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ϵ expansion for the free energy of the continuous three-state Potts model: evidence for a first-order transition

Joseph Rudnick†
Department of Physics, Technion, Haifa, Israel

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Abstract. Low-order terms in an ϵ expansion for the free energy of the continuous three-state Potts model are displayed. The free energy has a scaling form and predicts a first-order transition to the order state. Two universal ratios are calculated to first order in ϵ from the expression. The results of this analysis are in good agreement with corresponding results of previous renormalization group analyses of the continuous Potts model.

In this paper are reported some of the results of a renormalization group analysis within the ϵ expansion of the continuous, field-theoretical version of the three-state Potts model. They agree with the results of the earlier renormalization group calculations of Golner (1973) and Amit and Shcherbakov (1974). For small ϵ ($\equiv 4$ minus the dimensionality of the system) the model has a discontinuous, or first-order, transition to its ordered state. If the transition is nearly continuous the free energy asymptotically close to the transition is given dominantly by a scaling form. Within this form certain combinations of thermodynamic quantities take on universal values at the transition. Low order in ϵ terms for the scaling form and the universal combinations will be presented.

The method by which the results were obtained is an extension of the continuous renormalization group method outlined elsewhere (Rudnick 1975). A detailed description of the method including its application to other systems will be given in a separate article. What is done is that Wilson-type differential equations for renormalized two-point, three-point and four-point vertices are generated graphically. These vertices replace the corresponding coefficients in a renormalized and rescaled free energy functional. The equations are integrated until an appropriate 'nearly Gaussian' free energy functional is generated. The free energy is then evaluated using this renormalized free energy functional.

The initial free energy functional has the following form (Amit and Shcherbakov 1974):

$$\begin{aligned}\mathscr{F}_{\mathrm{P}}\{s(\boldsymbol{q})\} = &\sum_{\boldsymbol{q}} (r+q^2)[s_1(\boldsymbol{q})s_1(-\boldsymbol{q})+s_2(\boldsymbol{q})s_2(-\boldsymbol{q})] \\ &+\frac{v}{\sqrt{N}}\sum_{\boldsymbol{q}_1,\boldsymbol{q}_2,\boldsymbol{q}_3}[s_1(\boldsymbol{q}_1)s_1(\boldsymbol{q}_2)s_1(\boldsymbol{q}_3)-3s_1(\boldsymbol{q}_1)s_2(\boldsymbol{q}_2)s_2(\boldsymbol{q}_3)]\delta_{\boldsymbol{q}_1+\boldsymbol{q}_2+\boldsymbol{q}_3} \\ &+\frac{u}{N}\sum_{\boldsymbol{q}_1-\boldsymbol{q}_4}[s_1(\boldsymbol{q}_1)s_1(\boldsymbol{q}_2)s_1(\boldsymbol{q}_3)s_1(\boldsymbol{q}_4)+s_2(\boldsymbol{q}_1)s_2(\boldsymbol{q}_2)s_2(\boldsymbol{q}_3)s_2(\boldsymbol{q}_4) \\ &+2s_1(\boldsymbol{q}_1)s_1(\boldsymbol{q}_2)s_2(\boldsymbol{q}_3)s_2(\boldsymbol{q}_4)]\delta_{\boldsymbol{q}_1+\boldsymbol{q}_2+\boldsymbol{q}_3+\boldsymbol{q}_4} \\ &-\sqrt{N}[H_1s_1(0)+H_2s_2(0)]. \end{aligned} \tag{1}$$

† Present address: Department of Physics, Case Western Reserve University, Cleveland, Ohio 44106, USA.

N is the number of spin modes in the system. If v were equal to zero this functional would describe a two-component Heisenberg-type spin system (Wilson and Kogut 1974). In such a system the transition to the ordered state—corresponding to a nonzero expectation value of $\boldsymbol{M} \equiv s(0)/\sqrt{N}$ in the limit $\boldsymbol{H} \to 0$—is continuous.

