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Testing Approximate Theories of First-Order Phase Transitions on the Two-Dimensional Potts Model

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The two-dimensional, q-state ($q > 4$) Potts model is used as a testing ground for approximate theories of first-order phase transitions. In particular, the predictions of a theory analogous to the Ramakrishnan–Yussouff theory of freezing are compared with those of ordinary mean-field (Curie–Wiess) theory. It is found that the Curie–Weiss theory is a better approximation than the Ramakrishnan–Yussouff theory, even though the former neglects all fluctuations. It is shown that the Ramakrishnan–Yussouff theory overestimates the effects of fluctuations in this system. The reasons behind the failure of the Ramakrishnan–Yussouff approximation and the suitability of using the two-dimensional Potts model as a testing ground for these theories are discussed.

KEY WORDS: First-order phase transitions; Curie–Weiss theory; Ramakrishnan–Yussouff theory; large-q expansions for q-state Potts models; Monte Carlo simulations of Potts models.

1. INTRODUCTION

The theoretical study of first-order phase transitions has lagged behind that of continuous phase transitions, even though the former occur much more often than the latter. The reason for this lag is simple: There are various universal quantities (e.g., critical exponents, scaling functions$^{(1,2)}$) assocated with continuous transitions; these universal quantities can be obtained by studying the simplest model in a given universality class.$^{(1,2)}$ Though there can be certain striking similarities between different first-order phase transitions (such as different freezing transitions$^{(3)}$), there are no strictly universal features associated with these transitions; thus, each model must be studied separately.

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The renormalization group provides, in principle, a way of studying first-order phase transitions in any model: Once a renormalization-group transformation has yielded a set of recursion relations for the coupling constants that characterize a model, the first-order phase boundary is obtained by finding all the points in the space of coupling constants that flow, under successive renormalization-group transformations, to a *discontinuity fixed point.*(4,5) Free energies and the jump in the order parameter at a first-order phase boundary are calculated in the standard way.(5) The only problem with the renormalization-group approach is that it is very hard to implement for most models, such as those that yield liquid-to-solid freezing transitions.[3] Only for very simple models, such as the Ising and Potts models, has it been possible to construct approximate, but nonperturbative, renormalization-group transformations that yield discontinuity fixed points and the associated first-order phase transitions.

Since the implementation of the renormalization-group method is often not feasible, it is necessary to find tractable aproximations that can be used to study first-order phase transitions in any model. The most common approximation of this type is the mean-field, Curie–Weiss (CW)(7) approximation[4]: uniform order parameters (there may be more than one order parameter) characterize the possible ordered phases; no fluctuations are allowed for in these order parameters; and n-body interactions ($n \geqslant 2$) are approximate by effective one-body interactions, or effective fields, which depend on the order parameters. In equilibrium, the order parameters assume values that minimize (globally) the free energy of the system.

The mean-field approximation described above does not work for a liquid–solid transition: The equations that have to be solved to obtain the order parameters contain the Fourier transform of the potential via which two particles interact; in all cases of physical interest, this potential diverges rapidly as the particles approach each other, so its Fourier transform does not exist. Thus, the equations for the order parameters are meaningless.

The simplest way out of this difficulty with the mean-field approximation for the liquid–solid transition is to replace the pair potential via which particles interact by a density–density correlation function.(8,9) The most successful theory of this type is due to Ramakrishnan and Yussouff.(3,9–11) In place of the pair potential, they advocate the use of the direct correlation function(12) measured in the liquid just before it freezes.

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[3] There have been some recent efforts to develop renormalization-group transformations for models of simple liquids,(6) but these are in their infancy.

[4] Landau expansions of the free energy to some low order in the order parameter are not suitable for strongly first-order transitions.

Except for this modification, the equations for the order parameters have exactly the same form as they do in the conventional mean-field approximation.

During the last few years, the Ramakrishnan–Yussouff (RY) theory has been widely used in the description of freezing transitions into crystals,(3,9–11,13–16) liquid crystals,(17,18) glasses,(19,20) and even the recently discovered quasicrystals.(21) Given this extensive use, we feel the conditions under which the RY approximation is reliable should be studied.[5] It is our purpose here to initiate such a study.

In particular, we study the first-order phase transition in the two-dimensional, q-state ($q > 4$) Potts model by using a man-field theory that is a direct generalization of the RY theory of freezing. The predictions of this theory are compared with those of conventional CW mean-field theory and with available exact results. Unfortunately, we have not been able to find clear criteria for the validity of the RY approximation. Our principal results are: (1) For all values of q considered here ($q \geqslant 10$), the CW theory is a better approximation than the RY theory. (2) For the two-dimensional Potts model, the RY theory overestimates the role of fluctuations in precipitating the first-order transition to the ordered phase. (3) The results obtained from a calculation in which effects of three-spin correlations (which are neglected in the simplest RY approximation) are included are also quite different from known exact results.

The remaining part of this paper is organized as follows. In Section 2, we review briefly the RY theory of the freezing of a liquid, develop a similar theory for the first-order transition in q-state ($q > 4$) Potts models in two dimensions, and show how it is related to the conventional CW mean-field theory of these models. In Section 3, certain thermodynamic functions needed as inputs to the RY theory are calculated by using the technique of large-q expension, and the accuracy of the large-q expansion is checked by comparing the results with those obtained from a Monte Carlo simulation for $q = 10$. In Section 4, we work out the predictions of the RY theory for the first-order transition in the two-dimensional Potts model and compare them with the results obtained from the CW approximation and with available exact results. We also describe the results obtained from a calculation (for $q = 10$) in which the effects of three-spin correlations are included. Section 5 contains a summary of our principal results and a few

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[5] The conditions under which conventional man-field theory is reliable have been investigated thoroughly. All thermodynamic properties are given exactly by mean-field theory for systems with sufficiently long-ranged potentials. Universal critical properties are predicted correctly by mean-field theory above the upper critical dimension d_u ($d_u = 4$ in the most common cases).

concluding remarks. In particular, we discuss the suitability of using the two-dimensional Potts model as a testing ground for the RY approximation.

