Critical temperatures of the spin-s Ising model

Theodore W. Burkhardt and Robert H. Swendsen
Institut für Festkörperforschung der Kernforschungsanlage Jülich, D-517 Jülich, West Germany
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Critical temperatures of the spin-s Ising model with nearest-neighbor interactions are calculated with an approach based on Kadanoff's lower-bound renormalization transformation. An initial transformation converts the spin-s Hamiltonian into a spin-1/2 Hamiltonian, which is then analyzed with a spin-1/2 renormalization transformation. The calculation is performed for the $d = 2$ square lattice and the $d = 3$ bcc lattice. For comparison the critical temperatures are also estimated from the ten-term high-temperature series for the susceptibility given by Camp and Van Dyke. The agreement is very good.

INTRODUCTION

Renormalization-group techniques have been used to calculate the critical behavior and the thermodynamic functions of the Ising model with considerable success.[1-3] The central ingredient in the approach is a transformation for converting a Hamiltonian with spin variables σ and interaction constants $\vec{K}$, into a Hamiltonian with new spin variables σ' and new coupling constants $\vec{K}'$. The mapping increases the lattice constant of the system but leaves the partition function unchanged.

When the spin-$\frac{1}{2}$ transformations of Refs. 1–3 are generalized to arbitrary spin s, one finds that the number of coupling constants involved increases rapidly with increasing s. In a simpler procedure for investigating the spin-s Ising model involving no more coupling constants than the spin-$\frac{1}{2}$ problem, an initial renormalization transformation is used to convert the spin-s Hamiltonian to a spin-$\frac{1}{2}$ Hamiltonian, which is then analyzed with a spin-$\frac{1}{2}$ renormalization transformation. In such an approach the critical behavior of the spin-s Ising model is determined by the fixed-point properties of the spin-$\frac{1}{2}$ transformation, and the universality principle,[4] according to which the critical exponents of the spin-s Ising model are independent of s, is automatically fulfilled.

Berker[5] has used a spin-s to spin-$\frac{1}{2}$ restructuring transformation in conjunction with the spin-$\frac{1}{2}$ results of Niemeijer and van Leeuwen[1] to calculate the critical temperatures of the spin-s Ising model for the two-dimensional triangular lattice. His results differ by less than 1% from critical temperatures estimated from the high-temperature series for the susceptibility.

In this paper we describe a restructuring transformation based on Kadanoff's lower-bound renormalization transformation.[3] Kadanoff's transformation has the advantages that it is quite simple and is not restricted to a particular dimension. Using the restructuring transformation followed by Kadanoff's spin-$\frac{1}{2}$ transformation, we compute the critical temperatures of the spin-s Ising model with nearest-neighbor interactions for the $d=2$ square lattice and the $d=3$ bcc lattice. We also estimate the critical temperatures from the coefficients in the high-temperature series for the susceptibility given by Camp and Van Dyke.[6] The two sets of results differ by less than 4% for the square lattice and by less than 3% for the bcc lattice. The deviation is a systematic one, for which the spin-$\frac{1}{2}$ rather than the spin-restructuring transformation appears to be primarily responsible. The renormalization-group calculation reproduces the basic s dependence of the critical temperature even for the largest values of s we considered.

RENORMALIZATION-GROUP CALCULATION

We write the Hamiltonian operator of the system in the form $H=-\sum h$. In the case $d=2$, the sum extends over all squares of a square lattice, and h depends on $n=4$ spin variables. In the case $d=3$, the sum extends over all cubes of a simple-cubic lattice, and h depends on $n=8$ spin variables. Kadanoff's lower-bound renormalization transformation[3] may be written in the form

$$h'(\sigma_1'\cdots\sigma_n') = \ln \mathrm{Tr}_\sigma \exp[p(\sigma_1'\sigma_1+\cdots+\sigma_n'\sigma_n) - \ln 2\cosh p(\sigma_1+\cdots+\sigma_n)+nh(\sigma_1\cdots\sigma_n)]. \quad (1)$$

The transformation yields a lower bound to the exact free energy. The lower-bound property holds even if σ' and σ represent Ising spin variables with different values of s. p is a variational parameter adjusted to optimize the calculation. A different value of p may be used each time the transformation is carried out.

