Critical behavior of the three-dimensional Ising model with nearest-neighbor, next-nearest-neighbor, and plaquette interactions

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The critical and multicritical behavior of the simple cubic Ising model with nearest-neighbor, next-nearest-neighbor, and plaquette interactions is studied using the cube and star-cube approximations of the cluster variation method and the recently proposed cluster variation–Padé approximant method. Particular attention is paid to the line of critical end points of the ferromagnetic-paramagnetic phase transition: its (multi)critical exponents are calculated, and their values suggest that the transition belongs to a different universality class. A rough estimate of the crossover exponent is also given. [S1063-651X(97)51201-3]

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The Ising model was introduced in the 1920s [1] for describing magnetic transitions and is still the subject of a very intense research activity. In particular, the Ising model with nearest-neighbor (NN), next-nearest-neighbor (NNN) and plaquette interactions on the simple cubic lattice has been considered as a simple model for the statistical mechanics of random surfaces [2–4], microemulsions [5], and also as a discretized string action (the so-called gonihedric model) [6–10]. The critical behavior of the square lattice version of this model has been studied for many years and is now well established [11], but very little has been done in the three-dimensional case. Previous mean-field calculations [3,12] have shown that the model exhibits a very rich phase diagram, with lamellar and ordered bicontinuous [13] phases, disordered structured and nonstructured regions [14,15], and coexisting ferromagnetic and paramagnetic phases with a first-order wetting transition [16].

The purpose of the present paper is to investigate the critical properties of the model beyond the mean-field level [17], focusing mainly on the multicritical and crossover properties of the line of critical end points of the ferromagnetic-paramagnetic phase transition. This will be done by means of the cluster variation method (CVM) [18,19] in its cube and star-cube [20] approximations, and the recently proposed cluster variation–Padé approximant method (CVPAM) [21–23]. Before turning to the description of our results, we now give a short account of both the model and the method.

The model is defined by the reduced Hamiltonian $\mathcal{H}=-\beta H$

$$\mathcal{H}=J_1\sum_{\langle ij\rangle} s_i s_j+J_2\sum_{\langle\langle ij\rangle\rangle} s_i s_j+J_3\sum_{[i,j,k,l]} s_i s_j s_k s_l, \qquad (1)$$

where $\sigma_i=\pm 1$ is the Ising variable associated with the site i of our simple cubic lattice, and sums are respectively over the NN pairs, NNN pairs, and plaquettes of the lattice.

In terms of the Peierls surfaces separating domains of spins with different sign, not only the area but also the bending and the intersections of the Peierls interfaces are weighted by the couplings J_1,J_2,J_3 [4]. If β_A,β_C,β_I are respectively the energy cost for a plaquette, a bending between two adjacent plaquettes and an intersection of four plaquettes sharing a common dual link of the Peierls interfaces, the relation with the couplings J_1,J_2,J_3 is $\beta_A=2J_1+8J_2$, $\beta_C=2(J_3-J_2)$, $\beta_I=-4(J_2+J_3)$ [3]. The model (1) can be considered as a discrete realization of a random surface model with an extrinsic curvature energy term [24,25]. Recently, the special case in which only bendings and intersections are taken into account and the area is not weighted at all (that is $J_1/\beta=2\kappa$, $J_2/\beta=-\kappa/2$, $J_3/\beta=(1-\kappa)/2$, where $\kappa=0$ is the case of phantom surfaces [26], while $\kappa\to\infty$ represents the limit of complete self-avoidance) has been put in connection with a discretized string model (the so-called gonihedric model) [6] and studied by Savvidy and Wegner [7]. This choice of the couplings corresponds to a zero temperature high degeneracy point where all possible sequences of ''+'' and ''−'' planes have the same energy. A phase transition has been found in this restricted parameter space with exponents different from the usual three-dimensional (3D) Ising exponents [8–10]. It has to be observed that this special case corresponds to the disorder line [27] $J_2=-J_1/4$ as calculated in the mean-field approximation [12] and that in the two-dimensional case there is no transition neither on the disorder line [28] nor on the line $J_2=-J_1/4$ [29].

We will concentrate on the study of the phase diagram around the region where the lamellar, the ferromagnetic and the paramagnetic phases coexist, which is close to the line $J_2=-J_1/4$, and we will explain the origin of the transition found in [8,9]. There is a particular physical interest in this region due to the extremely low values of the surface tension between coexisting phases [12], which is an important property for applications in real surfactant systems [5].