2. RAMAKRISHNAN–YUSSOUFF AND CURIE–WEISS APPROXIMATIONS

If F_l is the free energy of a uniform liquid with density ρ_l, then the free energy functional F for a nonuniform density $\rho(\mathbf{r})$ is$^{(13)}$

$$\begin{aligned}\beta(F-F_l) = {} & \beta \int d\mathbf{r}\, [\rho(\mathbf{r})-\rho_l]\, v_e(\mathbf{r}) \\ & + \int d\mathbf{r} \left\{ \rho(\mathbf{r}) \ln\left(\frac{\rho(\mathbf{r})}{\rho_l}\right) - [\rho(\mathbf{r})-\rho_l] \right\} \\ & - \frac{1}{2!\,\rho_l} \int d\mathbf{r}_1\, d\mathbf{r}_2\, C^{(2)}(\mathbf{r}_1,\mathbf{r}_2)[\rho(\mathbf{r}_1)-\rho_l][\rho(\mathbf{r}_2)-\rho_l] \\ & - \frac{1}{3!\,\rho_l^2} \int d\mathbf{r}_1\, d\mathbf{r}_2\, d\mathbf{r}_3\, C^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) \\ & \times [\rho(\mathbf{r}_1)-\rho_l][\rho(\mathbf{r}_2)-\rho_l][\rho(\mathbf{r}_3)-\rho_l] \\ & - \cdots \end{aligned} \tag{1}$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant, $v_e(\mathbf{r})$ is an external, one-body potential, and the correlation functions $C^{(2)}$, $C^{(3)}$, etc., are given by

$$C^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = [-\rho_l] \frac{\delta^2[\beta(F-F_l)]}{\delta\rho(\mathbf{r}_1)\,\delta\rho(\mathbf{r}_2)} \tag{2a}$$

$$C^{(3)}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3) = [-\rho_l^2] \frac{\delta^3[\beta(F-F_l)]}{\delta\rho(\mathbf{r}_1)\,\delta\rho(\mathbf{r}_2)\,\delta\rho(\mathbf{r}_3)} \tag{2b}$$

etc. Since the uniform liquid is rotationally invariant, $C^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = C(|\mathbf{r}_1-\mathbf{r}_2|)$, the direct correlation function. If we minimize $\beta(F-F_l)$ with respect to $\rho(\mathbf{r})$, we get

$$\begin{aligned}\frac{\rho(\mathbf{r})}{\rho_l} = \exp\Bigg\{ & -\beta v_e(\mathbf{r}) + \frac{1}{\rho_l}\int d\mathbf{r}_1\, C^{(2)}(\mathbf{r}-\mathbf{r}_1)[\rho(\mathbf{r}_1)-\rho_l] \\ & + \frac{1}{2\rho_l^2}\int d\mathbf{r}_1\, d\mathbf{r}_2\, C^{(3)}(\mathbf{r},\mathbf{r}_1,\mathbf{r}_2)[\rho(\mathbf{r}_1)-\rho_l][\rho(\mathbf{r}_2)-\rho_l] \\ & + \cdots \Bigg\} \end{aligned} \tag{3}$$

i.e., $\rho(\mathbf{r})/\rho_l$ assumes the value it would have in a noninteracting fluid with an effective, one-body potential (molecular field) given by

$$
\begin{aligned}
-\beta v_{\text{eff}}(\mathbf{r}) = {} & -\beta v_e(\mathbf{r}) + \frac{1}{\rho_l}\int d\mathbf{r}_1\, C^{(2)}(\mathbf{r}-\mathbf{r}_1)[\rho(\mathbf{r}_1)-\rho_l] \\
& + \frac{1}{2\rho_l^2}\int d\mathbf{r}_1\, d\mathbf{r}_2\, C^{(3)}(\mathbf{r}, \mathbf{r}_1, \mathbf{r}_2)[\rho(\mathbf{r}_1)-\rho_l][\rho(\mathbf{r}_2)-\rho_l] \\
& + \cdots
\end{aligned}
\tag{4}
$$

In the RY approximation, the terms containing $C^{(n)}$ with $n \geqslant 3$ are neglected in Eqs. (1), (3), and (4) and $C^{(2)}(\mathbf{r}_1-\mathbf{r}_2)$ is taken to be the direct correlation function measured in the liquid just before it freezes.

For a liquid in which the particles interact via a pair potential $V^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)$, the effective, one body-potential is

$$\frac{1}{\rho_l}\int d\mathbf{r}_1\, V^{(2)}(|\mathbf{r}-\mathbf{r}_1|)[\rho(\mathbf{r}_1)-\rho_l]$$

in the CW approximation. Thus, the RY approximation is the usual mean-field approximation for such a liquid with $V^{(2)}$ replaced by $-C^{(2)}/\beta$ in the self-consistent equation for $\rho(\mathbf{r})$ and the equation for the free energy functional $\beta(F-F_l)$. (In the remaining part of this paper we shall set $C^{(n)}=0$ for $n \geqslant 3$ unless stated otherwise.)

The phase into which the liquid freezes is characterized by an infinite number of order parameters, namely the expansion coefficients $\mu_{\mathbf{G}}$ in density waves

$$\frac{\rho(\mathbf{r})}{\rho_l} = 1 + \sum_{\mathbf{G}} \mu_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})$$

which represent the crystalline solid. In terms of these order parameters, Eq. (3) can be rewritten as ($C^{(n)}=0$, $n \geqslant 3$)

$$1 + \sum_{\mathbf{G}} \mu_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r}) = \exp\left[\sum_{\mathbf{G}} C_{\mathbf{G}}^{(2)} \mu_{\mathbf{G}} \exp(i\mathbf{G}\cdot\mathbf{r})\right] \tag{5}$$

where $C_{\mathbf{G}}^{(2)}$ is the Fourier transform of the direct correlation function ($C_{\mathbf{k}}^{(2)} = 1 - \rho_l S_{\mathbf{k}}^{-1}$, where $S_{\mathbf{k}}$ is the static structure factor of the liquid.)

For a liquid in which the particles interaact via a pair potential $V^{(2)}(|\mathbf{r}_1-\mathbf{r}_2|)$, the conventional mean-field approximation yields a formal expression like Eq. (5), with $C_{\mathbf{G}}^{(2)}$ replaced by $-\beta V_{\mathbf{G}}^{(2)}$, where $V_{\mathbf{G}}^{(2)}$ is the Fourier transform of $V^{(2)}(r)$. However, this formal expression is meaningless in all cases of physical interest because $V^{(2)}(r)$ diverges rapidly as $r \to 0$, so $V_{\mathbf{G}}^{(2)}$ does not exist. Hence, the conventional mean-field approximation fails for the freezing of a liquid.

Equation (5) is equivalent to an infinite set of coupled equations[6] for the order parameters $\mu_{\mathbf{G}}$. For the approximate solution of these equations and for the different choices of **G**'s that lead to different crystal structures,[7] we refer the reader to the original papers of Ramakrishnan and Yussouff$^{(3,9-11)}$ and to Refs. 13–16.

