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Determination of critical temperature for three-dimensional Ising systems

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Abstract. A real space renormalisation group method has been applied to find the critical temperature of the Ising model on cubic and octahedral lattices. The result obtained for a cubic lattice is in good agreement with that obtained from high-temperature series expansion and is better than the results of other papers. A modification of the transformation tested for a simple cubic lattice allowed us to find the critical temperature for an octahedral lattice. The latter has not so far been studied by any version of the real space renormalisation group method.

1. Introduction

The renormalisation transformation (RT) cannot be constructed within the real space renormalisation group (RSRG) theory unambiguously for different lattice systems. Even for systems of the same space symmetry and the same space dimensionality there is, to some extent, a flexibility in formulating and choosing the RT. Up to now, a lot of different schemes of realisation of the RSRG method have been proposed (Burkhardt and van Leeuwen 1982). In practice all these solutions are nót equivalent. At the present stage of development of the theory, the chosen form of the transformation can be checked as to its correctness only retrospectively. One of the earliest realisations of RSRG is the transformation proposed by Niemeijer and van Leeuwen (NVL) based on the cumulant expansion method (Niemeijer and van Leeuwen 1974). In this version the lattice is divided into cells. The intracell part of the Hamiltonian is treated exactly and the partition function is expanded in a cumulant expansion of powers of the intercell part of the Hamiltonian. In the present paper we describe the application of a modified NVL scheme to the studies of critical temperature of three-dimensional Ising models on simple cubic and octahedral lattices.

2. Renormalisation group transformation

Here we use the renormalisation transformation of the form

$$\exp \mathcal{H}'\{S'\} = \sum_{\{S\}} \prod_{i'} \tfrac{1}{2}[1 + S'_{i'} \operatorname{sign}(i'\text{th cell})] \exp \mathcal{H}\{S\}. \quad (1)$$

The spins $S'_{i'}$ form a new lattice isomorphic to the original one. On splitting the Hamiltonian $\mathcal{H}\{S\}$ into the zeroth part $\mathcal{H}_0\{S\}$ and the perturbational part $V\{S\}$, we can write the transformation relation (1) as

$$\mathscr{H}'\{S'\} = E_0 + \langle V\{S\}\rangle_0 + \tfrac{1}{2}(\langle V^2\{S\}\rangle_0 - \langle V\{S\}\rangle_0^2) + \dots \tag{2}$$

where the average $\langle\dots\rangle_0$ is defined by

$$\langle A\rangle_0 = \frac{\Sigma_{\{S\}} \Pi_{i'} \frac{1}{2}[1 + S'_{i'} \operatorname{sign}(i'\text{th cell})] \exp \mathscr{H}_0\{S\} A\{S\}}{\Sigma_{\{S\}} \Pi_{i'} \frac{1}{2}[1 + S'_{i'} \operatorname{sign}(i'\text{th cell})] \exp \mathscr{H}_0\{S\}}. \tag{3}$$

The transformation (1) is unequivocal if the value +1 is ascribed to half of the spins for which $\Sigma_n S_{i'}^n = 0$ ($n = 8$ or 6) or if the value -1 is ascribed to the other half of these spins (Nauenberg and Nienhuis 1974). The ambiguity of this transformation has been removed in different ways by Fields and Fogel (1975), Oitmaa and Barber (1977), Hsu and Gunton (1977) and Tatsumi (1978). In our calculations we take into account three coupling parameters, namely, magnetic field H, the nearest-neighbour pair interaction K, and the next-nearest-neighbour pair interaction L. Any possible long-range pair couplings as well as any complex (multispin) couplings generated by the transformation (2) are omitted. In such approximations the renormalisation group equations can generally be written at the fixed point as

$$0 = H^*(0, K^*, L^*), \qquad K^* = K^*(0, K^*, L^*), \qquad L^* = L^*(0, K^*, L^*). \tag{4}$$

Hereafter, the asterisks symbolising the fixed point values of the couplings are, for brevity, abandoned.

