 3 shows the cluster used to consider the system of the coupled chains in three dimensions. Also, in this case we take into considerations the contributions to the intrachain interactions from all nearest-neighbor rows of a given row.

To evaluate transformation (7) in both cases [two-dimensional (2D) and three-dimensional (3D)] 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 the Ising model all of these averages are known exactly, and for the spins from removed even rows (see, for example, Ref. 8),

$$\langle s_i^z\rangle = \frac{\sinh h}{\sqrt{\cosh^2 h + e^{-4k} - 1}}, \quad \langle s_i^z s_{i+n}^z\rangle = G_z^n, \tag{14}$$

where

$$G_z = \frac{1}{A^2}\left[\frac{4(B-A)}{B+A}e^{2h} + e^{4k}(e^{2h}-1)^2\right] \tag{15}$$

and

$$A = \sqrt{4e^{2h} + e^{4k} + e^{4(h+k)} - 2e^{2h+4k}}, \quad B = e^{2k} + e^{2(h+k)}, \tag{16}$$

whereas for decimated odd rows with four-spin block the averages of several spins have been presented above [Eqs. (10) and (11)] and for the two spin products they are given by

$$\langle S_{3i,j}S_{3i+1,j}\rangle = w_1 + w_0\sigma_{i,j} + w_{12}\sigma_{i+1,j} + w_2\sigma_{i,j}\sigma_{i+1,j},$$

$$\langle S_{3i,j}S_{3i+2,j}\rangle = w_2 + w_0\sigma_{i,j} + w_{12}\sigma_{i+1,j} + w_1\sigma_{i,j}\sigma_{i+1,j},$$

$$\langle S_{3i+1,j}S_{3i+3,j}\rangle = w_2 + w_{12}\sigma_{i,j} + w_0\sigma_{i+1,j} + w_1\sigma_{i,j}\sigma_{i+1,j},$$

$$\langle S_{3i+2,j}S_{3i+3,j}\rangle = w_1 + w_{12}\sigma_{i,j} + w_0\sigma_{i+1,j} + w_2\sigma_{i,j}\sigma_{i+1,j},$$

$$\langle S_{3i+1,j}S_{3i+2,j}\rangle = q_0 + q_1(\sigma_1+\sigma_2) + q_{12}\sigma_1\sigma_2,$$

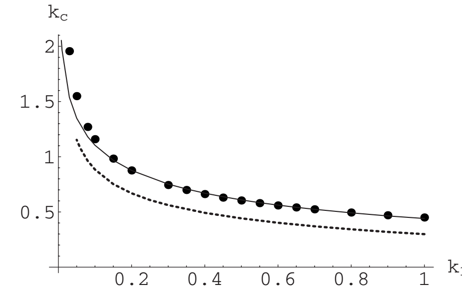

FIG. 4. Critical inverse temperature (k_c) of the Ising model as a function of interchain interaction (k_1); 2D (dots—LPRG; thin line—exact result) and 3D (dashed line—LPRG).

$$\langle S_{3i,j}S_{3i+3,j}\rangle = \sigma_{i,j}\sigma_{i+1,j}, \tag{17}$$

where w_i and q_i are presented in the Appendix.

Now we are able to evaluate numerically the renormalization transformation (7). In the second order in the cumulant expansion with clusters presented in Figs. 2 and 3 for 2D and 3D systems, respectively, the RG transformation has a form of the four recursion relations for four parameters, intrachain interaction $k=K^z$, interchain interactions (transverse $k_1=K_1^z/K_z$ and diagonal $k_2=K_2^z/K_z$), and magnetic field h. As usual, 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 $k_\alpha=\infty$ and infinite temperature $k_\alpha=0$. Figure 4 shows the critical inverse temperature as a function of the interchain interaction k_1 for $k_2=0$ in the absence of applied field. In 2D case as mentioned in our previous paper[4] the LPRG in the lowest nontrivial approximation gives, even for $k_1=k$ (standard Ising model), quite reasonable agreement with the exact result. The values of the inverse critical temperature found by using LPRG with cluster (8-10-8) for several values of the interchain interactions are listed in Table I. As seen for the interchain interaction $0.5>k_1>0.15$ the deviation from the exact values is less than 1% and for $1>k_1>0.15$ it is less than 2%. 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. For the system of the Ising chains in three dimensions in the lowest approximation, the LPRG leads to the critical inverse temperature $k_c=0.299$ for the standard Ising model with $k_1=k$ and $k_2=0$ which is rather far from the best estimation k_c