Let us now briefly discuss the methods we are going to use. The cluster variation method is a powerful generalized mean-field theory introduced by Kikuchi [18] and then refor-

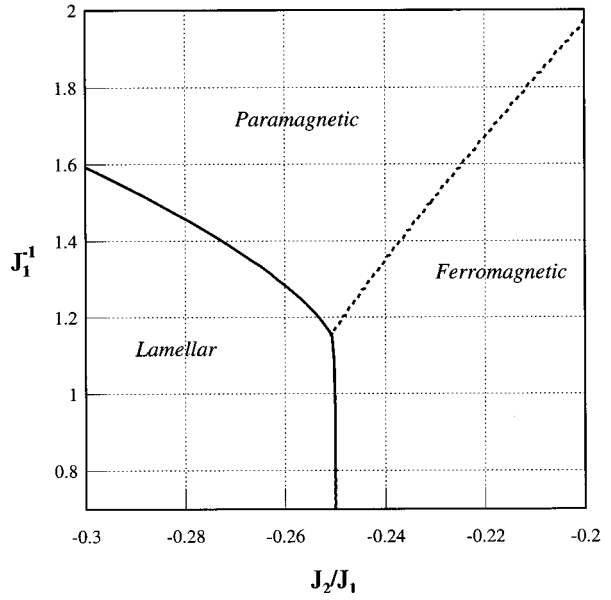

FIG. 1. The phase diagram of the model (1) for $J_3=0$. Solid and the dashed lines represent first- and second-order transitions respectively.

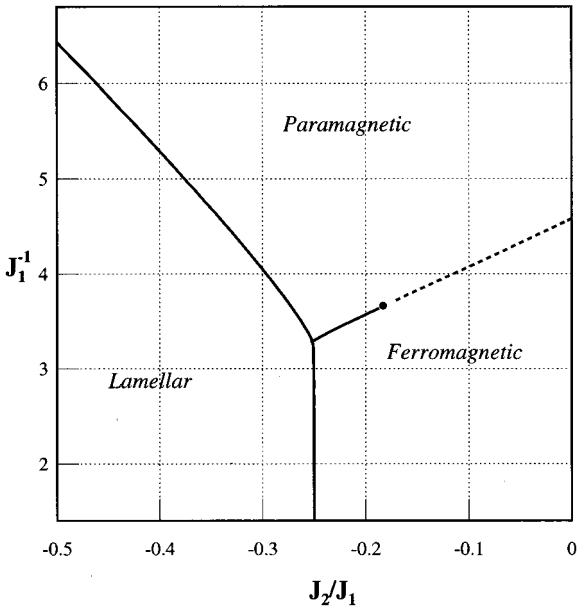

FIG. 2. The phase diagram of the model (1) for $\kappa=1/3$. Solid and the dashed lines represent first- and second-order transitions respectively.

mulated in a very elegant way [19] as a truncated cluster (cumulant) expansion of the variational principle of statistical mechanics. In the cube approximation of the CVM one has to minimize the free energy density functional

$$f[\rho_8]=\mathrm{Tr}(\rho_8 H_8)+\frac{1}{\beta}\Bigg[\mathrm{Tr}\ \mathcal{L}(\rho_8)-\frac{1}{2}\sum_{\text{plaquettes}}\mathrm{Tr}\ \mathcal{L}(\rho_{4,\text{plaq}})+\frac{1}{4}\sum_{\text{edges}}\mathrm{Tr}\ \mathcal{L}(\rho_{2,\text{edge}})-\frac{1}{8}\sum_{\text{sites}}\mathrm{Tr}\ \mathcal{L}(\rho_{1,\text{site}})\Bigg], \qquad (2)$$

where H_8 is the contribution of a single cube to the Hamiltonian (when splitting the total Hamiltonian H into single cube contributions one has to keep in mind that nearest-neighbor interactions are shared by four cubes and then will get a coefficient 1/4 in H_8, and similarly next-nearest-neighbor and plaquette interactions will get a coefficient 1/2), $\mathcal{L}(x)=x\ \ln x$, ρ_α with $\alpha=8$ (4, 2, 1) denotes the cube (respectively plaquette, edge, site) density matrix, and the sums in the entropy part are over all plaquettes (edges, sites) of a single cube (notice that we have not assumed any *a priori* symmetry property for our density matrices, and that the plaquette, edge and site matrices can be thought of as partial traces of the cube matrix). In the following we shall also use, for the ferromagnetic phase only, the star-cube approximation, introduced in [20], where it is described in great detail for the NN case (inclusion of NNN and plaquette interactions is indeed straightforward). For both approximations, the (numerical) minimization task is greatly simplified by the so-called natural iteration method [20,30].

