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On the critical temperature of a quasi-one-dimensional Ising model

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Abstract. Within the framework of a phenomenological renormalization group theory, the calculation of the critical temperature of the three-dimensional spatially anisotropic Ising model is carried out. In the calculation, clusters $n \times n \times \infty$ with $n = 1, 2, 3$ and 4 are used. The results are applied to estimate the reduced values of the interchain interactions in quasi-one-dimensional Ising magnets.

1. Introduction

In the present paper we shall consider a three-dimensional spin-$\frac{1}{2}$ Ising model on a simple cubic lattice with the coupling constant J along one spatial direction and with J' along the other two directions, with the assumption that the magnitude of $J' \leqslant J$. At present, the critical point of this model with fully isotropic interactions ($J' = J$) is known with great accuracy [1–3]: $kT_c/J = 2.25574 \pm 0.00007$ (the percentage error is 0.003%). Another state to be considered is the anisotropic case. Calculations available here can be divided into two groups. On the one hand, there are calculations within the framework of the high-temperature series expansions ([4], and references therein), simulations by the Monte Carlo method on stretched finite parallelepipeds $n \times n \times n'$ ($n' \geqslant n$) with subsequent extrapolation of results to the infinite system by a finite size scaling scheme [5] and calculations by the real-space renormalization group method [6]. These approaches work increasingly poorly the higher the anisotropy of the system. Thus, owing to the small number of terms in the high-temperature series, the results for kT_c/J given in [4] are restricted to $J'/J \geqslant 0.01$; because of the rather small stretch of the parallelepipeds ($n'/n \leqslant 6$) the estimates obtained in [5] for the temperature of a phase transition have a considerable error when $J'/J < 0.1$ and the renormalization group values [6] have been found only for $J'/J \geqslant 0.1$. On the other hand, there are calculations of the critical temperature based on the mean-field theory: the linear Ising chain in a mean field (here the intrachain interactions are taken exactly and the interchain interactions approximately) [7], the double Ising chain in the analogous field (part of interchain interactions is described rigorously) [8] and finally the extended Bethe–Peierls approximation (EBPA) when a cluster of the central chain and the four chains nearest to it is placed in a molecular field [9]. These approaches, unlike the previous ones, lead to satisfactory results only for high anisotropy of interaction.

The phenomenological renormalization group method [10, 11] combining the finite size scaling ideas and the transfer matrix technique is a powerful tool in investigating

phase transitions of various systems. Within this method, the critical temperature estimation is obtained from the renormalization group equation

$$(1/n)\xi_n(T_c^{(n)}) = [1/(n+1)]\xi_{n+1}(T_c^{(n)}) \tag{1}$$

connecting the correlation lengths of two clusters with transverse sizes n and $n+1$ (the pair $(n, n+1)$), with the correlation length itself being defined by the relation

$$\xi_n = 1/\ln(\lambda_1^{(n)}/\lambda_2^{(n)}) \tag{2}$$

where $\lambda_1^{(n)}$ and $\lambda_2^{(n)}$ are the largest and second-largest eigenvalues of the transfer matrix of the subsystem correspondingly. Even if three terms in the sequence $\{T_c^{(n)}\}$ are known, its relatively slow convergence can be, generally speaking, accelerated by using mathematical methods for extrapolation. One of the best ways to do this is the alternating ε-algorithm [11] for the first step of which the original sequence $\{a_l\}$ is transformed into the new sequence by the formula

$$a_l^{(1)} = (a_{l-1}a_{l+1} - a_l^2)/(a_{l-1} + a_{l+1} - 2a_l). \tag{3}$$

In this paper we apply the phenomenological renormalization group method to the Ising model under discussion. As partially finite subsystems, we choose clusters $n \times n \times \infty$ in the direction with a coupling J, we estimate the critical temperature for transverse sizes of clusters up to $n = 4$ and then from three points we extrapolate from equation (3) for each value J'/J. We use the theoretical results obtained to determine the magnitude (without consideration of the sign) J'/J in the Ising magnets $MCl_2 \cdot 2NC_5H_5$ where M = Co, Fe.

2. Calculation of the critical temperature

The correlation length in the linear Ising chain ($n = 1$) is given as

$$\xi_1(T) = 1/\ln[\coth(J/2kT)]. \tag{4}$$

Further, a cluster $2 \times 2 \times \infty$ belongs to the two-dimensional Ising models on a cylinder for which the eigenvalues of the transfer matrix are known in analytical form for any number of chains [12]. In the case when four chains form the cluster under consideration, the dominant eigenvalues are equal to

$$\begin{aligned}\lambda_1^{(2)} = {} & [\![2\cosh(2K)\cosh(4K') + \sqrt{2}\sinh(4K') + \{[2\cosh(2K)\cosh(4K') \\ & + \sqrt{2}\sinh(4K')]^2 - 4\sinh^2(2K)\}^{1/2}]\![2\cosh(2K)\cosh(4K') \\ & - \sqrt{2}\sinh(4K') + \{[2\cosh(2K)\cosh(4K') - \sqrt{2}\sinh(4K')]^2 \\ & - 4\sinh^2(2K)\}^{1/2}]\!]\end{aligned} \tag{5}$$

and

$$\begin{aligned}\lambda_2^{(2)} = {} & 4\sinh(2K)[\![\cosh(2K)\cosh(4K') \\ & + \{[\cosh(2K)\sinh(4K')]^2 + 1\}^{1/2}]\!]\exp(4K')\end{aligned} \tag{6}$$

where $K = J/2kT$ and $K' = J'/2kT$. We use this cluster (as well as the subsequent clusters) with periodic boundary conditions to eliminate undesirable surface effects.