TABLE I. Critical inverse temperature of the Ising chains coupled by interchain interaction k_1 in two dimensions.

k_1	k_c (LPRG)	k_c (exact)	Error (%)
1	0.45	0.4407	2.1
0.5	0.604	0.609	0.8
0.2	0.876	0.876	0.0
0.15	0.983	0.968	0.8
0.1	1.159	1.104	5.0
0.05	1.549	1.349	14.8

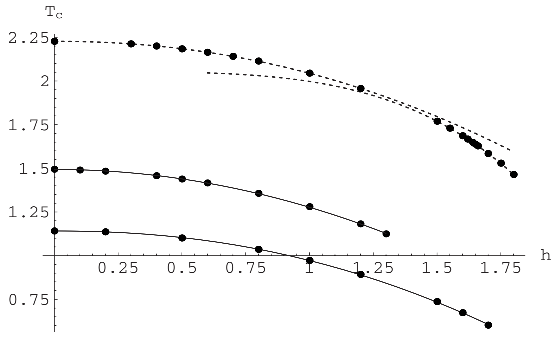

FIG. 5. Critical temperature as a function of field; top dots $k_1=k$ for 2D Ising antiferromagnet (dashed lines denote $T_c=2.2-0.18h^{2.1}$ and $T_c=2.0-0.06h^4$); bold lines $k_1=0.2k$ (bottom for 2D $T_c=1.1-0.17h^{2.2}$ and upper for 3D $T_c=1.5-0.22h^2$ Ising antiferromagnets).

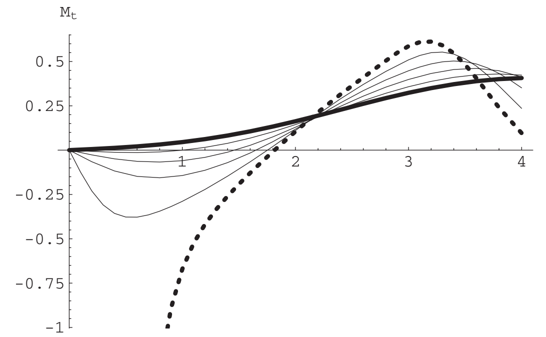

FIG. 6. Field dependence of the 2D Ising coupled chains magnetocaloric coefficient with $k_1/k=0.2$ for $k=0.9$ (dashed line), 0.8, 0.7, 0.6, 0.5 (thin lines, from bottom to the top), and 0.4 (solid line).

=0.21. Of course one expects that for the weaker interchain interaction the method should work better; unfortunately we have not found any results to be compared. The approximation can be improved by taking into account the higher orders in the cumulant expansion and by increasing the used cluster.

In zero magnetic field the critical temperature of the antiferromagnetic transition $(k<0)$ is identical to that of a ferromagnet $(k>0)$. Hereafter, in this section we will focus our attention on the Ising antiferromagnetic chains with the original intrachain interaction $k<0$ coupled by ferromagnetic interchain interaction $k_1=-\delta k$ with $\delta=1$ and 0.2 $(k_2=0)$ in the longitudinal field. In the presence of the longitudinal external field the antiferromagnetic phase transition of the Ising model in opposition to the ferromagnetic one survives, and the critical temperature is shifted to the lower temperature with increasing field. This shift is presented in Fig. 5 for $\delta=1$ in two dimensions and $\delta=0.2$ in two dimensions and three dimensions. For the chains coupled by the weak interchain interaction $\delta=0.2$ in both cases, 2D and 3D, the critical temperature is shifted according to the power law

$$t_c - t_c(h) \propto h^{\omega}, \tag{18}$$

with ω close to 2 (2 for 3D system and 2.2 for 2D one). For the field small enough the similar behavior is observed also for the model with $\delta=1$ in two dimensions. In the latter case for higher fields the results can be satisfactorily fitted to the power law with ω close to 4.