As discussed in detail in Ref. 7, difficulties arising from an extra relevant variable are encountered if Kadanoff's transformation is used to

calculate the critical surface outside the invariant subspace of Hamiltonians in which $h(\sigma_1 \cdots \sigma_n)$ is completely symmetric in the n-spin variables. We therefore confine our attention entirely to the symmetric subspace. Since the initial Hamiltonian we wish to consider, which involves only nearest-neighbor interactions, lies outside the symmetric subspace, we initially perform an exact decimation transformation[3] to enter the subspace. In the square-lattice calculation, the decimation eliminates every other spin, leaving a square lattice with a lattice constant increased by the factor $\sqrt{2}$. In the bcc calculation, the decimation eliminates all the spins on one of the two simple-cubic sublattices, leaving a simple-cubic lattice with the same lattice constant as the original bcc lattice. After the decimation is performed,

$$h(\sigma_1 \cdots \sigma_n) = \ln \mathrm{Tr}_\tau \exp[K_{\mathrm{nn}}(\sigma_1 + \cdots + \sigma_n)\tau]. \quad (2)$$

In Eq. (2) K_{nn} is the nearest-neighbor coupling constant in the initial Hamiltonian. τ and σ represent the decimated and the surviving Ising spin variables, respectively, and take the values $s, s-1, \ldots, -s$.

To reduce the spin-s problem to spin $\frac{1}{2}$, we insert Eq. (2) into Eq. (1), taking the σ' and σ variables to be spin-$\frac{1}{2}$ and spin-s variables, respectively. As discussed in Ref. 3, for the case of zero magnetic field $h'(\sigma_1' \cdots \sigma_n')$ contains a constant term and two-spin, four-spin, ..., n-spin interactions with corresponding coupling constants K_0', $K_2', \ldots, K_n'$. The spin-s to spin-$\frac{1}{2}$ transformation is followed by repeated applications of the spin-$\frac{1}{2}$ renormalization transformation, which is Eq. (2), with σ' and σ both representing spin-$\frac{1}{2}$ variables. In the spin-$\frac{1}{2}$ to spin-$\frac{1}{2}$ transformations, p was set equal to the value p^* reported in Ref. 3, which maximizes the free energy of the fixed-point Hamiltonian. The value of p used in the spin-s to spin-$\frac{1}{2}$ spin-restructuring transformation was chosen to maximize the contribution of the transformation to the free energy. For this particular value of p, $\partial K_0'/\partial p = 0$, where K_0' is the constant term in the Hamiltonian generated by the decimation and spin-restructuring transformations.

To obtain values for the critical temperature T_c of the s-spin Ising model, we sought the value of $K_{\mathrm{nn}}^c \propto T_c^{-1}$ in Eq. (2), which is mapped onto the critical surface of the spin-$\frac{1}{2}$ transformation by the decimation and spin-restructuring transformations. We confined our attention to low values of s to avoid excessive computing times. Since the trace in Eq. (1) contains $(2s+1)^n$ terms, the time required to perform the spin-restructuring transformation increases rapidly with s. T_c normalized by its mean-field value[8] is shown for various values of s in Table I. A graph of the results is given in Fig. 1.

TABLE I. T_c divided by its mean-field value for various values of s. r.g. denotes the renormalization-group results and h.t.s. the results from the high-temperature series for the susceptibility.

	$d=2$, square lattice		$d=3$, bcc lattice	
	r.g.	h.t.s.	r.g.	h.t.s.
$\frac{1}{2}$	0.546	0.567	0.771	0.7942
1	0.615	0.633	0.816	0.8350
$\frac{3}{2}$	0.639	0.655	0.831	0.8476
2	0.649	0.665	0.837	0.853
$\frac{5}{2}$	0.655	0.670		0.856
3	0.658	0.673		0.858
4	0.662	0.677		0.860
10	0.667	0.681		0.862
25		0.683		0.863
∞		0.683		0.863

