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Low-temperature phase of the three-state antiferromagnetic Potts model on the simple-cubic lattice

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The three-state antiferromagnetic Potts model on the simple-cubic lattice is investigated using the cluster variation method in the cube and the star-cube approximations. The broken-sublattice-symmetry phase is found to be stable in the whole low-temperature region, contrary to previous results obtained using a modified cluster variation method. The tiny free-energy difference between the broken-sublattice-symmetry and the permutationally-symmetric sublattice phases is calculated in the two approximations and turns out to be smaller in the (more accurate) star-cube approximation than in the cube one. [S1063-651X(96)50212-6]

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The three-state antiferromagnetic Potts model on the simple-cubic lattice has been intensively studied in the last two decades, because of its unusual and rather obscure low-temperature and critical properties [1–16]. The model Hamiltonian is very simple and can be written as

$$\mathcal{H}=J\sum_{\langle ij\rangle}\delta(s_i,s_j), \tag{1}$$

where $J>0$ is the interaction strength, the summation is over all nearest-neighbor (NN) pairs, δ denotes Kronecker's delta, and the variables s_i can take on three different values, say $\{1,2,3\}$.

It is now commonly accepted that the model exhibits a continuous phase transition at temperature $T_c=1.23$ (in units of J/k_B, with k_B Boltzmann's constant), belonging to the universality class of the three-dimensional XY model, as suggested by the value of the critical exponents recently calculated by means of extensive Monte Carlo simulations [13] and the coherent-anomaly method [14]. The nature of the ordered phase, however, is not yet as clear as the critical behavior.

In the past some authors suggested that the ordered phase should be one with algebraically decaying correlations like a Kosterlitz-Thouless phase [1,5,7,8], or an incompletely ordered phase [10]. Other studies, however, indicated the existence of a long-range ordered phase called broken-sublattice-symmetry (BSS) phase [2–4,9]. In this phase the simple-cubic lattice is split into two interpenetrating sublattices, say A and B, such that a site in A has all its nearest neighbors belonging to B and vice versa. In terms of the site expectations $p_{k,\alpha}=\langle\delta(s_i,k)\rangle, i\in\alpha$, with $k=1,2,3$ and $\alpha=A,B$, the BSS phase can be roughly described, at very low temperatures, by $p_{1,A}=1$, $p_{1,B}=0$ and $p_{k,A}=0$, $p_{k,B}=1/2$ for $k=2,3$ (it can be easily verified that the phase is sixfold degenerate). To be more precise, even at very low temperature, there is a small probability to find $s_i=2$ or 3 in sublattice A, too, because this causes no increase in energy when the neighboring sites are all in the state 3 or 2, respectively. This implies that the long-range order does not saturate even at zero temperature, and that the zero temperature entropy per site is slightly larger than the value $\frac{1}{2}\ln 2\simeq 0.346\,574$ one would predict naively.

Furthermore, in a recent investigation of the Blume-Emery-Griffiths model by Rosengren and Lapinskas [11], based on a modified cluster variation method, a new phase was found in an intermediate temperature region $(0.78<T<T_c)$ between the BSS and the disordered phase.

This phase, of degeneracy twelve, is characterized by the relation $p_{1,A}=p_{2,B}>p_{3,A}=p_{3,B}>p_{2,A}=p_{1,B}$ between the site expectations, and has been called the permutationally-symmetric-sublattices (PSS) phase by the authors. The result is qualitatively similar to that obtained in the Bethe approximation (which, of course, predicts higher transition temperatures), and has received a partial confirmation by a Monte Carlo investigation by the same authors and Kundrotas [16]. On the other hand, a different Monte Carlo investigation by Kolesik and Suzuki [15] suggests that an intermediate phase might exist but cannot be the PSS phase predicted by Rosengren and Lapinskas. Kolesik and Suzuki have computed the free energies of the BSS and PSS phases, finding indications that the BSS free energy is lower in the low temperature region, up to a temperature which is higher (slightly below 1.0) than the transition temperature proposed by Rosengren and Lapinskas. For even higher temperatures, the free energy difference between the BSS and PSS phases is indistinguishable from zero, although the authors conclude that they cannot definitely rule out the possibility that it vanishes only at the critical point.