As usual except for the effective spin-dependent terms, the renormalized Hamiltonian $\mathcal{H}'(\sigma)$ contains also a constant term $F(k_i,h)$ which can be used to calculate numerically the free energy per spin according to the formula

$$f = \sum_{n=1}^{\infty} \frac{F(k_i^{(n)},h^{(n)})}{3^n}. \tag{19}$$

Using the recursion relations for the parameters k_i and h and formula (19) one can find the thermodynamic quantities of the model under consideration. Figure 6 shows the field dependence of the magnetocaloric coefficient of the antiferromagnetic Ising chains coupled by weak interchain interaction $\delta=0.2$ for several values of inverse temperature k. For the highest temperature $k=0.4$ $(t=2.5)$ the magnetocaloric coefficient is positive for all values of field. For $k>0.4$ there is a range of the field for which M_T is negative, and the point of the sign changing is shifted toward the smaller fields for decreasing temperature. The dashed line denotes the curve for the temperature $t=1/0.9$, lower than zero-field critical temperature of the system $t_c=1/k_c=1/0.876$ (Table I). In this case $(k=0.9)$ M_T diverges at $h_c=0.443$. So, similarly as in one-dimensional case if only the temperature and field are small enough M_T is negative in the higher-temperature (disordered) phase of the Ising antiferromagnet.

III. *XY* CHAIN IN TRANSVERSE FIELD

Below in this section, we consider a one-dimensional quantum spin *XY* model with $K^x=K^y$, where $K^z=0$ in a transverse field. For a quantum system, because of the noncummutavity of several terms of Hamiltonian (2) the decimation transformation cannot be carried out exactly and we apply the approximate decimation proposed by Suzuki and Takano.[5] The Suzuki-Takano procedure takes quantum effect into account within a single block and neglects the effect of noncommutativity of several blocks. Thus, in opposition to the Ising case the results depend on the division of the chain into blocks, i.e., on the size of the block. In our previous paper[7] we used the smallest nontrivial for the antiferromagnetic chain block size $m=3$ (four spin in a block). In the present paper we extend our study to larger blocks, six and eight spins. In Fig. 7 and Table II the results of the linear renormalization group (LRG) for the zero-field *XY* chain free energy obtained by using four-, six-, and eight-spin blocks are compared with the exact results found by Katsura.[9] 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 eight-spin block is about 6%, and for $t=1$ it is about 1%. So, for sufficiently high-temperature LRG should lead to reasonable results also for the quantum models.

Applying transformation (7) to Hamiltonian (3) with $K^x=K^y=K>0$, $K^z=0$, one obtains the transformed Hamiltonian

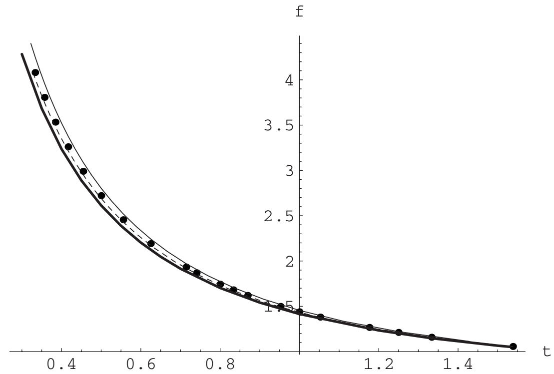

FIG. 7. Temperature dependence of the one-dimensional *XY* model free energy found by using the four-spin (thin line), six-spin (dotted line), and eight-spin (dashed line) blocks. The solid line denotes the exact result found by Katsura (Ref. 9).

