

Nonuniversality of ratios of critical and tricritical parameters in the three-state Potts model with symmetry-breaking perturbations

Marcia C. Barbosa and W. K. Theumann

*Instituto de Física, Universidade Federal do Rio Grande do Sul, Caixa Postal 15051, 91 500 Porto Alegre,
Rio Grande do Sul, Brazil*

(Received 26 November 1986; revised manuscript received 25 May 1988)

Fluctuation corrections to symmetry-breaking perturbations are shown to yield *nonuniversal* ratios for t_c/t_i , h_c/h_i , and M_c/M_i , between the reduced temperature t , magnetic field h , and magnetization M of the underlying XY model at the critical and tricritical points of the three-state Potts model. When applied to the trigonal-to-pseudotetragonal phase transition in uniaxially stressed SrTiO_3 along $[1+\delta, 1+\delta, 1-2\delta]$, $\delta \ll 1$, we find a non-negligible break to the universality of δ_i/δ_c , in distinction to previous work.

I. INTRODUCTION

There are interesting phase transitions that are known to be described by the three-state Potts model,¹ as the two-dimensional lattice-gas transition of He and other atoms on Grafoil;² the magnetic transition in a cubic ferromagnet with easy axes along the cube axes when placed in a magnetic field along the $[111]$ diagonal;³ the trigonal to pseudotetragonal structural phase transition in perovskites like SrTiO_3 subject to stress along the $[111]$ direction;⁴ transitions in ^3He - ^4He mixtures that can be described by suitable forms of the Blume-Emery-Griffiths model.⁵

Symmetry-breaking perturbations are crucial in determining the nature of a phase transition.⁶ In a recent work by Blankshtein and Aharony⁷ on the continuum version of the three-state Potts model with quadratic symmetry breaking (QSB) in an external field, given by the effective Hamiltonian

$$\mathcal{H}_0 = \int d\mathbf{x} \left\{ \frac{1}{2} [r\varphi^2 + g(\varphi_1^2 - \varphi_2^2) + (\nabla\varphi)^2] + w(\varphi_1^3 - 3\varphi_1\varphi_2^2) + u(\varphi^2)^2 - h_1\varphi_1 \right\}, \quad (1.1)$$

where $\varphi = \{\varphi_1(\mathbf{x}), \varphi_2(\mathbf{x})\}$ is a two-component field in d -dimensional space, it was shown that the Landau (mean-field) theory⁸ yields critical and tricritical points in nonzero field h_1 .

A typical phase diagram, shown in Fig. 1, has three phase transitions involving a disordered phase and two ordered phases. Denoting by $\bar{\varphi}_1$ and $\bar{\varphi}_2$ the mean-field solutions that minimize the free energy, in phase I, $\bar{\varphi}_1 \neq 0$ and $\bar{\varphi}_2 = 0$ but $\bar{\varphi}_1 \rightarrow 0$ as $h_1 \rightarrow 0$; in phase II, $\bar{\varphi}_1 \neq 0$ and $\bar{\varphi}_2 = 0$ but $\bar{\varphi}_1 \rightarrow 0$ as $h_1 \rightarrow 0$; in phase III, $\bar{\varphi}_1 \neq 0$ and $\bar{\varphi}_2 \neq 0$. The first-order line I-II ends at a critical point with a nonzero magnetization $\bar{\varphi}_{1c}$, while the first-order line I-III changes into a second-order line at a "normal" tricritical point, in the form discussed by Straley and Fisher.⁹ The critical point is associated with the ordering of the "longitudinal" component $\bar{\varphi}_1$, while the second-order line, in particular the tricritical point, involves the ordering of the "transverse" component $\bar{\varphi}_2$. Eventually, under ap-

propriate QSB, the first-order line I-II and the critical point may disappear leaving a single phase-transition line to the ordered phase III. A change in sign of the QSB term may turn the tricritical point into a critical end point,⁸ where the first-order line I-III disappears.