Being an approximate variational theory, the CVM yields necessarily classical values of the critical exponents. In order to overcome this major drawback, one of us has proposed the cluster variation–Padé approximant method [21–23]. The basic idea of the CVPAM is that, since the CVM with 7–8 point or larger clusters is very accurate at high and low enough temperatures, one can extrapolate the results at such temperatures using D log Padé approximants [31] (see [23] for an application of the more sophisticated Adler's methods) in order to extract accurate information about the critical behavior, i.e., improved critical temperatures and nonclassical, precise critical exponents. In test applications, indeed, the CVPAM has produced results of quality almost comparable to state of the art Monte Carlo simulations, but with a much smaller numerical effort.

We can describe our results. The ground states of the model have been thoroughly investigated in [3]; here we shall consider the restricted parameter space J_1, J_2 and $\kappa>0$ with $J_3/J_1=(1-\kappa)/(4\kappa)$. In this region, the line $J_2/J_1=-1/4$ is always the boundary between ferromagnetic and lamellar ground states.

In Fig. 1 the phase diagram of the model (1) as given by the CVM cube approximation is depicted in the plane $J_3=0$. The line separating the paramagnetic and the ferromagnetic phase (dashed line) is a second order line, with the usual critical Ising transition at $J_1=0.218$ (shifted to $J_1=0.222$ by application of the CVPAM [21]), to be compared with the best estimate $J_1=0.22165$ [32]. The lamellar phase—here consisting of alternate planes of different sign—is separated from the paramagnetic and the ferromagnetic phase by a coexistence line (solid line) [33], which is asymptotically close to the line $J_2=-J_1/4$ at low temperature. The second-order line ends onto the first order one with a critical end point at $J_1^{\text{end}}=0.865\pm0.005$ and $J_2^{\text{end}}=-0.2176\pm0.0006$. In the case of the gonihedric model [6] with $\kappa=1$, our value for the inverse critical temperature is $\beta_c=0.427$ to be compared with the value $\beta_c=0.44$ found by Monte Carlo simulations [8] and the upper bound $\beta_c=1.49$ calculated in [9]. Notice that, since the lamellar-ferromagnetic coexistence line is slightly bent toward the lamellar phase (and this feature persists at $J_3\neq0$), the critical point of the gonihedric model is extremely close to our critical end point, and this has important consequences on the meaning of the exponents that one can define, as we shall see.

TABLE I. Inverse critical temperatures $J_c(R)=1/T_c(R)$ and order parameter amplitudes for $\kappa=1$.

R	-0.14	-0.15	-0.16	-0.17	-0.18	-0.19	-0.20	-0.21	-0.22	-0.23	-0.24
$J_{1,c}(R)$	0.360	0.378	0.398	0.421	0.447	0.476	0.511	0.552	0.602	0.663	0.743
$B(R)$	1.84	1.87	1.90	1.95	2.01	2.06	2.17	2.28	2.47	2.68	3.15

The topology of the phase diagram at varying κ remains the same as at $J_3=0$, but in the range $0<\kappa<\kappa^*$, with $\kappa^*\simeq 0.8$, there is a tricritical point (see Fig. 2) on the ferromagnetic-paramagnetic transition line at negative values of J_2 [34]. The transition line becomes of first order before reaching the lamellar phase.

The critical behavior suggested by the phase diagram of Fig. 1 can be now discussed. The first important point is that the critical end point we have found (actually a line of critical end points, since κ can vary), which does not exist in two dimensions [11], must be described by critical exponents which differ from the usual three-dimensional Ising ones, which apply to the ferromagnetic-paramagnetic critical surface. As a consequence, in the vicinity of the line of critical end points, which bounds the critical surface, it is natural to expect some crossover phenomenon.

In Ref. [10] we have already calculated with the CVPAM the order parameter critical exponent β of the gonihedric model (using CVM results up to a temperature which was less than half the transition temperature), finding $\beta=0.062\pm 0.003$ (together with the improved estimate for the inverse critical temperature $\beta_c=0.434$), which agrees well with the Monte Carlo estimates $\beta/\nu=0.04(1)$ and $\nu=1.2(1)$ [8]. In view of the above considerations this must be regarded as an effective exponent (in our picture the critical transition of the gonihedric model lies on the universal ferromagnetic-paramagnetic critical surface, and hence has to be described by the usual 3D Ising exponents), induced by a crossover phenomenon. Nevertheless, the critical transition of the gonihedric model is extremely close to our critical end point (CEP) and this means that the corresponding exponents are very good approximations to the critical end point ones. Thus from now on we shall use the estimate $\beta_{\mathrm{CEP}}=0.062\pm 0.003$. In order to calculate also γ_{CEP}, we have determined the high temperature susceptibility for $J_3=0$ and $J_2=-J_1/4$ in the cube approximation of the CVM and, according to the CVPAM prescriptions, we have determined D log Padé approximants (biased with our improved β_c) to it, and from these we have deduced $\gamma_{\mathrm{CEP}}=1.41\pm 0.02$.