for the effective spin operators σ^{α} with effective parameters K' and h', and as usually generated by the transformation interaction parameter $(K^z)'$. Using the recursion relations for these three parameters obtained with eight-spin block, and the formula for free energy (19), we find the field and temperature dependences of the magnetocaloric coefficient (M_T) and two-point longitudinal correlation function (G),

$$G = \langle S_i^z S_{i+1}^z \rangle. \tag{20}$$

Figure 8 shows the field dependence of M_T for several values of the inverse critical temperature $K=1/t$. For temperatures small enough $1/t=1.25$ and 0.8 there is a region of the field where M_T is negative which points to the existence of out-of-plane antiferromagnetic correlations. Of course for the *XY* model the existence of such correlations does not depend on the sign of the in-plane interaction (K). In Figs. 9 and 10 the temperature dependences of the correlation function G and M_T for several values of the field are presented. For $h<2$ correlation function is negative for the sufficiently low temperature, whereas for $h>2$ it tends to the saturation value $G=1$. This behavior is a symptom of the zero-temperature phase transition between the critical state and the state with the spins directed along the field, perpendicularly to the plane *XY*. The same behavior can be observed for M_T which can be easily measured by using the method mentioned above. As seen in Fig. 10 for $h<2$, M_T changes sign at some value of temperature, whereas for $h>2$, M_T is positive for all values of temperature.

TABLE II. Free energy of the quantum *XY* model for several values of temperature found by using four-, six-, and eight-spin clusters and exact result.

t	$f_{4\text{-site}}$	$f_{6\text{-site}}$	$f_{8\text{-site}}$	f_{exact} (Ref. 9)
0.08	18.4	17.33	16.9	15.93
0.278	5.14	4.908	4.818	4.62
1.05	1.394	1.381	1.375	1.36
1.333	1.166	1.158	1.155	1.148
2.5	0.844	0.843	0.843	0.842
4.0	0.754	0.754	0.754	0.754

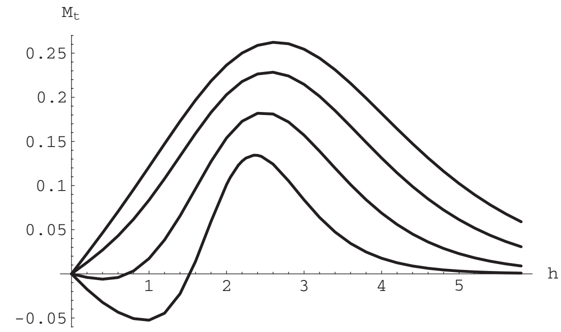

FIG. 8. Field dependence of the magnetocaloric coefficient of the 1D *XY* model in a transverse field for inverse temperature $1/t=0.5$, 0.6, 0.8, and 1.25 from top to the bottom.

IV. HEISENBERG ANTIFERROMAGNETIC CHAIN IN FIELD

In this section we shall apply linear RG transformation (7) with weight operator (6) and $m=7$ (eight-spin cluster) to study Heisenberg chain (3) $(K^x=K^y=K^z=K)$ in the magnetic field. Figure 11 shows the field dependence of M_T for ferromagnetic $(K>0)$ and antiferromagnetic $(K<0)$ interactions at several temperatures $t=K^{-1}$. In the ferromagnetic case M_T has a maximum at some characteristic value of the field h_{max} and linearly tends to zero as $h\to 0$. For increasing temperature from $t=1$ to $t=3.3$ the height of this maximum is almost constant but the location is shifted toward higher field values according to the power law $h_{\text{max}}\propto t^{3/2}$ (Fig. 12). In the antiferromagnetic case for sufficiently low temperature there is a field value at which M_T changes sign and then shows a maximum. Similarly as for the ferromagnet this maximum is shifted toward higher fields with increasing temperature. However, in this case the maximum height grows with temperature and the shift can be fitted to the law $h_{\text{max}}-h_0\propto t^{5/4}$ (Fig. 12).