An important issue in critical phenomena is the search of *universal ratios* of *nonuniversal* quantities, and most attention concentrated so far on amplitude ratios of thermodynamic properties above and below a critical point.¹⁰ Universal amplitude ratios arise whenever relevant perturbations of the *same form* drive a system away from a critical point to states above and below.

In the limit of a vanishingly small w , i.e., in the neighborhood of the underlying XY model, where the renormalization group (RG) in $d = 4 - \epsilon$ dimensions¹¹ may be used, Blankshtein and Aharony⁷ (BA-I) found nontrivial *universal amplitude ratios* for t_c/t_i , h_c/h_i , and M_c/M_i ,

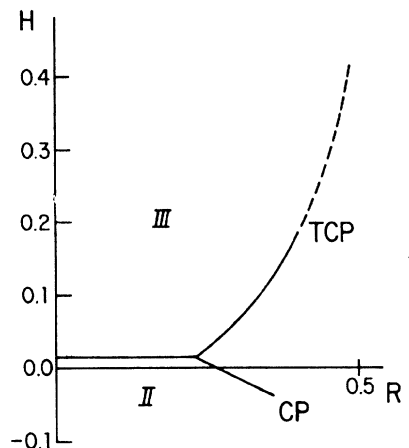


FIG. 1. Typical phase diagram for the three-state Potts model with symmetry-breaking perturbations taken from Ref. 19 and similar to one in BA-I. Dimensionless temperature and field variables, $R = (4u_1/9w^2)r$ and $H = (16u_1^2/27w^3)h_1$ are used. The solid lines represent first-order transitions ending at a critical point (CP) or a tricritical point (TCP) and the broken line indicates a second-order transition.

between the reduced temperature t , external field h , and magnetization M of the underlying XY model at the critical and tricritical points of the Potts model.

If $t = (T - T_c)/T_c$ and $\hat{t} = (T - T_t)/T_t$ define the reduced temperatures of the underlying XY model, T_c and T_t being the true critical and tricritical temperatures of the model, then $t_c = [T_c(w) - T_c]/T_c$ and $t_t = [T_t(w) - T_t]/T_t$ in which $T_c(w)$ and $T_t(w)$ are the true critical and tricritical temperatures of the Potts model.

One may argue, on general grounds, that ratios of critical-to-tricritical *parameters* should not be universal. It is important to note, however, that the situation may be different with appropriately chosen parameters, as those of BA-I. Indeed, based on the existence of a *single* perturbation parameter w , that drives the system away from XY -model behavior either to a critical or to a tricritical point, a scaling argument valid in the limit of small w was shown by BA-I to yield the explicit forms

$$\begin{aligned} t_c(w) &= A_c f_{t_c}(G) w^{1/\phi_w}, \\ h_c(w) &= B_c f_{h_c}(G) w^{\Delta/\phi_w}, \\ M_c(w) &= C_c f_{M_c}(G) w^{\beta/\phi_w}, \end{aligned} \quad (1.2)$$

for the critical point of the Potts model, and similar ones for the tricritical point, with the *same exponents*, particularly the crossover exponent ϕ_w that rules crossover behavior away from the XY model with a ratio w/t^{ϕ_w} . Here, $f_{t_c}(G)$, $f_{h_c}(G)$, and $f_{M_c}(G)$ are *universal functions* of the dimensionless QSB parameter $G = (4u/9w^2)g$, while A_c , B_c , and C_c are nonuniversal coefficients. In ratios of critical-to-tricritical parameters the dependence on w would then drop out and one would expect a cancellation of nonuniversalities in the coefficients to take place, leaving overall *universal ratios*, a precise analogy with the usual reasoning that leads one to expect universal amplitude ratios of thermodynamic properties.¹⁰ It is this universality that seems to be confirmed by the RG calculations of BA-I.

If correct, the universality of ratios of critical-to-tricritical parameters in the three-state Potts model could have important implications. Indeed, in further work Blankschtein and Aharony¹² suggested that the three-state Potts model with QSB in an external field should describe the trigonal-to-pseudotetragonal phase transition of uniaxially stressed SrTiO₃ with *weak off*-diagonal stress along the $[1 + \delta, 1 + \delta, 1 - 2\delta]$ direction.