RESULTS FROM THE HIGH-TEMPERATURE SUSCEPTIBILITY SERIES

For comparison with the renormalization-group results, we have also estimated the critical temperatures from the ten-term high-temperature series for the susceptibility given by Camp and Van Dyke.[6] In order to provide consistency checks and error estimates, a variety of techniques[9] were used. Padé approximants were made to the logarithmic derivatives and to the γ^{-1} power of the susceptibility, both with and without prior Euler transforms to shift the antiferromagnetic singularity away from the origin. The ratio method was applied to each of these series as well as to the original series, and Neville tables were used to extrapolate the results. Finally we used the variation of the ratio method due to Domb and Sykes,[10] in which γ is set equal to the known value.

The internal consistency of the Padé and Neville tables is generally excellent. In some cases, the apparent uncertainty is confined to the fifth significant digit. However, a comparison between the results of the different methods suggests more conservative estimates of the error.

Our final results are shown in Table I and in Fig. 1. We believe the third digit to be reliable, and for small s in the case of the bcc lattice we give a fourth digit because of the consistency between methods. For spin $\frac{1}{2}$ our results agree with the exact square-lattice result and with the bcc result obtained from a 15-term series.[11]

CONCLUSION

The critical temperatures calculated with renormalization-group methods are in very good agreement with the essentially exact results from the high-temperature series for the susceptibility. For the square lattice, the two sets of results differ by less than 4%, and for the bcc lattice, by less than 3%. It can be seen in Fig. 1 that the renormalization-group calculation clearly reproduces the basic s dependence. The renormalization-group critical temperatures are uniformly lower than the series temperatures. This would appear to be primarily a consequence of the spin-$\frac{1}{2}$ transformation rather than the spin-restructuring transformation, since the systematic deviation is also present in the critical temperature for spin $\frac{1}{2}$. The spin-restructuring approach seems to work remarkably well, even for the largest values of s we considered.

The greater accuracy (better than 1%) which Berker[5] obtains with his spin-restructuring transformation probably rests in the exceptionally accurate critical surface for spin $\frac{1}{2}$ calculated by Niemeijer and van Leeuwen[1] with a seven-spin cluster approximation. Their renormalization transformation, which involves 11 different couplings, yields a critical temperature 0.2% higher than the exact value. For $d=2$ and $p=p^*$ Kadanoff's transformation, which involves only a two-spin and a four-spin coupling, yields a critical temperature 4% lower than the exact value. Our spin-restructuring transformation offers the same basic advantages as the Kadanoff method in general. It is simpler than Berker's transformation and is not restricted to $d=2$.

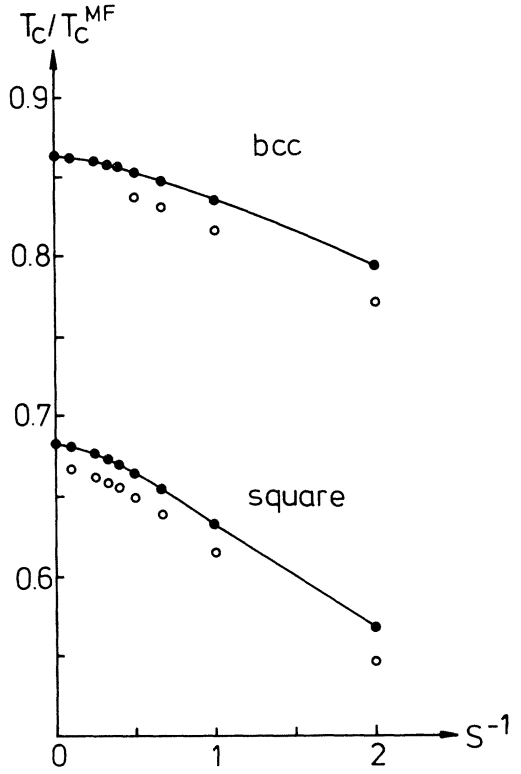

FIG. 1. T_c divided by its mean-field value as a function of s^{-1}. The empty circles indicate renormalization-group results, and the curves indicate the results from the high-temperature series for the susceptibility.

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