The magnetocaloric coefficient M_T is measured at constant temperature but its temperature dependence at constant field can yield some hint about the short-range order and zero-temperature phase transition in systems without finite temperature long-range order. In Fig. 13 the results for M_T

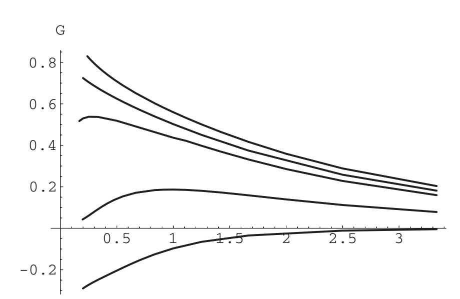

FIG. 9. *XY* model. Temperature dependence of G for several values of the field $h=1.0$, 1.5, 1.9, 2.0, and 2.1 from bottom to the top.

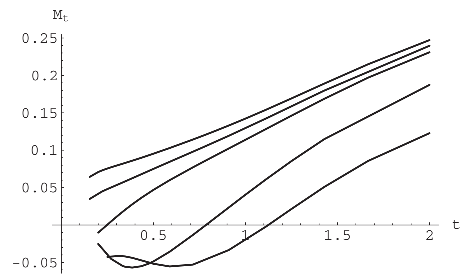

FIG. 10. *XY* model. Temperature dependence of M_t for several values of the field $h=1.0$, 1.5, 1.9, 2.0, and 2.1 at $t=1$ from bottom to the top.

are shown for various magnetic fields below as well as above the saturation field $h_c=4$. For low fields (0.5 and 1 in Fig. 13) M_T is negative and then for sufficiently high temperature it is positive, which means that magnetization first increases with increasing temperature and then decreases. For the field strong enough above the saturation field $h \geq h_c$ (4 and 5 in Fig. 13) the magnetization decreases with increasing temperature. For intermediate values of the field M_T changes sign twice. Because the method used in this paper is the high-temperature approximation we were not able to find accurately the range of the field. The origin of this behavior is the competition between the applied magnetic field and antiferromagnetic interactions and can be explained in the same way as a two-peak structure of the specific heat observed for the system under consideration.[10]

V. CONCLUSION

The linear real-space renormalization-group transformation has been used to calculate the isothermal magnetocaloric coefficient for three spin systems. We start with the weakly coupled Ising chains in two and three dimensions. In this paper the LPRG method[4] has been improved by taking into account all contributions from the nearest-neighbor rows to the nearest and next-nearest effective interchain interactions, whereas in our previous papers we confined ourselves to the smallest nontrivial cluster. The LPRG transformation is obtained by two approximations: (i) the abbreviation of the cumulant expansion which is reasonable if the intrachain interaction is weaker than interchain one ($k_1 < k$) and (ii) the truncation of the interchain interaction generated by transformation (7). Usually, in the higher-order calculation the RG transformation generates different interactions. In our case

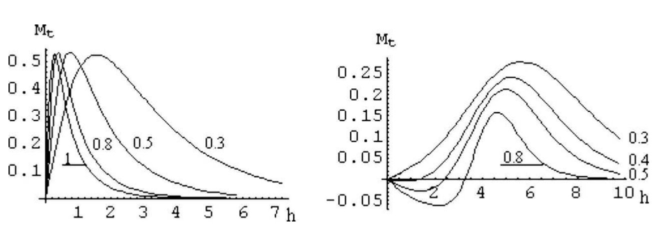

FIG. 11. Field dependence of the magnetocaloric coefficient for one-dimensional Heisenberg ferromagnet for inverse temperature $1/t=0.3$, 0.5, 0.8, and 1.0 from right to the left, and antiferromagnet for $1/t=0.3$, 0.4, 0.5, and 0.8 from top to the bottom, respectively.