The analysis of the crossover phenomenon is a considerably more difficult task, and we have tried to give an estimate of the crossover exponent ϕ [35] proceeding along the lines described in [22]. From now on we set $J_2/J_1=R$. Assuming that near the critical end point, but still in the ferromagnetic phase, the order parameter has a multicritical scaling law given by

$$m\simeq t^{\beta_{\mathrm{CEP}}} f(z), \quad z=\frac{R-R_{\mathrm{CEP}}}{t^{\phi}}, \tag{3}$$

where t is the deviation from the critical temperature and R_{CEP} can be well approximated by $-1/4$ (see also below), one can derive the scaling laws

$$T_c(R)-T_c(R_{\mathrm{CEP}})\propto (R-R_{\mathrm{CEP}})^{1/\phi} \tag{4}$$

for the ferromagnetic critical temperature and

$$B(R)\propto (R-R_{\mathrm{CEP}})^{-\omega}, \quad \omega=\frac{\beta_{\mathrm{Ising}}-\beta_{\mathrm{CEP}}}{\phi}, \tag{5}$$

where $\beta_{\mathrm{Ising}}\simeq 0.327$ [36] is the usual three-dimensional Ising exponent (a high-order CVPAM analysis on the simple cubic lattice predicted $\beta_{\mathrm{Ising}}=0.325(4)$ [23]), for the critical amplitude $B(R)$, which is defined by

$$m\simeq B(R)(T_c(R)-T)^{\beta_{\mathrm{Ising}}}, \quad R>R_{\mathrm{CEP}}. \tag{6}$$

Using the CVPAM we have extrapolated the low-temperature ferromagnetic order parameter (the smallest value used being 0.89) given by the CVM star-cube approximation, to calculate the critical temperatures and amplitudes in the range $-0.24\leqslant R\leqslant -0.14$ for $\kappa=1,2$ and 10. $T_c(R)$ was determined by requiring that $T_c(R)$-biased D log Padé approximants gave $\beta_{\mathrm{Ising}}=0.327$ and then the critical amplitude could be obtained by making approximants to $(T_c(R)-T)^{-\beta_{\mathrm{Ising}}}m$. As a check, for the simple NN Ising model (that is $\kappa=0$ and $R=0$) we have obtained $B(0)\simeq 1.626$, to be compared with the value 1.691 904 5 reported by Blöte and Talapov. The results for $\kappa=1$ are reported in Table I. Several fits were then made. The fits on the basis of Eq. (4) gave $\phi=1.13$, 1.09, and 1.03 for $\kappa=1,2$ and 10 respectively, while the fits to Eq. (5) gave $\phi=1.16$ and 1.20 for $\kappa=1$ and 2 and were inconclusive for $\kappa=10$. A fit with R_{CEP} free was also made to Eq. (5) for $\kappa=1$, and the result was $R_{\mathrm{CEP}}=-0.249\,774$, confirming that $R_{\mathrm{CEP}}=-1/4$ is a very good approximation.

A reasonable final estimate for the crossover exponent might then be $\phi=1.1(1)$, but it must be taken with some care for several reasons. Apart from the various approximations involved in the calculations of ϕ, it is a matter of fact that a similar calculation in the case of the semi-infinite Ising model [22] gave a result differing by 10–30 % from extensive computer simulations, and furthermore the true multicritical scaling law for the order parameter might be more complicated than our Eq. (3) (e.g., the scaling axes might not be parallel to the T and R axes), although the relatively good quality of the fits seems to indicate that Eq. (3) is fairly good.

Summarizing, we have studied the critical and multicritical behavior of the simple cubic Ising model with NN, NNN, and plaquette interactions, calculating the exponents of a line of critical end points which does not exist in two dimensions and might be relevant for some surfactant system. We have also tried to give an estimate of the crossover exponent, but this can certainly be refined using, e.g., Monte Carlo simulations or series expansions combined with the partial differential approximants method [37].