3. Simple cubic lattice: Results and critical exponents

For the case of the simple cubic (SC) lattice equations (4) in the second-order cumulant approximation have the following form

$$\begin{aligned}
K &= (16KL + 32L^2)f_1^2 + (32KL + 64L^2)f_1^2 f_2 + (16KL + 32L^2)f_1^2 f_3 \\
&\quad - (64KL + 128L^2)f_1^4 + 4(K + 2L)f_1^2 \\
L &= (4K^2 + 16KL + 20L^2)f_1^2 + (12K^2 + 48KL + 56L^2)f_1^2 f_2 \\
&\quad + (12K^2 + 48KL + 52L^2)f_1^2 f_3 - (28K^2 + 112KL + 128L^2)f_1^4 \\
&\quad + 2Lf_1^2 \\
&\quad f_\alpha = n_\alpha / z \qquad (\alpha = 1, 2, 3) \\
z &= \exp(12K + 12L) + 8\exp(6K + 6L) + 12\exp(4K) + 12\exp(4L) \\
&\quad + 24\exp(2K - 2L) + 24\exp(-2K - 2L) + 8\exp(-6K + 6L) \\
&\quad + 3\exp(4K - 4L) + 3\exp(-4K - 4L) + 12\exp(-4K) + 12\exp(-4L) \\
&\quad + \exp(-12K + 12L) + 8 \qquad (5) \\
n_1 &= \exp(12K + 12L) + 6\exp(6K + 6L) + 6\exp(4K) + 6\exp(4L) \\
&\quad + 6\exp(2K - 2L) + 6\exp(-2K - 2L) + 2\exp(-6K + 6L) + 2 \\
n_2 &= \exp(12K + 12L) + 4\exp(6K + 6L) + 4\exp(4K) + 4\exp(2K - 2L) \\
&\quad - 4\exp(-2K - 2L) - 4\exp(-6K + 6L) + \exp(4K - 4L) \\
&\quad - \exp(-4K - 4L) - 4\exp(-4K) - \exp(-12K + 12L)
\end{aligned}$$

$$n_3 = \exp(12K + 12L) + 4\exp(6K + 6L) + 4\exp(4L) - 4\exp(2K - 2L) - 4\exp(-2K - 2L) + 4\exp(-6K + 6L) - \exp(4K - 4L) - 4\exp(-4L) + \exp(-12K + 12L).$$

The fixed point of these relations is found to be $K = 0.151\,95$, $L = 0.033\,18$. The critical temperature $K_c = J/k_B T_c$ has been calculated by analysing the flow diagram in which the fixed point has been reached, starting from the initial values $K_0 = K_c$, $L_0 = 0$. In the second order of expansion this leads to the result $K_c = 0.224\,01$ (while $K_c^I = 0.297\,80$ in the first order). The data for a comparison between our result for T_c and the results obtained by other methods, are given in table 1, (Tatsumi 1978, Onyszkiewicz 1974, 1980, Strieb *et al* 1963, Yang and Wang 1975) where the value resulting from the high-temperature series technique (HTSE) is assumed to be 1.00. It is remarkable that RSRG methods yield results that are in far better agreement with the HTSE value than the five other representative approaches taken into consideration in table 1. Moreover, the RT presented in this paper gives a better result than other RSRG transformations based on the cumulant expansion.

Table 1. Critical temperature results for the simple cubic lattice.

0.99	LTSE
1.00	HTSE
1.01	RPA
1.33	MFA
1.30	Oguchi approx.
1.14	BPW
1.14	constant coupling
1.14	HDEM (Onyszkiewicz)
0.92	HDEM (Horwitz and Callen)†
0.93	RSRG (Hsu and Gunton)
0.98	RSRG (Tatsumi)
0.98	RSRG (Oitmaa and Barber)
0.99	RSRG (present paper)

HDEM, high-density expansion method
LTSE, low-temperature series expansion
† discontinuous phase transition.

In the works of Hsu and Gunton as well as of Oitmaa and Barber the calculations are performed up to the second order of the expansion while in that of Tatsumi to the third order. For the sake of comparison, table 2 presents the values of the critical indices obtained by them and the results of this paper. The thermal and magnetic

Table 2. Critical eigenvalues and exponents for the SC lattice.