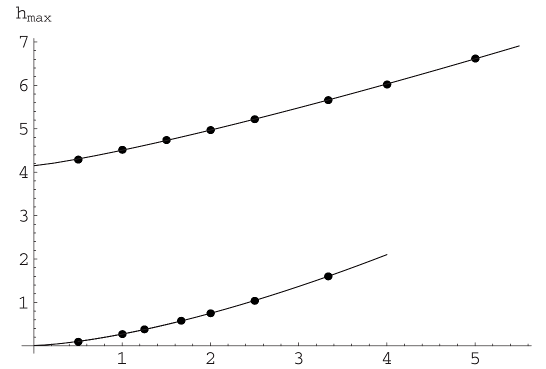

FIG. 12. The characteristic field of the magnetocaloric coefficient maximum as a function of temperature for Heisenberg ferromagnet—the bottom solid curve denotes $h_{max}=0.26t^{3/2}$—and antiferromagnet—the upper solid curve denotes $h_{max}=4.15 + 0.36t^{5/4}$.

the number of these different interactions already in the second-order cumulant expansion is infinite for an infinite system. Thus, in order to carry out the LPRG transformation we have to confine ourselves to a finite cluster which is justified if only the temperature is not too low. So, the LPRG method can be used for a weak interchain interaction but not too weak because in the latter case the critical temperature is shifted to very low temperatures. In the range of the approximation validity ($0.5k > k_1 > 0.15k$ in Table I) the results for T_c differs by less than 1% from the exact value. However, even in the case of the standard Ising model where the interchain interaction is equal to the intrachain one, we have found the value for the inverse critical temperature $k_c \approx 0.45$ which differs by 2% from the exact one; in the previous paper this difference was about 7%. The LPRG method has been also used to study the critical temperature of the weakly interacting Ising chains system in three dimensions. In this case the value of the inverse critical temperature $k_c \approx 0.299$ found for the standard Ising model ($k_1 = k$) is not satisfactory in comparison with the best estimate $k_c \approx 0.21$. Of course, one expects that the result should be better for the weakly interacting chains where the present approximation is valid, but it also seems that for the system in three dimensions one should consider a bigger cluster and the higher cumulant expansion.

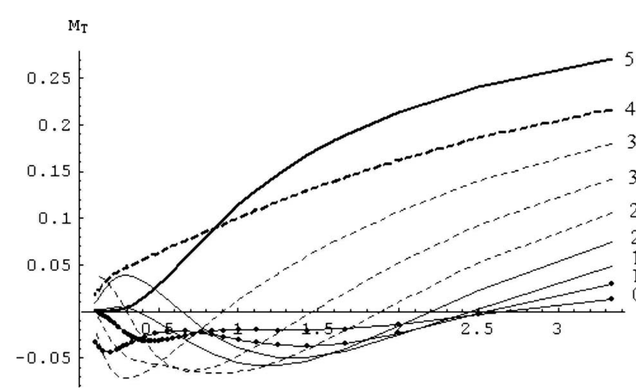

FIG. 13. Heisenberg model. Temperature dependence of M_t for several values of field $h=0.5-5.0$.

For a quantum system, because of the noncommutativity of several terms of Hamiltonian (3), the renormalization transformation cannot be carried out exactly even for a 1D lattice and in zero magnetic field. Thus, in opposition to the classical Ising model even in one dimension, one has to make some approximation to obtain the explicit form of the RG transformation. The simplest approximation is based on the Suzuki-Takano idea[5] of finding the chain averages considering only a few spin blocks. It means that the results of the decimation depend on the one-dimensional block size. We have compared the temperature dependence of the quantum XY model free energy found by using four-, six-, and eight-spin blocks with that obtained rigorously by Katsura.[9] As one expects for sufficiently high temperatures $t>2.5$ (Table II) independent of the block size, the LRG leads to the correct values of the free energy. However, for lower temperature the results depend on the block size and, for example, for $t=4/3$ the free-energy value found with eight-spin block differs from the exact value by 0.6%, whereas that found with four-spin block differs by 1.6%. The deviation is of course much larger for low temperatures, and the free energy at $t=0.278$ differs from the exact value by 4% and 11% for eight- and four-spin blocks, respectively. So, it should be noted here that the used approximation is high-temperature approximation especially in the case of the quantum spin models.