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[1] E. Ising, Z. Phys. **31**, 253 (1925).
[2] See, e.g., *Statistical Mechanics of Membranes and Surfaces*, edited by D.R. Nelson, T. Piran, and S. Weinberg (World Scientific, Singapore, 1989).
[3] A. Cappi, P. Colangelo, G. Gonnella, and A. Maritan, Nucl. Phys. **B370**, 659 (1992).
[4] M. Karowski, J. Phys. A **19**, 3375 (1986).
[5] For a recent review see G. Gompper and M. Schick, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, London, 1994), Vol. 16.
[6] R. V. Ambartzumian, G. S. Sukiasan, G. K. Savvidy, and K. G. Savvidy, Phys. Lett. B **275**, 99 (1992).
[7] G. K. Savvidy and F. J. Wegner, Nucl. Phys. B **413**, 605 (1994); G. K. Savvidy, K. G. Savvidy, and F. J. Wegner, *ibid.* **443**, 565 (1995).
[8] D. A. Johnston and R. P. K. C. Malmini, Phys. Lett. B **378,** 87 (1996); hep-lat/9508026.
[9] R. Pietig and F. J. Wegner, Nucl. Phys. B **466,** 513 (1996).
[10] E. N. M. Cirillo *et al.*, Phys. Lett. A (to be published); hep-lat/9607078.
[11] See, e.g., J. M. J. van Leeuwen, Phys. Rev. Lett. **34**, 1056 (1975); for the relation with the 8-vertex model see [28].
[12] G. Gonnella, S. Lise, and A. Maritan, Europhys. Lett. **32**, 735 (1995).
[13] L. E. Scriven, Nature (London) **263**, 123 (1976).
[14] B. Widom, J. Chem. Phys. **90**, 2437 (1989).
[15] P. Colangelo, G. Gonnella, and A. Maritan, Phys. Rev. E **47**, 411 (1993).
[16] G. Gompper and M. Schick, Phys. Rev. Lett. **65**, 1116 (1990).
[17] Actually, Monte Carlo simulations have been performed [3,4] to investigate the critical behavior of model (1), but only in the region close to the usual Ising transition point, where tricritical points with classical exponents have been found on the ferromagnetic-paramagnetic transition line.
[18] R. Kikuchi, Phys. Rev. **81**, 988 (1951).
[19] G. An, J. Stat. Phys. **52**, 727 (1988); T. Morita, *ibid.* **59**, 819 (1990).
[20] A. Pelizzola, Physica A **211**, 107 (1994).
[21] A. Pelizzola, Phys. Rev. E **49**, R2503 (1994).
[22] A. Pelizzola, J. Magn. Magn. Mater. **140-144**, 1491 (1995).
[23] A. Pelizzola, Phys. Rev. E **53**, 5825 (1996).
[24] W. Helfrich, Z. Naturforsch. **28C**, 693 (1973).
[25] A. M. Polyakov, Nucl. Phys. B **268**, 406 (1986).
[26] Surfaces without excluded volumes are sometimes called phantom surfaces.
[27] The disorder line is the line limiting in the paramagnetic phase the region where the structure function has a peak at a transferred momentum diferent from zero. In the 2D 8-vertex model it has been calculated by J. Stephenson, J. Math. Phys. (N.Y.) **11**, 420 (1970).
[28] R.J. Baxter, *Exactly Solved Models in Statistical Mechanics* (Academic, London, 1982).
[29] In the case $J_3=0$ see D. P. Landau and K. Binder, Phys. Rev. B **31**, 5946 (1985).
[30] R. Kikuchi, J. Chem. Phys. **60**, 1071 (1974).
[31] A. J. Guttmann, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic, London 1989), Vol. 13.
[32] See, for example, A. M. Ferrenberg and D. P. Landau, Phys. Rev. B **44**, 5081 (1991).
[33] Our calculations show that the ferromagnetic-lamellar transition line, even if quite close, does not exactly coincide with the line $J_2=-J_1/4$ as it was assumed in [8].
[34] More extensive studies of the phase diagram and of the tricritical end point will appear elsewhere.
[35] For crossover scaling theory see, e.g., M. E. Fisher, Rev. Mod. Phys. **46**, 597 (1974) and, in a slightly different context, D. P. Landau and K. Binder, Phys. Rev. B **41**, 4633 (1990).
[36] A. L. Talapov and H. W. J. Blöte, J. Phys. A **29,** 5727 (1996); preprint cond-mat/9603013.
[37] See, e.g., M. E. Fisher and D. F. Styer, Proc. R. Soc. London, Ser. A **384**, 259 (1982); **388**, 75 (1983).