λ_T	λ_H	ν	η	
		0.638	0.041	series expansion results
2.362	5.670	0.807	−0.007	Tatsumi (third order)
2.339	6.324	0.816	−0.322	Oitmaa and Barber
2.274	5.483	0.844	0.090	Hsu and Gunton
2.452	6.664	0.773	−0.473	present paper

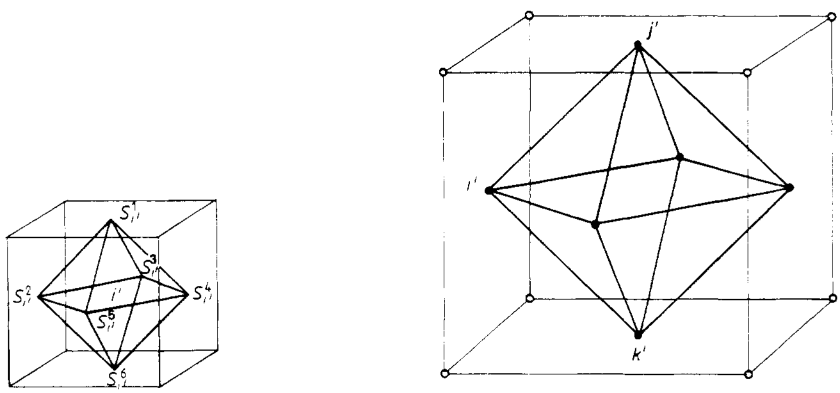
eigenvalues following from the application of this RT, differ from expected values by 19% and 18%, respectively. This leads to a better value of ν than in other papers, and to a worse value of η. It is to be noted that the same RG approach has been utilised for a nearest-neighbour Ising model on a SC lattice with free-surface boundary condition (Dunfield and Noolandi 1980) giving better results than other approaches.

4. Application to the octahedral lattice: Critical temperature calculation

So far only a cubic lattice has been studied by other authors, using the NVL method in the cumulant approximation applied to three-dimensional Ising models. The differences in various versions of the transformation (1) rely only on different definitions of the weight factor

$$P(S', S) = \prod_{i'} \tfrac{1}{2}[1 + S'_{i'} \operatorname{sign}(i'\text{th cell})]. \tag{6}$$

However, any modification of this factor is not in itself sufficient to obtain critical temperatures and other non-universal quantities of three-dimensional Ising models on lattices of every symmetry. It is rather easy to notice that in most of the three-dimensional lattices it is not possible to construct the lattices which would be isomorphic to the original one and would be built from all lattice points, i.e., without dropping any of spins. As an example let us now consider the octahedral lattice being a sublattice of a real lattice composed of the spins of manganese ions in Mn_3GaC (figure 1(*a*)). The geometric centres of the octahedrals do not however form an octahedral lattice. Therefore, using the RT of equation (1) for the octahedral lattice one cannot construct an isomorphic one. In fact the blocks formed in the RG approach consist of the spins lying on the walls of the cube, as depicted in figure 1(*b*), whereas the spins placed at the corners of this cube do not belong to any block. Obviously, the 'redundant' spins cannot be arbitrarily neglected, and thus the RT of equation (1) does not preserve the symmetry of the lattice. In order to arrive at a new lattice isomorphic to the original one, we avail ourselves of the decimation transformation for these spins. Accordingly,



(*a*) (*b*)

Figure 1. Octahedral lattice: (*a*) an elementary cell composed of six spins of manganese ions, (*b*) the centres of the six cells *i'*, *j'*, *k'*, ... also form an octahedron. The centres of the eight cells at the corners of the cube do not belong to the new lattice.

the RT used here for the octahedral lattice consists of two steps, namely, the transformation of (1) and then the decimation transformation for 'redundant' spins.