Mean-field calculations¹² predict a first-order transition for rather small values of δ that either ends at a critical point or changes over into a continuous transition at a tricritical point for nonzero δ_c and δ_t , respectively. Experiments on SrTiO₃ that have alignment problems that, at present, do not enable one to assert accurately the values of δ , yield apparently a first-order transition if δ is

zero,⁴ and the critical and tricritical points for nonzero δ have, to our knowledge, not yet been found.

The parameters δ_c and δ_t are, of course, nonuniversal but their ratio is expected to be universal *if* that is the case with the ratios of critical-to-tricritical parameters in the three-state Potts model, as argued by Blankschtein and Aharony¹² (BA-II).

There are two important aspects in which the above arguments are incomplete. The first one is the effect of the higher-order symmetry-breaking terms that are generated by fluctuations through the RG procedure whenever there is a QSB term, even for vanishingly small w . This is a point that is often omitted in RG calculations.

Specifically, \mathcal{H}_0 has to be replaced by the effective Hamiltonian

$$\begin{aligned} \mathcal{H} = \int d\mathbf{x} \{ & \frac{1}{2}[r\varphi^2 + g(\varphi_1^2 - \varphi_2^2) + (\nabla\varphi)^2] \\ & + w_1[\varphi_1^3 - 3(w_2/w_1)\varphi_1\varphi_2^2] \\ & + u_1(\varphi^2)^2 + u_2(\varphi_1^4 + \varphi_2^4) - h_1\varphi_1 \}, \end{aligned} \quad (1.3)$$

with new couplings w_1 , w_2 , u_1 , and u_2 where even w_1 and u_1 do not follow the same RG equations as w and u in Eq. (1.1). As it turns out, \mathcal{H} is indeed the Hamiltonian that remains invariant in form under RG transformations, within a φ^3 - φ^4 theory. The origin of the new terms is referred to below.

As will be shown here, the higher-order symmetry-breaking terms lead to *nonuniversal* ratios of critical-to-tricritical parameters in $d = 4 - \epsilon$ dimensions. When similar calculations are carried out for SrTiO₃ a non-negligible break in universality for δ_c/δ_t is obtained.

A second important issue that deserves to be studied is the effect of fluctuations on symmetry-breaking perturbations in $d = 6 - \epsilon$ dimensions, where the full size of the trilinear terms in w_1 and w_2 come into play.¹³ Detailed calculations that were also done for this case are deferred to a separate publication.¹⁴

The outline of the paper is the following. In Sec. II we present the solutions of the RG equations for the Potts model that involve the basic temperature, magnetization, and external-field variables that are the main issue of the present work. In Sec. III we discuss the results for the critical and tricritical points of the model and consider the application to SrTiO₃ in Sec. IV. We conclude with a further discussion in Sec. V.

II. RENORMALIZATION-GROUP EQUATIONS

Our starting Hamiltonian, given by Eq. (1.3), arises when all symmetry-breaking terms up to fourth order are kept in the Hubbard-Stratonovich transformation¹⁵ on the discrete-spin Hamiltonian for the three-state Potts model with an anisotropic exchange interaction.

In the presence of the external field h_1 , the magnetiza-

tion $M_1 = \langle \varphi_1 \rangle \neq 0$ already in the disordered phase, and one writes as usual

$$\varphi_1 = \bar{\varphi}_1 + M_1, \quad \varphi_2 = \bar{\varphi}_2, \quad (2.1)$$

where $\bar{\varphi}_1$ and $\bar{\varphi}_2$ are the fluctuating parts, with $\langle \bar{\varphi}_1 \rangle = \langle \bar{\varphi}_2 \rangle = 0$. The effective Hamiltonian becomes then