In the present work we examine carefully the issue of the type of ordered phase(s) by means of two high order approximations of the cluster variation method (CVM) [17–19]. The CVM is a simple and powerful variational method for Ising-like models, based on a cumulant expansion of the variational principle of statistical mechanics. The full (and generally unaffordable) variational principle is based on the minimization of the functional

$$\mathcal{F}[\rho_\Lambda]=\mathrm{Tr}(\rho_\Lambda\mathcal{H}+k_BT\rho_\Lambda\ln\rho_\Lambda), \tag{2}$$

where Λ is the lattice, ρ_Λ the corresponding trial density matrix, and Tr stands for trace. In the CVM one chooses a set of maximal clusters to take into account and considers the approximate variational functional

$$F[\{\rho_\alpha,\alpha\in M\}]=\sum_{\alpha\in M}\mathrm{Tr}(\rho_\alpha\mathcal{H}_\alpha+k_BTa_\alpha\rho_\alpha\ln\rho_\alpha), \tag{3}$$

where M is the set of the maximal clusters and all their subclusters, ρ_α the reduced trial density matrix for the cluster α, $\mathcal{H}_\alpha$ the Hamiltonian contribution associated to the cluster α (in the present case $\mathcal{H}_\alpha=0$ if α is not a nearest-neighbor pair), and the a_α's are constant, geometry-dependent coefficients that can be easily obtained by solving a suitable set of linear equations [18,19]. The approximate functional F has to be minimized with respect to the cluster density matrices (which, for a classical model, are diagonal), with the constraints (normalization and compatibility, respectively)

$$\mathrm{Tr}\rho_\alpha=1,\quad \alpha\in M \quad\text{and}\quad \mathrm{Tr}_{\alpha\setminus\beta}\rho_\alpha=\rho_\beta,\quad \beta\subset\alpha\in M. \tag{4}$$

In this work we shall use two different approximations in the CVM scheme, the cube and the star-cube ones. The cube approximation [17] is obtained by selecting as maximal clusters the cubic cells of the lattice, and the corresponding functional (free energy per site) is

$$f[\rho_8]=3\mathrm{Tr}(\rho_2\mathcal{H}_2)+k_BT\Big[\mathrm{Tr}(\rho_8\ln\rho_8)-3\mathrm{Tr}(\rho_4\ln\rho_4)+3\mathrm{Tr}(\rho_2\ln\rho_2)-\frac{1}{2}\mathrm{Tr}(\rho_{1A}\ln\rho_{1A})-\frac{1}{2}\mathrm{Tr}(\rho_{1B}\ln\rho_{1B})\Big], \tag{5}$$

where ρ_8, ρ_4, ρ_2, and $\rho_{1\alpha}$ denote the density matrices for the cube, square, nearest-neighbor pair, and site (with a sublattice index $\alpha=A,B$) clusters, respectively. f can be regarded as a functional of ρ_8 only, since the compatibility constraints can be easily solved by *defining* the other density matrices as partial traces of ρ_8. In principle, ρ_8 has $3^8=6561$ different diagonal elements, but symmetry considerations reduce this number to 495, which (apart from the normalization constraint, which can be easily dealt with) is the final number of independent variables for this approximation. Despite this large number of variables, the local minima corresponding to the various phases are easily obtained by means of the so-called natural iteration method (NIM) [20].