The transfer matrices of the Ising models on cylinders $n \times n \times \infty$ with transverse sizes $n = 3$ and $n = 4$ have dimensions 512 and 65536, respectively. To solve the eigenvalue

Table 1. Critical temperature of the three-dimensional Ising model with spatially anisotropic interactions: the calculation by a phenomenological renormalization group method with use of the cluster pairs (1, 2), (2, 3) and (3, 4) and the extrapolation from equation (3); in the last column the non-physical values are included in parentheses.

	kT_c/J			
J'/J	(1, 2)	(2, 3)	(3, 4)	Extrapolation
1.0	2.32977	2.34298	2.29052	(2.33242)
0.9	2.19274	2.18445	2.13485	(2.19440)
0.8	2.05015	2.02275	1.97665	(2.09029)
0.7	1.90117	1.85737	1.81538	(0.84121)
0.6	1.74468	1.68757	1.65029	1.58020
0.5	1.57907	1.51226	1.48023	1.45073
0.4	1.40194	1.32971	1.30338	1.28827
0.3	1.20921	1.13684	1.11654	1.10862
0.2	0.99298	0.92728	0.91317	0.90931
0.1	0.73242	0.68315	0.67518	0.67364
0.09	0.70181	0.65494	0.64759	0.64622
0.08	0.66983	0.62556	0.61881	0.61759
0.07	0.63619	0.59473	0.58859	0.58752
0.06	0.60051	0.56211	0.55658	0.55564
0.05	0.56221	0.52715	0.52223	0.52142
0.04	0.52038	0.48901	0.48473	0.48405
0.03	0.47346	0.44623	0.44261	0.44205
0.02	0.41823	0.39581	0.39289	0.39245
0.01	0.34579	0.32939	0.32729	0.32698
0.009	0.33666	0.32099	0.31898	0.31868
0.008	0.32694	0.31203	0.31012	0.30983
0.007	0.31650	0.30239	0.30058	0.30031
0.006	0.30515	0.29190	0.29020	0.28994
0.005	0.29262	0.28030	0.27872	0.27848
0.004	0.27849	0.26718	0.26573	0.26551
0.003	0.26197	0.25181	0.25051	0.25031
0.002	0.24148	0.23268	0.23155	0.23138
0.001	0.21248	0.20548	0.20458	0.20444

problem of these matrices which are real, symmetric and dense, we used an invariance of the subsystems under the transformations of the group $\mathbf{Z}_2 \otimes \mathbf{T}_n \otimes \mathbf{C}_{4v}$ ($\mathbf{Z}_2$ is a group of spin inversions; $\mathbf{T}_n$ is a group of translations in the transverse directions of a cluster; $\mathbf{C}_{4v}$ is a group of rotations around the axis of a system at angles $\pi/2$ and the reflections in planes through this axis; $\otimes$ and $\otimes$ are the symbols of the direct and semidirect products, respectively). By virtue of the indicated symmetry the matrices can be reduced to a block diagonal form in which the leading eigenvalues, as it turns out, are located in different subblocks; in the case $n = 3$ both subblocks have a dimension of only 13 and in the case $n = 4$ the largest eigenvalue $\lambda_1^{(4)}$ lies in the subblock of 433rd order and $\lambda_2^{(4)}$ in that of 372nd order†. We have carried out these quasi-diagonalizations after which we performed numerically the solution of the transcendental equation (1) including the required diagonalization of the corresponding subblocks.

In table 1 the critical temperature values that we calculated within a phenomenological renormalization group theory approximation are collected; in the last column

† For the cluster, of the next size, $5 \times 5 \times \infty$ the transfer matrix has an order $2^{25} = 33\,554\,432$ and the dimension of each two subblocks containing the extreme eigenvalues equals 86056.

Table 2. A comparison of critical temperatures of the quasi-one-dimensional Ising model found by different methods.

Method	kT_c/J			
	$J'/J = 1$	$J/J' = 10^{-1}$	$J/J' = 10^{-2}$	$J/J' = 10^{-3}$
EBPA [9]	2.4053	0.6959	0.3335	0.2072
Table 1, (3, 4)	2.2905	0.6752	0.3273	0.2046
Table 1, extrapolation	—	0.6736	0.3270	0.2044
Exact [3]	2.25574			
Series [4]	2.2553	0.6715	0.325	

the three-point extrapolation results are given. In this connection it is necessary to note the following. Since we use a degenerate cluster $1 \times 1 \times \infty$, some anomalies take place for small anisotropy of the system. For instance, when $J' = J$ the (1, 2) estimate of a phase transition point is nearer to the true value than that with the (2, 3) pair. Moreover, the extrapolation does not lead obviously to improvements up to $J'/J = 0.7$ (that is why we have put the formally extrapolated values in parentheses). However, on further increase in anisotropy (by about $J'/J = 0.5$) the extrapolation (3) begins to give improved values which, if judged by analogy with the two-dimensional variant (for a check we have performed such a calculation for the exactly solved flat anisotropic Ising model using strips with $n = 1, 2, 3$ and 4 and also with cyclic boundaries in finite directions), are the upper estimates of the rigorous critical temperatures; the percentage errors of these estimates monotonically decrease with decrease in J'/J.