The use of the RT of (1) leads to effective (renormalised) couplings of three types. The first one concerns interactions between the spins belonging to new octahedrals, the second one refers to the coupling between 'redundant' spins, and the last one comprises the mixed interactions, i.e., interactions between the spins belonging to new octahedrals and the 'redundant' spins. These types of couplings are illustrated in figure 2, where typical graphs obtained in the second-order approximation of expansion (2) are shown. The same kind of graph can correspond to these three types of interactions, since each graph symbolises an appropriate class of interaction. In such cases the proportion of the number of topologically equivalent graphs belonging to the first type to those belonging to the two remaining types reads 3:1. This enables us to simplify the use of the decimation procedure. Applying the same technique as previously for SC lattice, we derive the following RG equations at the fixed point:

$$K = \tfrac{4}{3}(2K^2+7KL+5L^2)f_1^2 + 4(2K^2+5KL+3L^2)(f_2-2f_1^2)f_1^2 + 2(K+L)f_1^2$$

$$L = \tfrac{8}{3}(K^2+2KL+L^2)f_1^2 + \tfrac{16}{3}(K^2+KL+L^2)f_1^2 f_2 + \tfrac{8}{3}(K^2+2KL+L^2)f_1^2 f_3$$
$$- 8(2K^2+3KL+2L^2)f_1^4 + Lf_1^2$$

$$f_\alpha = n_\alpha / z \qquad (\alpha = 1, 2, 3)$$

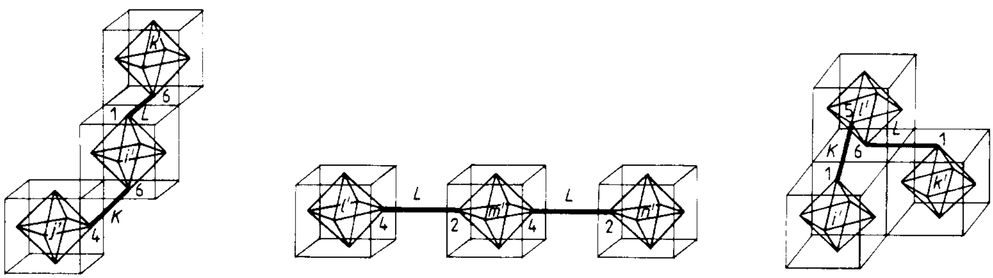
$$z = \exp(3L+12K) + 6\exp(L+4K) + 12\exp(-L) + 3\exp(3L-4K)$$
$$+ 6\exp(L-4K) + 4\exp(-3L)$$

$$n_1 = \exp(3L+12K) + 4\exp(L+4K) + \exp(3L-4K) + 4\exp(-L)$$

$$n_2 = \exp(3L+12K) + 2\exp(L+4K) - \exp(3L-4K) - 2\exp(L-4K)$$

$$n_3 = \exp(3L+12K) + 2\exp(L+4K) - 4\exp(-L) + 3\exp(3L-4K)$$
$$+ 2\exp(L-4K) - 4\exp(-3L). \qquad (7)$$

where the symbols H, K and L refer to the octahedral lattice and not to the SC lattice considered previously. The inverse critical temperature K_c has been determined to be of 0.2860 in the second and 0.2922 in the first order of cumulant expansion. However, in the case of the octahedral lattice, relatively accurate determination of the critical



(*a*) (*b*) (*c*)

Figure 2. Examples of second-order graphs of the cumulant expansion. (*a*) the case of the renormalised coupling between 'octahedral' spins, (*b*) the case of the interaction between 'redundant' spins (lattice points l', m', n' indicate 'redundant' spins), (*c*) the case of 'mixed' coupling (lattice point l' stands for 'redundant' spin).

exponents which should be the same as for the SC lattice, requires more precise approximation. Thus, it follows that within the RT applied the character of the lattice topology influence the values of the exponents.

5. Concluding remarks

RSRG method based on the cumulant expansion has been applied to analyse critical behaviour of the Ising model on cubic lattice at the ferromagnetic fixed point. The inverse critical temperature K_c as well as the exponents ν and η have been calculated. The temperature obtained is very close to the expected value. Also, the obtained value of ν is satisfactory and closer to the expected result than those values reported in other papers. However, the value of the critical exponent η is found to be unacceptable. More accurate calculation of η would be possible by including a larger number of interactions and by extending the cumulant expansion to an order higher than two.

The possibility of applying the RSRG method to non-cubic lattices has also been shown in this paper. With this purpose the cumulant expansion has been combined with decimation method, and with the renormalisation transformation obtained in this way, the critical temperature for the octahedral lattice has been calculated. Although the simple method applied in this paper does not guarantee satisfactory results of the critical exponents, it seems to be efficient in the calculation of the critical temperatures of more complicated three-dimensional systems.

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