We now develop the analogs of Eqs. (1) and (3)–(5) for a q-state Potts model, which is defined by the Hamiltonian

$$H = -\sum_{i>j} J_{ij}\delta_{\sigma_i,\sigma_j} - \sum_i h_i^e(q\delta_{\sigma_i,1} - 1)/(q-1) \tag{6}$$

where the Potts spins σ_i can assume values 1, 2,..., q for all sites i, h_i^e is an external field [the analog of v_e in Eq. (1)] which is conjugate to the order parameter

$$m_i = \frac{1}{(q-1)} \langle (q\delta_{\sigma_i,1} - 1) \rangle$$

(the angular brackets denote a thermal average), and, for specificity, we choose J_{ij} to be equal to J if i, j are nearest neighbor pairs of sites on a two-dimensional, square lattice, and $J_{ij} = 0$ otherwise.

For $q > 4$, the model (6) with $h_i^e = 0$ for all i goes from a disordered state ($m_i = 0$) to an ordered one ($m_i \neq 0$) at a finite temperature T_c via a first-order phase transition.$^{(23)}$,[8] This transition is much simpler than the liquid–solid transition because the ordered state is uniform and there is only one order parameter. Also, the conventional mean-field approximation$^{(24)}$ is not meaningless for the Potts-model transition as it is for the liquid–solid transition.

To obtain the conventional mean-field and RY approximations for model (6), we write the density matrix ρ as a product $\prod_i \rho_i$, with the one-particle density matrices

$$\rho_i = \exp[-\beta H_{\text{eff}}(\sigma_i)]/\mathrm{Tr}\exp[-\beta H_{\text{eff}}(\sigma_i)] \tag{7}$$

$$H_{\text{eff}}(\sigma_i) = -h_i^{\text{eff}}(q\delta_{\sigma_{i,1}} - 1)/(q-1) \tag{8}$$

$$h_i^{\text{eff}} = h_i^e + h_i^r \tag{9}$$

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[6] This can be seen by multiplying both sides of Eq. (4) by $\exp(-i\mathbf{G}\cdot\mathbf{r})$ and integrating over a unit cell.

[7] In the simplest, one-order-parameter approximation, the magnitude of **G** is set equal to the value of **k** at which the structures factor $S_{\mathbf{k}}$ has its principal maximum.

[8] See Wu$^{(22)}$ for a review of phase transitions in two-dimensional Potts model.

where eff stands for effective and r for response. Conventional mean-field theory$^{(24)}$ is obtained by minimizing $\psi(\rho) \equiv k_B T \operatorname{Tr}(\rho \ln \rho) + \operatorname{Tr}(\rho H)$ with respect to h_i^{eff} and with $\rho = \prod_i \rho_i$. This yields

$$h_i^{\text{eff}} = h_i^e + \frac{q-1}{q} \sum_j J_{ij} m_j \tag{10}$$

In addition, the order parameter

$$m_i = \frac{\langle (q\delta_{\sigma_{i},1} - 1) \rangle_{\rho_i}}{q-1}$$

must satisfy the self-consistency relation

$$\beta h_i^{\text{eff}} = \frac{q-1}{q} \ln \frac{1+(q-1)m_i}{1-m_i} \tag{11}$$

The minimization of $\psi(\rho)$ with respect to h_i^{eff} is equivalent to the minimization of

$$\begin{aligned} F = & -\sum_i h_i^e m_i - \frac{q-1}{q} \sum_{i>j} J_{ij} m_i m_j \\ & + \frac{k_B T}{q} \sum_i \{[1+(q-1)m_i] \ln[1+(q-1)m_i] \\ & + (q-1)(1-m_i)\ln(1-m_i)\} - k_B T \ln q \end{aligned} \tag{12}$$

with respect to m_i; the resulting self-consistent equation for m_i is the same as the one obtained by combining Eqs. (10) and (11). For a uniform external field ($h_i^e = h^e$ for all i), the order parameter is uniform ($m_i = m$ for all i) at the global minimal of F, so the response field

$$h_i^r = zJ(q-1)m/q \tag{13}$$

where z is the coordination number of the lattice ($z = 4$ for the two-dimensional square lattice considered here).

This expression for the response field is not employed in the RY approximation. Instead, we expand h_i^r as [cf. Eq. (4)]

$$\beta h_i^r = \sum_j C_{ij}^{(2)} m_j + \frac{1}{2} \sum_{j,k} C_{ijk}^{(3)} m_j m_k + \cdots \tag{14}$$

and, as before, write the density matrix ρ as $\prod_i \rho_i$, with ρ_i given by Eqs. (7)–(9). Again, this yields the self-consistency relation (11). Substituting $h_{\text{eff}}^i - h_i^e$ for h_i^r in Eq. (14) and using Eq. (11), we get

$$C_{ij}^{(2)} = -(q-1)(\chi^{-1})_{ij} + (q-1)\delta_{ij} \tag{15}$$

where

$$(\chi^{-1})_{ij}=\frac{\beta}{q-1}\frac{\partial h_i^e}{\partial m_j}\bigg|_{\{m_i\}=0}$$

are the elements of the inverse susceptibility matrix. We define the nonlocal susceptibility as

$$\chi_{ij}\equiv(q-1)\frac{\partial m_i}{\partial(\beta h_j^e)}\bigg|_{\{h_i^e\}=0}$$

Given the Hamiltonian (6), the expression (14) for βh_i^r cannot be obtained by minimizing $\chi(\rho)=k_B T\,\mathrm{Tr}(\rho\ln\rho)+\mathrm{Tr}(\rho H)$. Instead, it is obtained by minimizing

$$\begin{aligned}\tilde{F}= &-\sum_i h_i^e m_i\\ &-k_B T\left[\frac{1}{2!}\sum_{ij}C_{ij}^{(2)}m_i m_j+\frac{1}{3!}\sum_{ijk}C_{ijk}^{(3)}m_i m_j m_k+\cdots\right]\\ &+\frac{k_B T}{q}\sum_i\{[1+(q-1)m_i]\ln[1+(q-1)m_i]\\ &+(q-1)(1-m_i)\ln(1-m_i)\}-k_B T\ln q \end{aligned}\tag{16}$$

with respect to m_i. Equation (16) is the Potts analog of Eq. (1). To obtain the RY approximation, we set $C^{(n)}=0$, for $n\geqslant 3$, in Eqs. (14) and (16).