$$\begin{aligned} \mathcal{H} = \mathcal{H}(M_1) + \int d\mathbf{x} \{ & \frac{1}{2} [\bar{r}_1 \bar{\varphi}_1^2 + \bar{r}_2 \bar{\varphi}_2^2 + (\nabla \bar{\varphi})^2] \\ & + \bar{w}_1 \bar{\varphi}_1^3 - 3\bar{w}_2 \bar{\varphi}_1 \bar{\varphi}_2^2 + \bar{u}_1 (\bar{\varphi}^2)^2 \\ & + \bar{u}_2 (\bar{\varphi}_1^4 + \bar{\varphi}_1^2 \bar{\varphi}_2^2) - \bar{h}_1 \bar{\varphi}_1 \}. \end{aligned} \quad (2.2)$$

Here $\mathcal{H}(M_1)$ is the mean-field part that consists of the spatial and thermal fluctuation-independent terms, and the new parameters are given by

$$\begin{aligned} \bar{r}_1 &= r_1 + 6w_1 M_1 + 12(u_1 + u_2) M_1^2, \\ \bar{r}_2 &= r_2 - 6w_2 M_1 + 4(u_1 + \frac{1}{2}u_2) M_1^2, \\ \bar{w}_1 &= w_1 + 4(u_1 + u_2) M_1, \\ \bar{w}_2 &= w_2 - \frac{4}{3}(u_1 + \frac{1}{2}u_2) M_1, \\ \bar{u}_1 &= u_1, \quad \bar{u}_2 = u_2, \\ \bar{h}_1 &= h_1 - r_1 M_1 - 3w_1 M_1^2 - 4(u_1 + u_2) M_1^3, \\ r_1 &= r + g, \quad r_2 = r - g, \end{aligned} \quad (2.3)$$

where M_1 is to be determined from $\langle \bar{\varphi}_1 \rangle = 0$.

New RG recursion relations to one-loop order in $d = 4 - \epsilon$ dimensions were derived in this work,¹⁶ in terms of the rescaling parameter $b = e^l$, assuming that $w_i^2 = O(\epsilon)$. The solutions, written in standard way,¹⁷ are given by

$$\begin{aligned} \bar{r}_1(l) &= T_1 - 6(u_1 + u_2)[1 - \bar{r}_1 \ln(1 + \bar{r}_1)] - 2(u_1 + \frac{1}{2}u_2)[1 - \bar{r}_2 \ln(1 + \bar{r}_2)] \\ &+ 9\bar{w}_1^2 \left[\ln(1 + \bar{r}_1) + \frac{\bar{r}_1}{1 + \bar{r}_1} \right] + 9\bar{w}_2^2 \left[\ln(1 + \bar{r}_2) + \frac{\bar{r}_2}{1 + \bar{r}_2} \right], \end{aligned} \quad (2.4)$$

$$\bar{r}_2(l) = T_2 - 6u_1[1 - \bar{r}_2 \ln(1 + \bar{r}_2)] - 2(u_1 + \frac{1}{2}u_2)[1 - \bar{r}_1 \ln(1 + \bar{r}_1)] + 18\bar{w}_2^2 [\bar{r}_1 \ln(1 + \bar{r}_1) - \bar{r}_2 \ln(1 + \bar{r}_2)] / (\bar{r}_1 - \bar{r}_2), \quad (2.5)$$

$$\bar{h}_1(l) = H_1 + \frac{3}{2}\bar{w}_1[1 - \bar{r}_1 \ln(1 + \bar{r}_1)] - \frac{3}{2}\bar{w}_2[1 - \bar{r}_2 \ln(1 + \bar{r}_2)], \quad (2.6)$$

where

$$T_1(l) = t_1 - 9w^2/2u + 6w_1 M_1 + 12(u_1 + u_2) M_1^2, \quad (2.7)$$

$$T_2(l) = t_2 - 9w^2/2u - 6w_2 M_1 + 4(u_1 + \frac{1}{2}u_2) M_1^2, \quad (2.8)$$

$$H_1(l) = \hat{h}_1 - t_1 M_1 - 3w_1 M_1^2 - 4(u_1 + u_2) M_1^3, \quad (2.9)$$

are appropriate temperature and external-field variables. For notational simplicity, the l dependence of every term on the right-hand sides has been omitted.