The mean-field approximation is obtained by discarding the summations over q_i, replacing all q_i's by zero and $s(0)$ by $\boldsymbol{M}\sqrt{N}$. One then minimizes the resulting expression with respect to $\boldsymbol{M}$ for a given r, u, v and H (Straley and Fisher 1973). When $v \neq 0$ in this approximation the transition to the ordered state involves a discontinuous jump from zero to a finite $\boldsymbol{M}$. Because the free energy is invariant with respect to rotations of $\boldsymbol{M}$ by 120° in the (M_1, M_2) plane the transition to the ordered state is a symmetry-breaking transition.

An approximate numerical renormalization group calculation by Golner (1973) applied to this model also predicted a first-order transition to the ordered state in three dimensions. Amit and Shcherbakov (1974) searched for a fixed point of the free energy functional (1) and found it to be sufficiently unstable for small ϵ that the transition was predicted to be generally not continuous—or at least not a continuous transition that scales. On the other hand, high- and low-temperature expansions applied to the two-dimensional Potts model (Straley and Fisher 1973) and an exact analysis (Baxter 1974) indicate that the transition in two dimensions can be continuous. This is not necessarily inconsistent with the renormalization group results, but the issue of the order of the transition in three dimensions should not be considered absolutely resolved.

The principal advance over previous renormalization group results represented by the results reported here is that the free energy in this paper is explicit and is exact to the two lowest orders in ϵ. Golner (1973) reported an explicit numerical form but it was the result of an approximate method of undetermined accuracy for the three-state Potts model. On the other hand the results of Amit and Shcherbakov (1974), while exact to first order in ϵ and consistent with the conclusions reported here as to the extended scaling form of the asymptotic free energy, do not provide explicit evidence for the first-order nature of the ordering transition.

The main results of the calculation reported here are the two lowest-order terms in the ϵ expansion for the free energy of the continuous three-state Potts model when the transition is nearly continuous. The expression leading to this free energy is:

$$\begin{aligned} F(\tau, \boldsymbol{H}, v, \boldsymbol{M}) = |v|^{d/z}\Bigg[&\left(\frac{\tau_v^2}{d-2y} - \frac{2s\tau_v}{d-y-2z} + \frac{s^2}{d-4z}\right)\frac{d}{2} + (\tau_v - s)|\boldsymbol{M}_v|^2 \\ &+ \operatorname{sgn}(v)(M_{1v}^3 - 3M_{2v}^2 M_{1v}) + u^*|\boldsymbol{M}_v|^4 \\ &+ \tfrac{1}{2}(\tau_v - s + 4u^*|\boldsymbol{M}_v|^2 + D)^2[\ln(\tau_v - s + 4u^*|\boldsymbol{M}_v|^2 + D) - \tfrac{1}{2}] \\ &+ \tfrac{1}{2}(\tau_v - s + 4u^*|\boldsymbol{M}_v|^2 - D)^2[\ln(\tau_v - s + 4u^*|\boldsymbol{M}_v|^2 - D) - \tfrac{1}{2}]\Bigg], \end{aligned} \tag{2}$$

where

$$D = [9|\boldsymbol{M}_v|^2 + 4u^{*2}|\boldsymbol{M}_v|^4 + 12u^* \operatorname{sgn}(v)(M_{1v}^3 - 3M_{1v}M_{2v}^2)]^{1/2}.$$

In this expression:

$$d = 4 - \epsilon = \text{the dimensionality of the system}$$

$$u^* = \epsilon/40 + 17\epsilon^2/800 + O(\epsilon^3)$$

$$s = 90/\epsilon - 261/2 + O(\epsilon)$$
$$y = 2 - 2\epsilon/5 - 7\epsilon^2/50 + O(\epsilon^3)$$
$$z = 1 - \epsilon/10 - 3\epsilon^2/100 + O(\epsilon^3)$$
$$x = (d + 2 - \eta)/2;\ \eta = \epsilon^2/50 + O(\epsilon^3)$$
$$\boldsymbol{M}_v = \boldsymbol{M}|v|^{-(d-x)/z}$$
$$\boldsymbol{H}_v = \boldsymbol{H}|v|^{-x/z}$$
$$\tau_v = \tau|v|^{-y/z}$$
$$\tau_v = r_{\rm H} + sv^2.$$

$r_{\rm H}$ in the last definition corresponds to the reduced temperature in the Heisenberg system. The free energy for a given τ, H and v is obtained by minimizing the right-hand side of (2) with respect to M. It is quite straightforward to show that the free energy will have the form

$$|v|^{d/y} f(\tau|v|^{-y/z}, \boldsymbol{H}|v|^{-x/z}, \mathrm{sgn}(v)). \tag{3}$$

This is clearly a scaling form. y is the temperature scaling parameter of Kadanoff *et al* (1967) and x is their magnetic field parameter. The expressions for y and x above are just the lowest-order terms in the ϵ expansions for them for a two-component Heisenberg spin system (Wilson and Kogut 1974).