Henceforth we shall restrict ourselves to uniform external fields ($h_i^e=h^e$ for all i) and uniform order parameters ($m_i=m$ for all i). Thus, the self-consistent equation for m in both CW and RY approximations will be

$$m=\frac{\exp(\beta h^{\mathrm{eff}})-\exp[-\beta h^{\mathrm{eff}}/(q-1)]}{\exp(\beta h^{\mathrm{eff}})+(q-1)\exp[-\beta h^{\mathrm{eff}}/(q-1)]}\tag{17}$$

with

$$h^{\mathrm{eff}}=h^e+z(q-1)m/q\tag{18a}$$

in the CW case and

$$h^{\mathrm{eff}}=h^e+(m/\beta)(q-1)(1-1/\chi)\tag{18b}$$

in the RY case, where

$$\chi=\sum_j\chi_{ij}\tag{18c}$$

is the uniform susceptibility in the disordered phase. [In Eq. (18a) and in the rest of the paper, we have set $J=1$ and $k_B=1$, so that the temperature T is measured in units of J/k_B.] Thus, the CW self-consistent equation is obtained from the RY self-consistent quation by replacing $(1/\beta)(1-1/\chi)$ by z/q. As we shall see in Section 4, both these approximation yield a first-order phase transition[9] for $q \geqslant 3$.

We defer a comparison of the CW and RY approximations for the Potts model until Section 4. However, the following observation is worth making: It is wll known (e.g., Ref. 25) that

$$F_{\text{exact}} \leqslant F_{\text{CW}} \tag{19}$$

where F stands for the equilibrium free energy. However, it is not clear whether the Ramakrishnan–Yussouff free energy F_{RY} provides an upper bound for F_{exact}.[10]

3. LARGE-*q* EXPANSION AND COMPARISON WITH MONTE CARLO RESULTS

It is clear from Eqs. (17) and (18b) that an analysis of the RY theory of the phase transition in the Potts model requires knowledge of the temperature dependence of the uniform susceptibility χ in the disordered phase. A similar situation occurs in RY-type theories of freezing,(3,9–11,13–21) where the needed information about the direct pair correlation function in the liquid phase is obtained from experiments, numerical simulations, or approximate analytic calculations. We have used the technique of large-q expansion to calculate the susceptibility χ in zero external field as a function of temperature in the disordered phase. The large-q expansion for Potts models was developed by Ginsparg *et al.*(26) for zero external field, and later extended by Goldschmidt(27) to include the effects of an external field. This method has been shown(26) to yield accurate estimates of the critical value q_c of q at which the phase transition changes from second to first order ($q_c=4$ in two dimensions), and of the latent heat associated with the first-order transition. A brief description of our calculation of χ is given below. For further details about the large-q expansion procedure, the reader is referred to the original paper of Ginsparg *et al.*(26)

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[9] For the Ising model ($q=2$) the RY theory yields a continuous transition with the magnetization exponent $\beta=\gamma/2$, where γ is the *exact* susceptibility exponent. Thus, mean-field exponents obtain for dimension $d \geqslant 4$.

[10] F_{CW} and F_{RY} are obtained by evaluating F and $\tilde{F}$, respectively [Eqs. (12) and (16)] at their global minima.

If the external field h^e is equal to zero, then the susceptibility χ in the disordered phase can be written as

$$\chi(h^e=0) \equiv (q-1)\left.\frac{\partial m}{\partial \beta h^e}\right|_{h^e=0}$$

$$= \frac{1}{N(q-1)} \sum_{m,n} \langle (q\delta_{\sigma_{m},1}-1)(q\delta_{\sigma_{n},1}-1)\rangle \tag{20}$$

where N is the total number of spins. Using the fact that in the disordered phase, the quantity

$$\langle (q\delta_{\sigma_{m},\alpha}-1)(q\delta_{\sigma_{n},\alpha}-1)\rangle, \qquad \alpha=1,2,\dots,q$$

is independent of α, we can reduce Eq. (20) to the form

$$\chi = \frac{1}{N(q-1)} \sum_{m,n} \langle q\delta_{\sigma_m,\sigma_n}-1\rangle$$

$$= 1+\frac{2}{N}\frac{\operatorname{Tr} e^{-\beta H} \sum_{m>n} (q\delta_{\sigma_m,\sigma_n}-1)/(q-1)}{\operatorname{Tr} e^{-\beta H}} \tag{21}$$

where H is the Hamiltonian defined in Eq. (6) with all the external fields h_i^e equal to zero. The large-q expansion is then used to evaluate both the numerator and the denominator of the second term on the right-hand side of Eq. (21). As we shall see shortly, the expansion parameter in two dimensions is $w=1/\sqrt{q}$. This expansion involves a rearrangement of the high-temperature series in such a way that all terms to a given order in the expansion parameter w are collected together. Each order in w is therefore exact to all orders in β. The expansion for the partition function $Z = \operatorname{Tr} \exp(-\beta H)$ is obtained by writing it in the form

$$Z = \operatorname{Tr} \prod_{\langle ij\rangle} [(e^{\beta}-1)\,\delta_{\sigma_i,\sigma_j}+1]$$

$$= (1+uw)^{2N} \operatorname{Tr} \prod_{\langle ij\rangle} \left[1+\frac{uw}{1+uw}(q\delta_{\sigma_i,\sigma_j}-1)\right] \tag{22}$$

where $\langle ij\rangle$ stands for distinct nearest neighbor pairs and

$$u=(e^{\beta}-1)/\sqrt{q} \tag{23}$$

It is easy to show that $0<u<1$ for all temperatures higher than the exact transition temperature$^{(23)}$ $T_c^{\text{ex}}=1/\ln(1+\sqrt{q})$. This particular way of scaling the temperature variable ensures$^{(26)}$ that only a finite number of terms contribute to the expansion for a given order in w. The terms arising from the expansion of the product in the right-hand side of Eq. (22) are represented by diagrams in the standard way, and all diagrams contributing to a particular order in w are collected together. The diagrams contributing to orders w^2 and w^3 in the expansion for Z are shown in Fig. 1a, where each solid line represents the factor

$$uw(q\delta_{\sigma_i,\sigma_j}-1)/(1+uw)$$

We have carried out the expansion for Z through order w^5. The large-q expansion for the numerator of the second term in the right-hand side of Eq. (21) proceeds exactly along the same lines. The only difference is the presence of the extra factor

$$(q\delta_{\sigma_m,\sigma_n}-1)/(q-1)$$

The diagrams contributing to this expansion to orders w and w^2 are shown in Fig. 1b, where the dashed lines represent the factor

$$(q\delta_{\sigma_m,\sigma_n}-1)/(q-1)$$

This expansion was carried out through order w^4. The resulting expansion for χ therefore contains terms up to order w^4. In Ref. 27, the large-q expansion for the free energy of the Potts model on a square lattice in the presence of an external field [the definition of the external field used in Ref. 27 is somewhat different from the one given in Eq. (6)] was carried out

