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Critical behavior of the three-dimensional Ising model

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The simple-cubic Ising model has been investigated with the Monte Carlo renormalization-group method. The results are found to be consistent with the critical exponents obtained from series and ϵ expansions.

The Monte Carlo renormalization-group method (MCRG) has been successfully applied to several two-dimensional systems, including the Ising model, for which very good agreement with the exact critical exponents was obtained.[1-3]

In this paper, we extend the MCRG method to three dimensions. The Ising model is again used as an appropriate test case because of the availability of accurate estimates of the critical exponents from high- and low-temperature and high-field series[4-10] as well as ϵ expansions,[11] even though an exact solution is not available.

The MCRG method and the necessary equations have been presented elsewhere.[2,3] The basic calculation starts with an MC simulation of the system of interest at its critical temperature to obtain a sequence of configurations from which any desired correlation functions can be calculated. An RG transformation is then applied directly to the individual configurations, yielding a sequence of configurations for the block spins. This sequence of configurations is equivalent to what would have been obtained if the exact RG transformation had been applied to the original Hamiltonian and the renormalized Hamiltonian had been simulated. This process can be repeated and, because the original Hamiltonian was at criticality, the effective renormalized Hamiltonians will approach the fixed point. The MCRG equations then give a sequence of estimates for the eigenvalues of the linearized RG transformation that converges toward the fixed point values. The critical exponents, which are of physical interest, are obtained from these eigenvalues by standard methods.[12]

The RG transformation we have used consisted of dividing the system into $2\times2\times2$ blocks and assigning a block-spin value of ±1 by a modified majority rule in which one spin was given two votes to act as a tie breaker. (This RG transformation was chosen both for its simplicity and the fact that the corresponding transformation in two dimensions has proven particularly efficient.[3]) The RG transformation is exact for the finite lattice and differs negligibly from the infinite-lattice transformation if the range of the fixed-point Hamiltonian is smaller than the linear dimensions of the smallest lattice considered.

We have performed MC simulations of the simple-cubic Ising model on lattices with linear dimensions up to $N=32$ and periodic boundary conditions. After three RG iterations with scale factor $b=2$, the $N=32$ lattice was reduced to the dimensions $4\times4\times4$. A comparison with MC simulations involving smaller lattices (for example, $N=16$ and two RG iterations) showed no notable size effect (truncation of the effective renormalized Hamiltonian). In fact, although there were indications from some of our runs on smaller lattices that there is a size dependence when the lattice is reduced to $3\times3\times3$, the effect on the exponents is still much less than 1%.

For the analysis of the linearized RG transformation matrix, we included first- through fourth-nearest-neighbor interactions, four-spin interactions, the magnetic field, and three-spin interactions. For each RG iteration, we studied both the eigenvalues and eigenvectors and observed the effect of successively including more interactions (more elements of the transformation matrix).

The critical temperature can be determined self-consistently with the MCRG method by observing the flows to high- or low-temperature fixed points when the MC simulation is performed above or below the critical temperature. The results of MC simulations about 1% above or below the critical temperature given by series expansions[4] showed flows away from the critical fixed point as expected. Since this is consistent with the series estimate for the critical temperature (which is, in any case, much more accurate than the present calculation with the available computer time), we chose to perform our long-

est MC simulations at the series value for the critical coupling $K_c = 0.443\,38$.

Table I shows MCRG data for a lattice with linear dimensions $N = 32$ and, for comparison, Table II gives the corresponding data for a lattice with $N = 24$. In both cases, the number of digits displayed was chosen to demonstrate the trends and fluctuations clearly and does not indicate the accuracy of the calculation. Statistical errors are about 2% for the even eigenvalue exponents and less than 1% for the odd ones. Although the size effect is expected to negligible for $N = 32$, there is still a systematic error due to the finite number of RG iterations used. This effect could also be as large as 1%.

An inspection of the odd eigenvectors shows that the components corresponding to the three-spin interactions are very small and erratic. It can be seen from the tables that they still have a significant effect on the eigenvalues, tending to lower δ and raise η. This effect may be spurious and we have computed the tabulated values of β and δ including only the magnetic field. If the effect is real, it would imply that either the value of δ is somewhat lower than the accepted value, $\delta = 5$, or that more RG iterations are needed for an accurate determination.