To obtain explicit solutions of the RG equations we separate each coupling into a symmetric and a symmetry-breaking part in the form

$$\begin{aligned} t_1 &= t + \bar{g}, \quad t_2 = t - \bar{g}, \\ \bar{g} &\equiv g + \frac{9}{2} \frac{w}{u} g_w + 9 \frac{w^2}{u^2} g_{u_2} + \frac{3}{10} \frac{t}{u} g_{u_1}, \\ w_1 &= w + 3\bar{g}_w, \quad w_2 = w - \bar{g}_w, \\ \bar{g}_w &\equiv g_w + (\frac{3}{4}g_{u_1} + g_{u_2}) \frac{w}{u}, \\ u_1 &= u - (g_{u_1} + \frac{1}{3}g_{u_2}), \\ u_1 + u_2 &= u + g_{u_1} - \frac{1}{3}g_{u_2}, \\ \hat{h}_1 &= h + \frac{3}{4} \frac{w}{u} g + \frac{27}{8} \frac{w^2}{u^2} g_w + \frac{27}{16} \frac{w^3}{u^3} g_{u_1} \\ &\quad - \frac{3}{2} \frac{t}{u} \left[\frac{1}{2} g_w + \frac{w}{u} \left(\frac{9}{40} g_{u_1} + g_{u_2} \right) \right], \end{aligned} \quad (2.10)$$

where again all l dependence has been suppressed.

The solutions for the symmetric parts, taken from BA-I, are

$$t(l) = te^{2l} / [Q(l)]^{2/5}, \quad (2.11)$$

$$w(l) = we^{(1+\epsilon/2)l} / [Q(l)]^{3/5}, \quad (2.12)$$

$$u(l) = ue^{el} / Q(l), \quad (2.13)$$

$$Q(l) = 1 + (e^{el} - 1)u / u^*, \quad (2.14)$$

$$h(l) = he^{(3-\epsilon/2)l}, \quad (2.15)$$

$$M_1(l) = M_1 e^{(1-\epsilon/2)l}, \quad (2.16)$$

where $u^* = \epsilon/40$ is the fixed point for the symmetric quartic coupling [a factor $(8\pi^2)^{-1}$ is absorbed in u].

For later use we introduce the parameter

$$T(l) \equiv \frac{4}{9} t(l) [u(l) / w^2(l)]. \quad (2.17)$$

Solving explicitly for the symmetry-breaking parts in Eqs. (2.10) yields the results

$$G(l) \equiv \frac{4}{9} \frac{g(l)u(l)}{w^2(l)} = G, \quad (2.18)$$

$$G_w(l) \equiv \frac{g_w(l)}{w(l)} = \frac{G_w}{[Q(l)]^{2/5}}, \quad (2.19)$$

$$G_{u_1}(l) \equiv \frac{g_{u_1}(l)}{u(l)} = \frac{G_{u_1}}{[Q(l)]^{4/5}}, \quad (2.20)$$

$$G_{u_2}(l) \equiv \frac{g_{u_2}(l)}{u(l)} = \frac{G_{u_2}}{[Q(l)]^{1/5}}, \quad (2.21)$$

in which G , G_w , G_{u_1} , and G_{u_2} are the initial ($l=0$) parameters defined on the left in each equation. Except for the first one, which follows from BA-I, the others are new. Within the present work restricted, as in BA-I, to leading order in the symmetry-breaking perturbations, they depend only on the symmetric couplings u and u^* .

Note that $G(l)$ is dimensionless whether fluctuations are taken into account or not, whereas $T(l)$, $G_w(l)$, $G_{u_1}(l)$, and $G_{u_2}(l)$ become dimensionless only in the free (mean-field) theory ($u=0$). Through the RG they acquire various dimensions via the l dependence in $Q(l)$. At $u=u^*$,

$$G_w(l) = G_w \exp(-2\epsilon l/5),$$

$$G_{u_1}(l) = G_{u_1} \exp(-4\epsilon l/5),$$

and

$$G_{u_2}(l) = G_{u_2} \exp(-\epsilon l/5).$$

Compared to the quadratic symmetry-breaking parameter $G(l)$, Eq. (2.18), all these G 's look like irrelevant variables in the limit $l \rightarrow \infty$. This is the XY -model limit that is achieved when the initial trilinear couplings w_1 and w_2 go to zero.