The star-cube approximation [21] goes a step further, including in the set of maximal clusters also the ''stars'' formed by a site and its six nearest neighbors. This choice seems particularly useful here, since in view of the above remarks on the very low temperature properties of the BSS phase it should be particularly important to consider explicitly the local environment of a site. The resulting approximate functional has the form

$$\begin{aligned}f[\rho_8,\rho_{7A},\rho_{7B}]=3\mathrm{Tr}(\rho_2\mathcal{H}_2)+k_BT\Big[&\mathrm{Tr}(\rho_8\ln\rho_8)+\frac{1}{2}\mathrm{Tr}(\rho_{7A}\ln\rho_{7A})+\frac{1}{2}\mathrm{Tr}(\rho_{7B}\ln\rho_{7B})\\&-3\mathrm{Tr}(\rho_4\ln\rho_4)-4\mathrm{Tr}(\rho_{4'A}\ln\rho_{4'A})\\&-4\mathrm{Tr}(\rho_{4'B}\ln\rho_{4'B})+6\mathrm{Tr}(\rho_{3A}\ln\rho_{3A})\\&+6\mathrm{Tr}(\rho_{3B}\ln\rho_{3B})-3\mathrm{Tr}(\rho_2\ln\rho_2)\Big],\end{aligned}$$

where $\rho_{7\alpha}$, $\rho_{4'\alpha}$ and $\rho_{3\alpha}$ are the reduced density matrices (all with a sublattice index α referring to the central site) for the star cluster and its four- and three-site subclusters obtained by taking the central site and three or two of its nearest neighbors forming a solid angle or a plane angle, respectively. The functional now depends on ρ_8, ρ_{7A} and ρ_{7B} (subcluster matrices being defined as partial traces, as above), but the diagonal elements of these matrices are not all independent because of the compatibility constraints. Taking into account the lattice symmetries one finds 495 variables for the cube matrix, 168 variables for each star matrix, and two sets of 30 linear constraints.

It is important to notice here that the calculation which suggested the stability of the PSS phase [11,12] was based on a modification of the cluster variation method which, although considering many-point clusters (up to the cube cluster, like our cube approximation), does not take into account

properly the n-point correlations with $n>2$. In the modified CVM, in fact, the density matrices are written as $\rho_\alpha = \exp(-\mathrm{H}\alpha(\mathrm{eff}))$, where $H_\alpha^{(\mathrm{eff})}$ is an effective Hamiltonian which contains only one-site and two-site terms. This results in a reduced number of variational parameters and in violation of the compatibility constraints in Eq. (4) (for a full description of the method, see Ref. [22]; the authors of Refs. [11,12] do not report details of the method used, leaving them to Ref. [23], which in turn refers to [22]). The results for the ordered phases are then qualitatively similar to those obtained using the much simpler two-point (Bethe) approximation. The present work can then be regarded as an improvement of that described in [11] for two reasons: first, the CVM is used in its full form, i.e., without the restriction inherent to the modified version used in [11]; second, with the star-cube approximation we go one step further in the cumulant expansion of the variational principle.

Let us now turn to a brief description of our results. As far as very low temperatures are concerned, results from the cube approximation are in perfect agreement with the modified CVM at the cube level [11,12]. In particular we have $p_{1A}=0.939\,067$, $p_{2A}=p_{3A}=0.030\,467$ and $p_{1B}=0.000\,117$, $p_{2B}=p_{3B}=0.499\,942$, while the entropy per site is $s=0.366\,928$. The star-cube approximation introduces only very small corrections, giving $p_{1A}=0.939\,041$, $p_{2A}=p_{3A}=0.030\,480$ and $p_{1B}=0.000\,055$, $p_{2B}=p_{3B}=0.499\,972$, with an entropy per site of $s=0.366\,941$.

Also the critical temperature does not change much with respect to the modified CVM. In the cube approximation we obtain $T_c=1.268$, which is just 0.5% higher than the modified CVM results, a difference of the same sign and order of magnitude of the one found in the simple Ising case [22]. In the star-cube approximation the critical temperature is slightly lower, $T_c\simeq 1.263$. These results are to be compared with the most recent Monte Carlo estimate $T_c=1.23$ [13].

These estimates can be further improved by employing the recently introduced cluster-variation–Padé-approximants method (CVPAM) [24,25], from which one can try to extract also estimates for the critical exponents. Using the star-cube results for the susceptibility for values of $w=\tanh(1/T)$ up to $w_{\max}=0.48$ we have obtained (with simple Dlog Padé approximants) a critical temperature $T_c\simeq 1.24$ and a critical exponent γ ranging from 1.30 to 1.33, in agreement with the best recent estimates yielding $\gamma\simeq 1.31$ [13]. These CVPAM results are still affected by relatively large systematic errors, and an accurate CVPAM analysis would require both using larger maximal clusters and including corrections to scaling [25]. This is beyond the scope of the present paper, but our calculation of γ can at least be regarded as a check of the accuracy of the CVM results.