Finally, we have calculated the isothermal magnetocaloric coefficient M_T for several spin models in disordered phases—paramagnetic phase of the coupled Ising chains in two dimensions and three dimensions, and $s=1/2$ quantum spin chains. For the system with ferromagnetic coupling in a longitudinal field, M_T is always positive because the field supports the ferromagnetic interaction. It means that such a system under the field becomes more ordered and consequently the entropy decreases with increasing field. For the system with antiferromagnetic coupling in the longitudinal field, there is a region of field values for which M_T is negative and the entropy increases with increasing field. In the latter case there is a competition between the antiferromagnetic coupling and applied field, and as a result of this the system becomes less ordered. Of course for the field strong enough M_T changes sign and the entropy decreases with increasing field. The similar behavior is observed for the XY model in a transverse field. In this case the field plays again out-of-plane antiferromagnetic correlations existing in such a system.

It was shown[2,3] that M_T is a very useful tool, complementary to the specific heat C_H, for studying thermodynamic properties of superconductors and magnets mainly in the ordered phase. The authors have paid attention to significant advantage of M_T over C_H, the absence of phonon contribution, which usually dominates specific heat close to critical temperature. Thus, one can conclude that, in some cases, in order to find a phase diagram, it is better to resort to the measurements of magnetocaloric effect than specific heat. The calculations of M_T for the simple spin systems presented in this paper have shown that precise measurements of the magnetocaloric effect in a disordered phase can give some additional insight into properties of the system. First, by using the measurements of M_T as a function of magnetic field, one can detect a change in the short-range correlation character, which is pronounced in the changing of sign of M_T, for example, as shown above the existence of the antiferromagnetic correlations. Generally, M_T is negative if there is a competition between an external field and exchange interactions. Second, from $M_T(T)$ curves taken for several values of the field the existence of a zero-temperature phase transition can be deduced. As shown in Figs. 10 and 13 it is easy to see the changes in the shape of these curves at the critical values of the field: for the XY model in transverse field at $h_c=2$ and for Heisenberg antiferromagnet at $h_c=4$.

ACKNOWLEDGMENT

The author acknowledges valuable discussions with T. Plackowski.

APPENDIX

In this appendix we present coefficients w_i and q_i [Eqs. (11) and (15)] as functions of intrachain interaction k and magnetic field h,

$$w_0=\frac{1}{2R}(e^{4h}-1)(e^{4h}+2e^{8h}+7e^{4(h+k)}+2e^{8(h+k)}+e^{4(h+3k)}+4e^{2h+4k}+4e^{6h+4k}+4e^{2h+8k}+3e^{4h+8k}+4e^{6h+8k}),$$

$$w_1=\frac{1}{2R}e^{2h}(1+e^{2h})^2(e^{4k}-1)(3e^{2h}+2e^{4k}+2e^{4(h+k)}+e^{2h+8k}),$$

$$w_2=\frac{1}{2R}e^{4h}(e^{4k}-1)^2(1+4e^{2h}+e^{4h}+e^{4k}+e^{4(h+k)}),$$

$$w_{12}=\frac{1}{2R}e^{4h}(e^{4k}-1)(e^{4k}-1)^3, \tag{A1}$$

and

$$q_0=\frac{1}{R}(e^{4(h+3k)}+e^{2h+4k}-2e^{6h+4k}-e^{8h+4k}-e^{4h}-4e^{6h}-e^{8h}-e^{4(h+k)}+e^{10h+4k}+e^{2h+8k}+e^{6h+8k}+e^{10h+8k}+e^{12h+8k}+e^{8h+12k}),$$

$$q_1=\frac{e^{2h}(e^{4h}-1)(e^{4k}-1)}{(2e^{2h}+e^{4h}+e^{4k})(1+2e^{2h}+e^{4(h+k)})},$$

$$q_{12}=\frac{1}{R}e^{4h}(e^{4k}-1)^2(1+e^{2h}+e^{4h}+e^{2h+4k}), \tag{A2}$$

where

$$R=(2e^{2h}+e^{4h}+e^{4k})(1+2e^{2h}+e^{4(h+k)})(e^{2h}+e^{4k}+e^{4(h+k)}+e^{2h+4k}). \tag{A3}$$

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