Following BA-I, we take $w_i^2(l) = w_i^2 e^{2l} = O(\epsilon)$ and $u_i(l) = O(\epsilon)$ in $d=4-\epsilon$ dimensions, requiring that $w_i \ll O(\epsilon^{1/2})$ but finite, in order to have a Potts-model critical and tricritical point. As will be demonstrated below, the trilinear and quartic symmetry-breaking parameters become then *dangerous* irrelevant variables.¹⁸

III. RESULTS FOR THE POTTS MODEL

We follow BA-I to obtain the reduced Hamiltonians for the critical and tricritical point. For simplicity, we denote in all that follows the fields in Eq. (2.2) as φ_1 and φ_2 .

The main features of the mean-field phase diagram are used as a guide in what follows. Thus, if initially $\bar{r}_1 < \bar{r}_2$ with fluctuations that enhance the inequality under RG iterations, longitudinal ordering should yield to a critical point in finite field, with a *nonzero* critical magnetization. If, instead, one starts with $\bar{r}_2 < \bar{r}_1$ a tricritical point may appear with *nonzero* external field and magnetization, now for transverse ordering.

A. The critical point

If initially $\bar{r}_1 < \bar{r}_2$ and the RG iterations are carried out until $\bar{r}_2(l^*) = O(1)$, the transverse component φ_2 becomes noncritical. This is achieved when

$$T_2(l^*) = 1, \quad (3.1)$$

up to a higher-order part, according to Eq. (2.5). One may then integrate out the component φ_2 in the partition function to obtain the reduced Hamiltonian for the critical point,

$$\mathcal{H}_{\text{eff}} = \int d\mathbf{x} \left\{ \frac{1}{2} [r_{\text{eff}} \varphi_1^2 + (\nabla \varphi_1)^2] + w_{\text{eff}} \varphi_1^3 + u_{\text{eff}} \varphi_1^4 - h_{\text{eff}} \varphi_1 \right\}, \quad (3.2)$$

where

$$r_{\text{eff}} = T_1(l^*) - 6[u_1(l^*) + u_2(l^*)] \times \{1 - T_1(l^*) \ln[1 + T_1(l^*)]\} + 9\bar{w}_2^2(l^*), \quad (3.3)$$

while $w_{\text{eff}} = \bar{w}_1(l^*) + \theta(w^3)$, $u_{\text{eff}} = u_1(l^*) + u_2(l^*)$, and

$$h_{\text{eff}} = \hat{h}_1 - (t_1 - 9w^2/u)M_1 - 3w_1 M_1^2 - 4(u_1 + u_2)M_1^3 \quad (3.4)$$

all terms depending on l^* . Explicit expressions for these coefficients were obtained from the RG solutions, Eqs. (2.10)–(2.21).

A true effective temperature-like variable

$$t_{\text{eff}} = r_{\text{eff}} + 6u_{\text{eff}}[1 - r_{\text{eff}} \ln(1 + r_{\text{eff}})], \quad (3.5)$$

that takes fluctuations into account, is now introduced following the work of Rudnick and Nelson¹⁷ in $d=4-\epsilon$ dimensions assuming a vanishingly small w_{eff} . When combined with Eq. (3.3) this yields $t_{\text{eff}} = T_1(l^*) + O(\bar{w}^2)$.