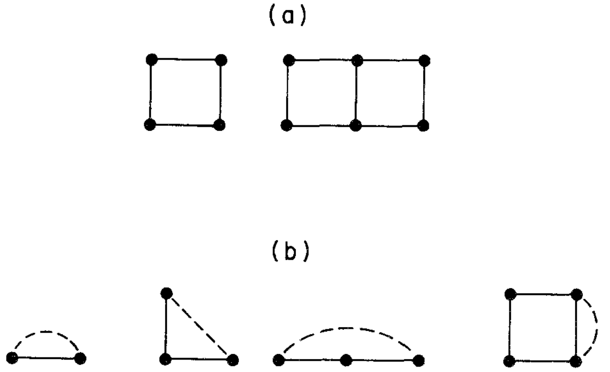

Fig. 1. Low-order diagrams contributing to the large-q expansions for (a) the partition function Z and (b) the susceptibility χ. The solid lines represent the nearest neighbor bonds $uw(q\delta_{\sigma_i,\sigma_j}-1)/(1+uw)$, and the dashed lines in (b) represent the factor $(q\delta_{\sigma_m,\sigma_n}-1)/(q-1)$. The first and the second diagrams in (a) are of order w^2 and w^3, respectively. The first diagram in (b) is of order w and the remaining three are of order w^2.

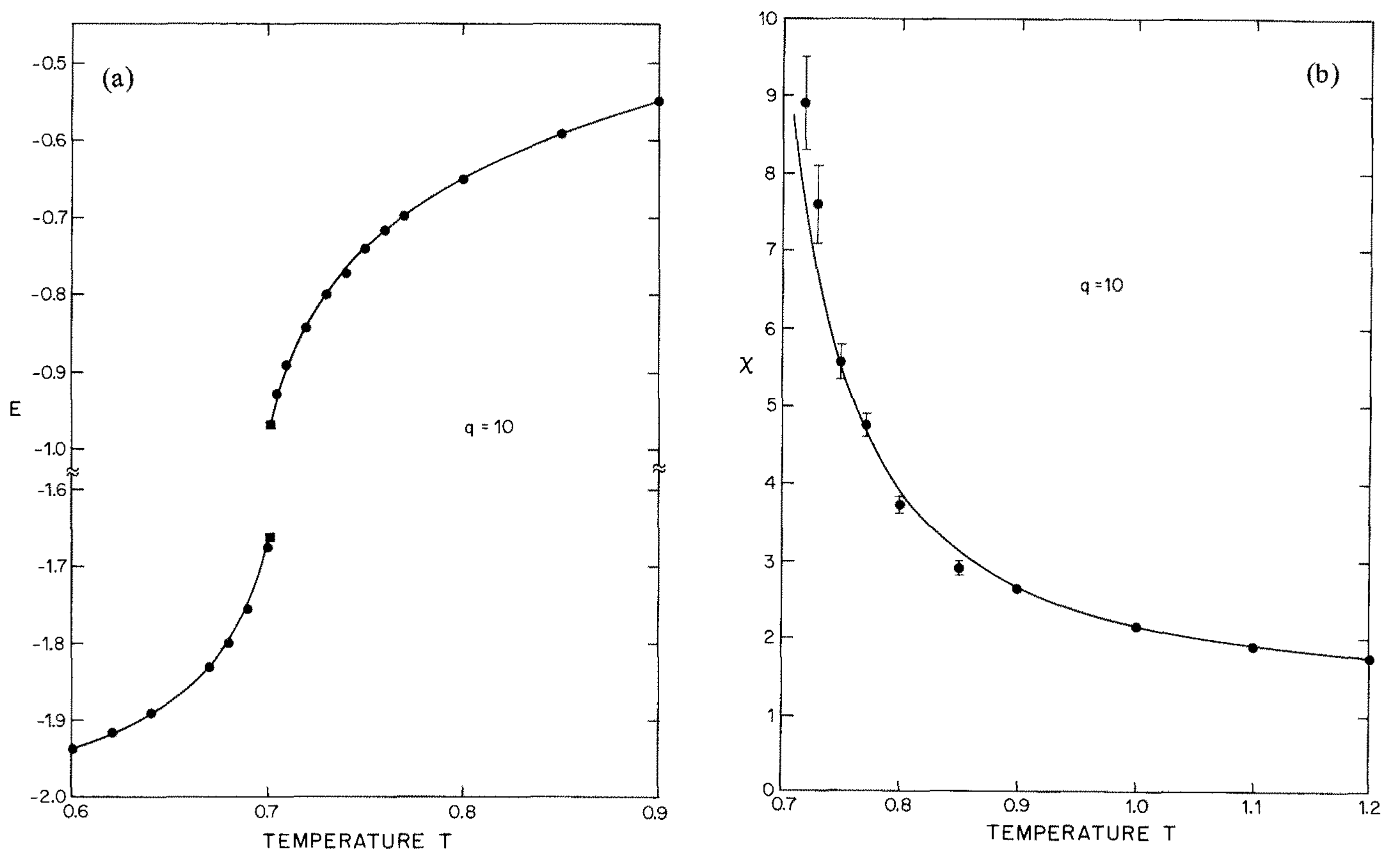

Fig. 2. (a) (—) The temperature dependence of the internal energy per spin E of the ten-state Potts model on a square lattice, calculated from the large q-expansion. (●) The results for E obtained from a Monte Carlo simulation. (■) The exact results for E as $T \to T_c^{\text{ex}}$ ($T_c^{\text{ex}} = 0.701$ for $q = 10$) from below and from above. Here and in Fig. 2b and Fig. 3, if no error bar is shown for the Monte Carlo result, the estimated error is less than the size of the data point. (b) (–) The result of the large-q expansion for the zero-field susceptibility χ of the ten-state Potts model in the disordered phase. (●) The Monte Carlo results for χ.

through order w^4. The first three terms (orders w^2, w^3, and w^4) of the expansion for Z and the first two terms (orders w and w^2) of the expansion for χ can be obtained from this work. Our results for these terms are in agreement with those obtained in Ref. 27.