3. Discussion

We compare the results obtained with the most qualitative calculations available at present. For comparison we have constructed table 2. From this table it is seen that our calculation perceptibly improves the estimates given by EBPA [9]. So, in the standard case $J' = J$ the error in the determination of a phase transition temperature decreases from 6.6% (EBPA) to 1.5% (phenomenological renormalization group; pair (3, 4)). It is interesting to note the following. For a three-dimensional Ising model with fully isotropic interactions there is a renormalization group calculation [13] also with the clusters $n \times n \times \infty$ ($n = 2, 3$ and 4) but with the screw (helical) boundary conditions of Kramers and Wannier (these boundary conditions break the symmetry $\mathbf{T}_n \otimes \mathbf{C}_{4v}$ and make the transfer matrix very sparse); this calculation gives $kT_c/J = 2.140$ (pair (2, 3)) and $kT_c/J = 2.231$ (pair (3, 4)), i.e. the screw boundary conditions lead, vice versa, to low estimates of the critical temperature. However, we return to the discussion of table 2. For small anisotropies the high-temperature series method [4] gives the most exact results. In the case of isotropic interactions the phase transition temperature determined by this method underestimates the accurate value by 0.02%. If we assume that for $J'/J = 0.1$ the exactitude here is preserved sufficiently well, then we come to the conclusion that our extrapolated value exceeds the true critical temperature by only 0.3%. Since $J'/J \to 0$ there are grounds to expect a further decrease in the error which is inserted in the approximation used, then it is rather clear that the results obtained in this paper are suitable for practical applications at least in the case of sufficiently anisotropic materials.

In $CoCl_2 \cdot 2NC_5H_5$ crystals possessing a pronounced quasi-one-dimensional mag-

netic Ising system with ferromagnetic intrachain and antiferromagnetic interchain interactions, $T_c = 3.17 \pm 0.02$ K and $J/k = 10.6 \pm 0.6$ K [14]. Hence, in keeping with the data of the previous section, $|J'|/J = 0.0069^{+0.0022}_{-0.0017}$. This value agrees with the earlier estimates $|J'|/J = 0.008$ [15] and $|J'|/J = 0.006$ [16]. In the compound $FeCl_2 \cdot 2NC_5H_5$ with the analogous structure, the magnetic phase transition occurs at the temperature $T_c = 6.6 \pm 0.3$ K and the constant of intrachain interactions is equal to $J/k \approx 25 \pm 2$ K [17]. Therefore, here, $|J'|/J = 0.0039^{+0.0031}_{-0.0018}$ with which, by and large, the ratio $|J'|/J =$ 0.006 found in [18] from a treatment of data on a zero-field powder susceptibility agrees.

References

[1] Pawley G S, Swendsen R H, Wallace D J and Wilson K G 1984 *Phys. Rev.* B **29** 4030
[2] Barber M N, Pearson R B, Toussaint D and Richardson J L 1985 *Phys. Rev.* B **32** 1720
[3] Guttmann A J 1987 *J. Phys. A: Math. Gen.* **20** 1855
[4] Navarro R and de Jongh L J 1978 *Physica* B **94** 67
[5] Graim T and Landau D P 1981 *Phys. Rev.* B **24** 5156
[6] da Silva L R, Tsallis C and Schwachheim G 1984 *J. Phys. A: Math. Gen.* **17** 3209
[7] Stout J W and Chisholm R C 1962 *J. Chem. Phys.* **36** 979
[8] Plascak J A and Silva N P 1982 *Phys. Status Solidi* b **110** 669
[9] Yurishchev M A 1985 *Phys. Status Solidi* b **128** 537
[10] Nightingale P 1982 *J. Appl. Phys.* **53** 7927
[11] Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J Lebowitz (New York: Academic) p 145
[12] Kaufman B 1949 *Phys. Rev.* **76** 1232
[13] Oguchi T and Taguchi Y 1986 *Prog. Theor. Phys. Suppl.* 87 23
[14] Takeda K, Matsukawa S and Haseda T 1971 *J. Phys. Soc. Japan* **30** 1330
[15] Pires A and Hone D 1978 *J. Phys. Soc. Japan* **44** 43
[16] Yurishchev M A 1983 *Fiz. Nizk. Temp.* **9** 851
[17] de Groot H J M, de Jongh L J, Thiel R C and Reedijk J 1984 *Phys. Rev.* B **30** 4041
[18] Yurishchev M A 1987 *Fiz. Nizk. Temp.* **13** 441