We obtain the following results from (2).

(i) To the two lowest orders in ϵ, the transition to the ordered state is first order. It occurs when

$$\tau_v = 10/\epsilon - \tfrac{7}{2} + 10\ln(\epsilon) - \tfrac{81}{8}\ln(90) + \tfrac{1}{8}\ln(10) + S + R_\tau. \tag{4}$$

R_τ stands for terms asymptotically smaller as $\epsilon \to 0$.

(ii) The limiting value of $|\boldsymbol{M}|$ just below the transition is

$$|\Delta \boldsymbol{M}| = |v|^{(d-x)/z}[-20/\epsilon + 27 - 4\ln(\epsilon) + \tfrac{9}{4}\ln(90) + \tfrac{7}{4}\ln(10) + R_M]. \tag{5}$$

R_M is similarly asymptotically smaller with respect to all other terms in the square brackets as $\epsilon \to 0$. To order ϵ^2 we have

$$(d-x)/z = 1 - 4\epsilon/10 + O(\epsilon^3). \tag{6}$$

(iii) Two universal quantities are χ_{T+}/χ_{T-} and C_{H+}/C_{H-}, the ratio of the isothermal longitudinal susceptibility just above the transition temperature to that just below the transition temperature and the ratio of the specific heat at zero $\boldsymbol{H}$ just above the transition to that just below the transition. To the two lowest orders in ϵ we have

$$\chi_{T+}/\chi_{T-} = 1 + (41\epsilon/40)\ln(9) - 11\epsilon/5 + O(\epsilon^2) \simeq 1 + \epsilon/20 + O(\epsilon^2) \tag{7}$$
$$C_{H+}/C_{H-} = \tfrac{1}{5} + 34\epsilon/125 + O(\epsilon^2). \tag{8}$$

With regard to result (ii), it is worth noting that in three dimensions (6) yields a spontaneous magnetization just below the transition temperature that goes as $|v|^{0\cdot 6}$ approximately. This is in good agreement with Golner's (1973) result that $|\Delta \boldsymbol{M}| \propto |v|^{0\cdot 56}$ approximately in three dimensions.

A troublesome feature of the ϵ expansion result is manifested in (5). Neglecting R_M, one obtains an expression that goes through zero when $\epsilon < 1$. Similarly it is worth noting that the ϵ expansion (8) for C_{H+}/C_{H-} is not rapidly convergent.

Finally we note that the form (2) for $F(\tau, \boldsymbol{H}, v, \boldsymbol{M})$ is only valid when

$$|v|^{1/z} \gtrsim |\tau|^{1/y}, \qquad |\boldsymbol{M}|^{1/(d-x)}.$$

This includes the region of the phase transition. Expressions for $F(\tau, \boldsymbol{H}, v, \boldsymbol{M})$ valid in other regions may be readily obtained. They are