Not much information is available on the convergence properties of the $1/\sqrt{q}$ expansion. Although it is known to yield accurate estimates for q_c and the latent heat, we are not aware of any test of the accuracy of this method in predicting the temperature dependence of thermodynamic functions. For this reason, we decided to check the accuracy of the results obtained from our truncated $1/\sqrt{q}$ expansion by comparing them with those obtained from a Monte Carlo simulation of the model with $q = 10$. The Monte Carlo simulations were carried out for a 40×40 sample. The standard Metropolis algorithm (e.g., Ref. 28) was used in the simulations. The results for the internal energy per spin E and the susceptibility χ obtained from the stimulations were compared with the predictions of the large-q expansion. The expansion for $E(T > T_c^{\mathrm{ex}})$ up to order w^5 was obtained from the high-temperature, large-q expansion for Z described above. The expansion for $E(T < T_c^{\mathrm{ex}})$, also up to order w^5, was obtained from the high-temperature result by using the exact duality transformation[(22)] that relates the partition function at a temperature $T < T_c^{\mathrm{ex}}$ to that at a temperature $T' > T_c^{\mathrm{ex}}$. The comparisons for E and χ are shown in Figs. 2a and 2b, respectively. It is clear that the truncated $1/\sqrt{q}$ expansion for E is in excellent agreement with the Monte Carlo results, and also with the exact results available for $T = T_c^{\mathrm{ex}}$. The expansion for χ also works quite well if the temperature is not very close to T_c^{ex}. The reason for the observed discrepancy near $T = T_c^{\mathrm{ex}}$ is not difficult to understand. The higher order terms in the large-q expansion on the high-temperature side contain large powers of the quantity u defined in Eq. (23). Since $u \to 1$ as $T \to T_c^{\mathrm{ex}}$, these terms become more important near the transition. We shall find in the next section that an analysis of the RY theory does not require knowledge of the behavior of χ at temperatures close to T_c^{ex}. Also, the accuracy of our expansion for χ is expected to get better for values of q larger than 10. For these reasons, we conclude that the large-q expansion for χ truncated at order w^4 (order $1/q^2$) is quite adequate for our present purpose.

4. RESULTS OF THE RAMAKRISHNAN–YUSSOUFF APPROXIMATION

As discussed in Section 2, the self-consistent equation (17) for the order parameter m in the RY approximation is identical to that in the CW theory. The only difference is in the form of the effective field h^{eff} [Eq. (18a) for the CW approximation, Eq. (18b) for the RY approximation; note that in the high-temperature limit, $\beta \to 0$, the susceptibility $\chi \to 1 + z\beta/q$, and the two expressions for h^{eff} become identical]. Thus, the analysis of the RY theory proceeds along the same lines as that of the CW theory.(24) We consider the situation where the external field h^e is equal to zero. Then, at high temperatures, the self-consistent equation (17) has only one solution at $m=0$. This solution corresponds to the only minimum of the free energy, F or $\tilde{F}$. As the temperature is decreased, two more solutions with $m>0$ develop for $q \geqslant 3$, one corresponding to a maximum and the other to a minimum of the free energy. The value of the free energy at the new minimum decreases relative to that at $m=0$ as the temperature is reduced. Eventually, at a temperature for which $\beta h^{\text{eff}} = 2(q-1)\ln(q-1)/q$, the free energy at the new minimum [which occurs at $m=(q-2)/(q-1)$ at this temperature] becomes equal to that at $m=0$. This signals a first-order phase transition in which the order parameter m changes discontinuously from zero to the value $(q-2)/(q-1)$. Thus, the transition temperature in the CW approximation in given by(24)

$$T_c^{\text{CW}} = \frac{2(q-2)}{(q-1)\ln(q-1)} \tag{24}$$

and the transition temperature in the RY approximation is to be determined from the condition

$$1 - \frac{1}{\chi(T_c^{\text{RY}})} = \frac{2(q-1)\ln(q-1)}{q(q-2)} \tag{25}$$

The values of T_c^{RY} for different values of q, determined via Eq. (25) and the large-q expansion for χ described in Section 3, are shown in Table I. Values of T_c^{CW} and the exact results for T_c [$T_c^{\text{ex}} = 1/\ln(1+\sqrt{q})$] are also listed for comparison. Both CW and RY approximations yield values of T_c that are higher than T_c^{ex}, with the RY approximation doing worse than the CW approximation for all the values of q ($q \geqslant 10$) considered here. We found in Section 3 that the results for χ obtained from the truncated large-q expansion for $q=10$ are indistinguishable from the Monte Carlo results for temperatures higher than $\sim 1.3 T_c^{\text{ex}}$. Since the value of T_c^{RY} for $q=10$ is $\sim 1.5 T_c^{\text{ex}}$, the large difference between T_c^{RY} and T_c^{ex} cannot be attributed to errors arising from our use of the large-q expansion for χ. Since the accuracy of the large-q expansion increases with q and the calculated value of the ratio $T_c^{\text{RY}}/T_c^{\text{ex}}$ also increases with q, the same argument applies to values of q higher than 10. The failure of the RY approximation in the $q \to \infty$ limit can, in fact, be demonstrated explicitly. In the $q \to \infty$ limit,

Table I. Values of the Transition Temperatures T_c^{RY} of the Two-Dimensional, q-State Potts Model on a Square Lattice Calculated from the RY Approximation[a]

q	T_c^{RY}	T_c^{CW}	T_c^{ex}
10	1.06	0.809	0.701
20	0.97	0.644	0.588
30	0.93	0.574	0.535
40	0.90	0.532	0.502
50	0.87	0.503	0.479
100	0.81	0.431	0.417
200	0.76	0.376	0.368
300	0.73	0.350	0.434
500	0.70	0.321	0.317
1000	0.67	0.289	0.287

[a] The results obtained from the CW approximation (T_c^{CW}) and the exact result (T_c^{ex}) are also listed for comparison.

only the first diagram in Fig. 1b needs to be included in the expansion for χ. This leads to the result

$$\chi|_{q\to\infty} \to 1 + 4(e^{\beta} - 1)/q \tag{26}$$

which, together with Eq. (25), implies that

$$T_c^{\mathrm{RY}}|_{q\to\infty} \to 1/\ln(\ln q) \tag{27}$$

The q dependence of T_c predicted by Eq. (27) is quite different from the exact result, $T_c^{\mathrm{ex}} \to 2/\ln q$ as $q \to \infty$, whereas the CW result [Eq. (24)] becomes exact in the $q \to \infty$ limit.

The accuracy of the $1/\sqrt{q}$ expansion for χ truncated at order $1/q^2$ is questionable for values of q close to 4. For this reason, RY treatments for $4 < q < 10$ were not attempted. Thus, we cannot rule out the unlikely possibility that the RY approximation works better than the CW approximation for these values of q.