Our results are consistent with the series[4–10] and ϵ-expansion [11] estimates, as well as the proposed set of exact fractions,[4] within the accuracy of our calculation. It should be noted, however, that these other estimates are not completely consistent with each other to the accuracy claimed for each. It has even been pointed out that the best series estimates suggest a (small) breakdown in hyperscaling.[13] Since our method automatically satisfies hyperscaling, it does not shed light on this last question, except insofar as convergence to a fixed point confirms our assumptions. On the other hand, with the rapidly advancing computer technology, we believe that a carefully optimized MC algorithm and perhaps a different RG transformation could substantially improve the accuracy of the present calculation—perhaps to the point of being competitive with series and ϵ expansions.

TABLE I. MCRG data for the $d = 3$ Ising model on a $32 \times 32 \times 32$ lattice with 7000 MC steps per site after discarding 3000 MC steps per site. Scale factor $b = 2$. Values of β and γ use the value of λ_1^0 including only the magnetic-field operator. ϵ-expansion estimates are from Ref. 11. Series estimates are from Ref. 6 (ν, η), Ref. 7 (α), Ref. 8 (δ), Ref. 9 (β), and Ref. 10 (γ).

RG iteration	Number of interactions	λ_1^e	ν	α	λ_1^o	δ	η	β	γ
1	1	2.6119	0.722	−0.166	5.5011	4.553	0.081	0.3910	1.384
	2	2.7143	0.694	−0.083	5.5012	4.553	0.081	0.3760	1.331
	3	2.7121	0.695	−0.084	5.5034	4.559	0.079	0.3763	1.332
	4	2.7082	0.696	−0.087				0.3768	1.334
	5	2.7075	0.696	−0.088				0.3769	1.334
2	1	2.8750	0.656	0.031	5.5365	4.649	0.062	0.3449	1.279
	2	2.9523	0.640	0.079	5.5105	4.578	0.076	0.3364	1.248
	3	2.9752	0.636	0.093	5.5122	4.583	0.075	0.3340	1.239
	4	2.9673	0.637	0.088				0.3349	1.242
	5	2.9411	0.643	0.072				0.3376	1.252
3	1	2.9645	0.638	0.087	5.6101	4.860	0.024	0.3208	1.272
	2	3.0171	0.628	0.117	5.5443	4.671	0.058	0.3157	1.252
	3	3.0389	0.624	0.129	5.5433	4.668	0.059	0.3137	1.244
	4	3.0117	0.629	0.114				0.3162	1.254
	5	2.9937	0.632	0.104				0.3179	1.260
ϵ-expansion			0.627(10)	0.119(30)		4.88(12)	0.021(20)	0.320(8)	1.2410(20)
Series			0.628^{+2}_{-1}	0.122(3)		5.00(5)	0.041^{+6}_{-3}	0.312(5)	1.250(1)
Exact (?) fractions			0.625	0.125		5	0	0.3125	1.25

TABLE II. Same as Table I for a $24 \times 24 \times 24$ lattice using 22500 MC steps per site after discarding 2250 MC steps per site.

RG iteration	Number of interactions	λ_1^e	ν	α	λ_1^o	δ	η	β	γ
1	1	2.5747	0.733	−0.199	5.4899	4.523	0.087	0.3981	1.402
	2	2.7028	0.697	−0.091	5.4887	4.519	0.087	0.3787	1.334
	3	2.6980	0.698	−0.095	5.4898	5.522	0.087	0.3794	1.336
	4	2.6940	0.699	−0.098				0.3799	1.338
	5	2.6864	0.701	−0.104				0.3810	1.342
2	1	2.7982	0.674	−0.021	5.5561	4.704	0.052	0.3543	1.312
	2	2.8839	0.655	0.037	5.5414	4.663	0.060	0.3442	1.275
	3	2.8933	0.652	0.043	5.5411	4.662	0.060	0.3431	1.271
	4	2.8957	0.652	0.044				0.3428	1.270
	5	2.8803	0.655	0.034				0.3446	1.276
3	1	2.9274	0.645	0.064	5.6398	4.948	0.009	0.3255	1.285
	2	3.0410	0.623	0.130	5.5588	4.712	0.051	0.3143	1.241
	3	3.0407	0.623	0.130	5.5466	4.678	0.057	0.3144	1.241
	4	2.9689	0.637	0.089				0.3213	1.269
ϵ-expansion			0.627(10)	0.119(30)		4.88(12)	0.021(20)	0.320(8)	1.241(2)
Series			0.638^{+2}_{-1}	0.122(3)		5.00(5)	0.041^{+6}_{-3}	0.312(5)	1.250(1)
Exact (?) fractions			0.625	0.125		5	0	0.3125	1.25

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