(*a*) $|\tau|^{1/y} \gtrsim |v|^{1/z}, |\boldsymbol{M}|^{1/(d-x)}$

$$\begin{aligned} F(\tau, \boldsymbol{H}, v, \boldsymbol{M}) = |\tau|^{d/y}\bigg[&\left(\frac{1}{d-2y} - \frac{2sv_\tau^2 \operatorname{sgn}(\tau)}{d-y-2z} + \frac{s^2 v_\tau^4}{d-4z}\right)\frac{d}{2} \\ &+ [\operatorname{sgn}(\tau) - sv_\tau^2]|\boldsymbol{M}_\tau|^2 + v_\tau(M_{1\tau}^3 - 3M_{1\tau}M_{2\tau}^2) + u^*|\boldsymbol{M}_\tau|^4 \\ &+ \tfrac{1}{2}[\operatorname{sgn}(\tau) - sv_\tau^2 + 4u^*|\boldsymbol{M}_\tau|^2 + D_\tau]^2[\ln(\operatorname{sgn}(\tau) - sv_\tau^2 + 4u^*|\boldsymbol{M}_\tau|^2 + D_\tau) - \tfrac{1}{2}] \\ &+ \tfrac{1}{2}[\operatorname{sgn}(\tau) - sv_\tau^2 + 4u^*|\boldsymbol{M}_\tau|^2 - D_\tau]^2[\ln(\operatorname{sgn}(\tau) - sv_\tau^2 + 4u^*|\boldsymbol{M}_\tau|^2 - D_\tau) - \tfrac{1}{2}] \\ &- \boldsymbol{H}_\tau . \boldsymbol{M}_\tau\bigg] \end{aligned} \tag{9}$$

where

$$\begin{aligned} \boldsymbol{M}_\tau &= \boldsymbol{M}|\tau|^{-(d-x)/y} \\ \boldsymbol{H}_\tau &= \boldsymbol{H}|\tau|^{-x/y} \\ v_\tau &= v|\tau|^{-z/y} \\ D_\tau &= [9v_\tau^2|\boldsymbol{M}_\tau|^2 + 4u^{*2}|\boldsymbol{M}_\tau|^4 + 12u^* v_\tau(M_{1\tau}^3 - 3M_{1\tau}M_{2\tau}^2)]^{1/2} \end{aligned}$$

(*b*) $|\boldsymbol{M}|^{1/(d-x)} \gtrsim |\tau|^{1/y}, |v|^{1/z}$

$$\begin{aligned} F(\tau, \boldsymbol{H}, v, \boldsymbol{M}) = |\boldsymbol{M}|^{d/(d-x)}\bigg[&\left(\frac{\tau_M^2}{d-2y} - \frac{2s\tau_M v_M^2}{d-y-2z} + \frac{s^2 v_M^4}{d-4x}\right)\frac{d}{2} + (\tau_M - sv_M^2) + v_M \cos 3\theta + u^* \\ &+ \tfrac{1}{2}(\tau_M - sv_M^2 + 4u^* + D_M)^2[\ln(\tau_M - sv_M^2 + 4u^* + D_M) - \tfrac{1}{2}] \\ &+ \tfrac{1}{2}(\tau_M - sv_M^2 + 4u^* - D_M)^2[\ln(\tau_M - sv_M^2 + 4u^* - D_M) - \tfrac{1}{2}] - H_{M11}\bigg] \end{aligned} \tag{10}$$

where

$$\begin{aligned} \tau_M &= \tau|\boldsymbol{M}|^{-y/(d-x)} \\ v_M &= v|\boldsymbol{M}|^{-z/(d-x)} \\ H_{M11} &= \boldsymbol{H} . \frac{\boldsymbol{M}}{|\boldsymbol{M}|}|\boldsymbol{M}|^{-x/(d-x)} \\ \cos\theta &= \frac{M_1}{|\boldsymbol{M}|} \\ D_M &= (9v_M^2 + 4u^{*2} + 12u^* v_M \cos 3\theta)^{1/2}. \end{aligned}$$

It can be verified that expressions (2), (9) and (10) for $F(\tau, \boldsymbol{H}, v, \boldsymbol{M})$ match to the two lowest orders in ϵ when $|\tau|^{1/y} \simeq |v|^{1/z} \simeq |\boldsymbol{M}|^{1/(d-x)}$.

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References

Amit D J and Shcherbakov A 1974 *J. Phys. C: Solid St. Phys.* 7 L96–8
Baxter R 1974 *J. Phys. C: Solid St. Phys.* **6** L445–8
Golner E 1973 *Phys. Rev.* B **8** 3419–22
Kadanoff L P *et al* 1967 *Rev. Mod. Phys.* **39** 395–431
Rudnick J 1975 *Phys. Rev.* B **11** 363–76
Straley J P and Fisher M E 1973 *J. Phys. A: Math., Nucl. Gen.* **6** 1310–26
Wilson K G and Kogut J 1974 *Phys. Rep.* **12C** 76–199