Other quantities of interest at the first-order transition include Δm, the discontinuity of the order parameter at the transition, and ΔS, the change in entropy per spin across the transition. The value of Δm is equal to $(q-2)/(q-1)$ in both CW and RY approximations. For the q-values considered here, this prediction yields values of Δm which are slightly higher than the exact results,(23) with the difference going to zero as $q \to \infty$. The CW and RY predictions for the entropy change at the transition can be obtained from the corresponding expressions (12) and (16) for the free energy. The results are

$$(\Delta S)_{\mathrm{CW}} = (q-2)\ln(q-1)/q \tag{28a}$$

$$(\Delta S)_{\mathrm{RY}} = -\frac{(q-2)^2}{2(q-1)} \frac{T_c^{\mathrm{RY}}}{[\chi(T_c^{\mathrm{RY}})]^2} \left.\frac{\partial\chi}{\partial T}\right|_{T=T_c^{RY}} \tag{28b}$$

We find that the CW result for ΔS is always higher than the exact value,(23) with the difference going to zero in the $q \to \infty$ limit. The value of ΔS obtained from the CW approximation is smaller than $\ln q$, as expected, for all values of $q \geqslant 3$. If we use the high-temperature, large-q expansion for χ to calculate the derivative $\partial\chi/\partial T$ in Eq. (28b), then we obtain values of $(\Delta S)_{\mathrm{RY}}$ that are larger than $\ln q$ for all values of $q \geqslant 10$. This obviously unphysical result is partly caused by the largeness of the calculated value of T_c^{RY} appearing in the RY expression (28b) for ΔS. If we consider the quantity $\Delta S/T_c$ instead of ΔS, then we obtain more sensible results. The values of $\Delta S/T_c$ obtained from the RY approximation are closer to the exact results than those obtained from the CW approximation if q is in the range $13 \leqslant q \leqslant 92$. At $q = 46$, the RY approximation yields almost the exact result for $\Delta S/T_c$. For $10 \leqslant q < 13$, the RY values for $\Delta S/T_c$ are higher than the CW values, whereas for $q > 92$, the RY values are smaller than the exact results, with

$$|(\Delta S/T_c)_{\mathrm{RY}} - (\Delta S/T_c)_{\mathrm{ex}}| > [(\Delta S/T_c)_{\mathrm{CW}} - (\Delta S/T_c)_{\mathrm{ex}}]$$

Thus, we find that the simple CW approximation works better than the RY approximation for all values of q $(q \geqslant 10)$ considered here. This result is somewhat unexpected in view of the fact that that the RY approximation takes into account some of the effects of fluctuations, whereas all fluctuation effects are neglcted in the CW approximation. If the usual mean-field expression for the zero-field susceptibility in the disordered phase

$$\chi = \frac{1}{1 - \beta z/q} \tag{29}$$

is used in Eq. (18b) to calculate the h^{eff}, then one obtains the CW result, Eq. (18a). Thus, our calculation shows that using a more accurate estimate (the large-q expansion) for χ in Eq. (18b) actually leads to worse results. This result, which we find rather surprising, indicates that the basic ingredient of the RY approximation, namely truncating the Taylor expansion for the response field h^r [Eq. (14)] at order m while using the exact susceptibility to evaluate the coefficients $C^{(2)}$, leads to some inconsistency for the two-dimensional Potts model. In this system, the RY prescription appears to overestimate the effects of fluctuations. In the RY picture, the phase transition takes place when spontaneous fluctuations having the symmetry of the ordered phase grow to a certain magnitude. The fact that the calculated values of T_c^{RY} are much higher than T_c^{ex} may therefore be considered as evidence that the RY approximation overemphasizes the ordering effect of these fluctuations. The reasons behind this problem are not fully understood. One obvious candidate is the truncation of the expansion in Eq. (14) at linear order. In order to examine the effects of this truncation, we carried out an analysis in which the first two terms (orders m and m^2) of the expansion were retained. In the uniform situation ($h_i^e = h^e$ and $m_i = m$ for all i), Eq. (14) then takes the form

$$\beta h^r = C_2 m + \tfrac{1}{2} C_3 m^2 \tag{30}$$

where

$$C_2 \equiv \sum_j C_{ij}^{(2)} = (q-1)(1 - 1/\chi)$$

as before, and

$$C_3 \equiv \sum_{j,k} C_{ijk}^{(3)} = \left.\frac{\partial^2(\beta h^r)}{\partial m^2}\right|_{m=0} \tag{31}$$

After a little algebra, Eq. (31) can be reduced to the form

$$C_3 = -(q-1)(q-2) + (q-1)^3 \chi^{(3)}/\chi^3 \tag{32}$$

where

$$\chi^{(3)} \equiv \left.\frac{\partial^2 m}{\partial(\beta h^e)^2}\right|_{h^e=0} \tag{33}$$

is a higher order susceptibility, which, in the disordered phase, can be written as

$$\chi^{(3)} = \frac{1}{N}\left\langle \left[\frac{1}{q-1} \sum_i (q\delta_{\sigma_{i,1}} - 1)\right]^3 \right\rangle \tag{34}$$

Thus, in the approximation in which the truncation is made at order m^2, the counterpart of Eq. (18b) for the effective field is

$$h^{\mathrm{eff}} = h^e + \frac{m(q-1)}{\beta}\left(1 - \frac{1}{\chi}\right) + \frac{1}{2\beta}\left[\frac{(q-1)^3 \chi^{(3)}}{\chi^3} - (q-1)(q-2)\right] m^2 \tag{35}$$

and the expression for the free energy becomes

$$\begin{aligned}\frac{\beta\tilde{F}}{N} = &-\beta h^e m - \frac{q-1}{2}\left(1-\frac{1}{\chi}\right)m^2 - \frac{1}{6}\left[\frac{(q-1)^3\chi^{(3)}}{\chi^3} - (q-1)(q-2)\right]m^3 \\ &+ \frac{1}{q}\{[1+(q-1)m]\ln[1+(q-1)m] \\ &+ (q-1)(1-m)\ln(1-m)\} - \ln q \qquad (36)\end{aligned}$$

For an analysis of the behavior predicted by these equations, it is necessary to have information about the temperature dependence of $\chi^{(3)}$. It is possible to develop a large-q expansion for this quantity by using the procedure outlined in Section 3. This calculation, however, is very complicated,