The central result of our paper, qualitatively different from the modified CVM, is, however, that the free energy of the BSS phase is always lower (although slightly) than that of the PSS phase. In Fig. 1 we have plotted the free energy difference δf vs temperature as given by the two approximations. It is important to notice that the numerical errors involved in the estimation of the free energy are several order of magnitudes smaller than δf. From Fig. 1 one can see that δf is very small in the cube approximation, and

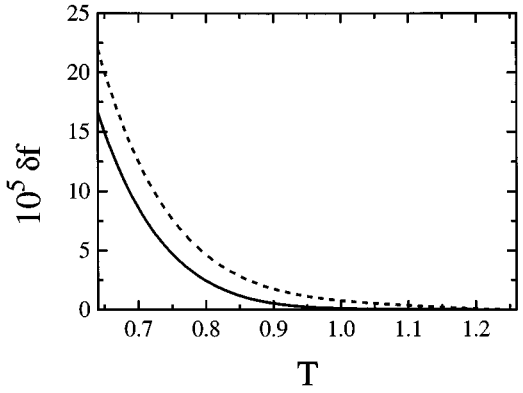

FIG. 1. Free energy difference between the PSS and the BSS phases, as given by the cube (dashed line) and the star-cube approximation (solid line)

becomes even smaller in the more accurate star-cube approximation. In both approximations δf vanishes only at the critical point, but in the star-cube approximation it becomes negligibly small at a temperature slightly below 1.0, like in the Monte Carlo simulations by Kolesik and Suzuki [15]. Furthermore, the numerical values of δf are of the same order of magnitude as those reported by these authors.

Although it is difficult to judge on the basis of our results which is the exact ordered phase, some conclusions can certainly be drawn. First of all, the results found by Rosengren and Lapinskas with the modified CVM [11] are ruled out and attributed to the neglect of high-order correlations (remember that a simple Bethe approximation yields the same qualitative results). This means also that the phase diagram they proposed for the Blume-Emery-Griffiths model [12] is incorrect and must be reconsidered. On the other hand, the present CVM predictions are compatible with the Monte Carlo results by Kolesik and Suzuki [15]. The Monte Carlo simulations tends to favor the possibility that the free energy difference δf vanishes below the critical point, giving rise to a new intermediate phase. The CVM results seems to support this possibility, the free energy difference δf being strongly depressed, while going from the cube to the star-cube approximation, in the same temperature region. In order to make this explicit, we have plotted in Fig. 2 the ratio between the two values of δf reported in Fig. 1. It can be seen

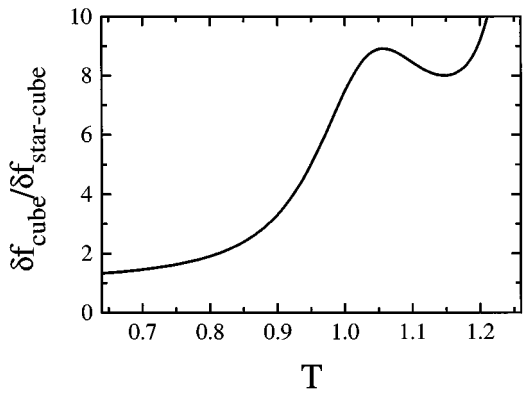

FIG. 2. Ratio of the free energy differences given by the cube and the star-cube approximations

that this ratio increases very quickly for temperatures between 0.9 and 1.0, and this could be a signal that upon going to larger and larger maximal clusters the free energy difference tends to zero. Both the Monte Carlo simulations and the cluster variation method, however, leave open also the possibility that the free energy difference vanishes only at the critical point, and further investigations are therefore welcome.

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