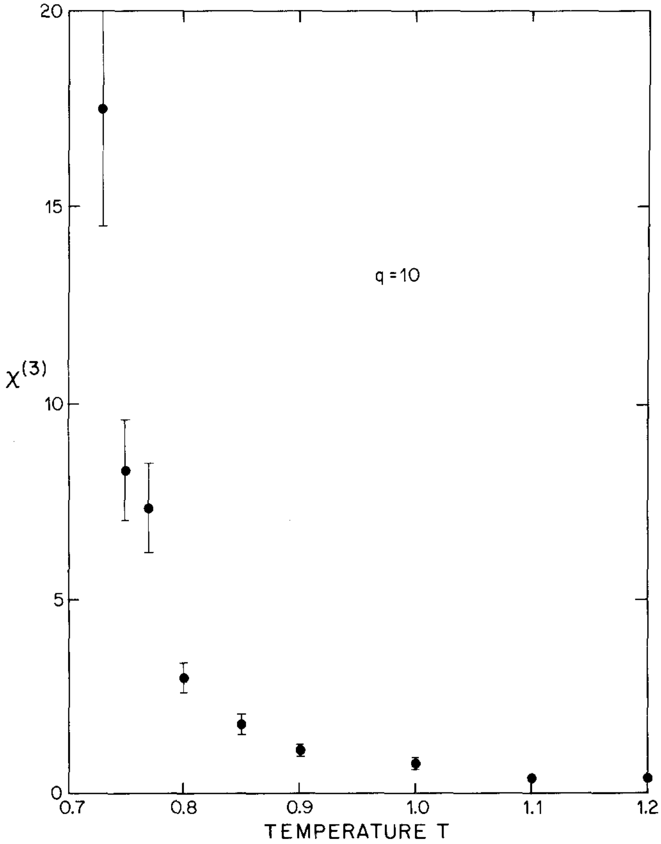

Fig. 3. Results for the susceptibility $\chi^{(3)}$ (see text) for $q = 10$ obtained from a Monte Carlo simulation.

involving a large number of diagrams for even the low-order terms. Also, the convergence of the expansion for $\chi^{(3)}$ is anticipated to be slower than that for χ. For these reasons, a large-q expansion for $\chi^{(3)}$ was not attempted. Instead, we calculated $\chi^{(3)}$ as a function of T for $q=10$ from our Monte Carlo simulations. The results are shown in Fig. 3. At high temperatures, $\chi^{(3)}$ is small and weakly dependent on T. As T approaches T_c^{ex} from above, the value of $\chi^{(3)}$ increases sharply. Due to large fluctuations, the values of $\chi^{(3)}$ for $T \sim T_c^{\mathrm{ex}}$ and for $T < T_c^{\mathrm{ex}}$ (in the supercooled metastable state) could not be determined with high accuracy from our Monte Carlo runs, which consisted of 10,000 Monte Carlo steps per spin. Using the Monte Carlo estimates for χ and $\chi^{(3)}$ in Eq. (32), we find that the coefficient C_3 is always negative. The magnitude of C_3 increases from ~ 10 at $T=1.2$ to ~ 40 as $T \to T_c^{\mathrm{ex}}$. The negative sign of C_3 implies that the m^2 term in Eq. (35) tends to inhibit the transition to the ordered phase. This effect goes in the right direction in the sense that it tends to compensate for the overestimation of the ordering effect of fluctuations found in the approximation in which the truncation is made at order m. However, the correction produced by the m^2 term appears to have too large a magnitude, so that the net result is an underestimation of the effects of fluctuation. A numerical search for the minima of the free energy given in Eq. (36) [with $h^e=0$ and the Monte Carlo values for χ and $\chi^{(3)}$] does not show any minimum other than the one at $m=0$ for temperatures higher than T_c^{ex}. Due to large numerical uncertainties in the Monte Carlo estimates for χ and $\chi^{(3)}$ at temperatures close to T_c^{ex}, we cannot rule out the possibility of a transition taking place at a temperature slightly higher than or below T_c^{ex}. However, our numerical analysis of Eq. (36) shows that if such a transition does occur, it would have a very small value (<0.2) of Δm. Thus, the inclusion of the order m^2 term in the expansion for h^r completely changes the predicted behavior, but yields results that are again quite different from the exact ones. This observation suggests that the Taylor expansion for h^r in powers of m is a poorly convergent one at best, and may very well be asymptotic for the values of m of interest here.

5. SUMMARY AND CONCLUDING REMARKS

We have found that a man-field theory analogous to the RY theory of freezing does not work well for the first-order phase transition in the two-dimensional Potts model. The basic ingredient of the RY approximation is an expansion of the response field in powers of the order parameter. The coefficients of this expansion are determined from the correlation functions in the disordered phase. The usual RY approximation corresponds to a truncation of this expansion at linear order. We have found that the analogous approximation for the Potts model yields results that are worse than those obtained from the simple CW approximation. Retaining the second term in the expansion completely changes the RY predictions. However, the results obtained from this two-term approximation are again quite different from known exact results. These observations indicate that for the two-dimensional Potts model, the Taylor-series expansion for the response field is a poorly convergent one, and a truncation of this expansion at a low order is not a good approximation.

A question that naturally arises from this study is whether the convergence problem found here is generic to the RY approximation or is peculiar to the system considered here. For an answer to this question, it is necessary to understand the suitability of using the two-dimensional Potts model as a testing ground for the validity of RY-type approximations. Generally speaking, the errors arising from a truncation of the expansion for the response field at a low order are expected to be small if (a) the discontinuity of the order parameter at the transition is small (since the Taylor expansion is used to describe both the disordered and the ordered phases, the higher order terms in the expansion would be less important if the order parameter has a small value at $T = T_c^-$), and (b) fluctuations at temperatures near T_c are small. (If large pseudocritical fluctuations are present, then the expansion coefficients $C^{(2)}$, $C^{(3)}$, etc. are expected to have large values.) In the two-dimensional Potts model, the first criterion is not satisfied for large values of q because the magnitude of the order-parameter jump at the transition increases with q. Since the transition is of second order for $q \leqslant 4$, the second criterion is not satisfied if q is close to 4. Thus, one may expect the RY approximation to work well only over a limited range of intermediate values of q. Our calculation shows that such a range of q values does not exist. This result may be a reflection of the fact that the jump in the order parameter at the transition is quite large for relatively small values of q ($\Delta m \simeq 0.86$ for $q = 10$), while fluctuations at temperatures close to T_c^{ex} remain large (the specific heat and the susceptibilities show large enhancements near T_c^{ex}, as can be seen in Figs. 2a, 2b, Fig. 3) for values of q as large as 10. Thus, it is possible that the choice of the two-dimensional Potts model as a testing ground for the RY approximation is a particularly unfavorable one. It is, however, interesting to note in this context that convergence problems similar to those encountered here (but less severe in the quantitative sense) were discovered in a recent analysis(29) of RY-type theories of the freezing of the hard-sphere liquid. In this study, it was found that if an approximate analytic representation of the direct pair correlaltion function is used in the calculation, then the inclusion of a part of the direct triplet correlation function contribution worsens the predictions considerably. A systematic analysis of the sensitivity of the predictions of RY-type theories of freezing to the level of truncation is very difficult because not much information is available about the higher order direct correlation functions in the liquid phase. Thus, tests of RY-type approximations on other simple models exhibiting first-order phase transitions (e.g., the Blume–Emery–Griffiths model(30) and the Ising antiferromagnet is a uniform external field(4)) would be interesting and useful.

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