The critical point at which φ_1 orders is that of the original Hamiltonian in Eq. (2.2), as discussed above, given now by the equations

$$t_{\text{eff}} = w_{\text{eff}} = h_{\text{eff}} = 0. \quad (3.6)$$

Thus, the first equation for the critical point, to leading order, becomes

$$T_1(l^*) = 0. \quad (3.7)$$

The second relation, $w_{\text{eff}} = 0$ in Eq. (3.6), yields now with Eqs. (2.3),

$$\begin{aligned} M_c e^{(1-\epsilon/2)l^*} &= M_c(l^*) \\ &\equiv -\frac{w(l^*)}{4u(l^*)} [1 + 3G_w(l^*) + \frac{5}{4}G_{u_1}(l^*) \\ &\quad + \frac{10}{3}G_{u_2}(l^*)]. \end{aligned} \quad (3.8)$$

When this is used in Eqs. (2.7) and (2.8) for $T_1(l)$ and $T_2(l)$, Eqs. (3.7) and (3.1) become

$$T(l^*)[1 + \frac{3}{10}G_{u_1}(l^*)] + G(l^*) - \frac{7}{3} - \frac{7}{6}G_{u_1}(l^*) + \frac{17}{9}G_{u_2}(l^*) = 0, \quad (3.9)$$

$$T(l^*)[1 - \frac{3}{10}G_{u_1}(l^*)] - G(l^*) - \frac{11}{9} + \frac{11}{18}G_{u_1}(l^*) - \frac{43}{27}G_{u_2}(l^*) = 1, \quad (3.10)$$

respectively, where $T(l)$ is defined in Eq. (2.17). In the absence of quartic symmetry-breaking terms, Eqs. (3.9) and (3.10) coincide with those in BA-I. This becomes more transparent following these authors noting that the initial value of $t(l) = te^{2l}[Q(l)]^{-2/5}$ in Eq. (2.11), at $l=0$, is the reduced critical temperature t_c of the underlying XY model at the critical point of the Potts model, when determined through Eqs. (3.9) and (3.10).

The explicit solution of Eqs. (3.9) and (3.10) yields first

$$e^{-2l^*} = \frac{w^2}{u} f_c \equiv \frac{9}{4} \frac{w^2}{u} \left(\frac{10}{9} - 2G + \frac{17}{45}G_{u_1} - \frac{94}{27}G_{u_2} \right) \quad (3.11)$$

to leading (zero-loop) order, the G 's being the amplitudes on the right-hand sides in Eqs. (2.18)–(2.21). Next, with $u = u^*$, and eliminating the l^* dependence through Eq. (3.11) we find that

$$t_c = \frac{9}{4} \left(\frac{7}{3} - G + \frac{7}{15} G_{u_1} - \frac{17}{9} G_{u_2} \right) f_c^{1/\phi_c - 1} \left(\frac{w^2}{u^*} \right)^{1/\phi_c}, \quad (3.12)$$

where

$$\phi_c = 1 + \frac{\epsilon}{10} - \frac{1}{10} \left(\frac{4}{5} G_{u_1} - \frac{17}{21} G_{u_2} \right) \epsilon + O(\epsilon^2). \quad (3.13)$$

If it were not for the terms involving G_{u_1} and G_{u_2} , this would be the crossover exponent $\phi = 1 + \epsilon/10 + O(\epsilon^2)$ for the XY model that gives the scaling form for t_c , Eq. (1.2), with $\phi_w = \phi/2$. Note that the apparently irrelevant quartic symmetry-breaking terms have become *dangerous* in modifying the exponent of w^2/u^* .

The reason for restricting u to its fixed-point value u^* , in the above and in what follows, is that already in this case the ratios of critical-to-tricritical parameters become nonuniversal, as will be seen below.

Turning now to Eq. (3.8), we find for the magnetization at the critical point,

$$M_c = - \left(1 + 3G_w + \frac{5}{4} G_{u_1} + \frac{10}{3} G_{u_2} \right) \frac{1}{4u^{*1/2}} f_c^{\lambda_c - 1/2} \left(\frac{w^2}{u^*} \right)^{\lambda_c}, \quad (3.14)$$

where

$$\lambda_c = \frac{1}{2} - \frac{\epsilon}{5} + \left(\frac{3}{5} G_w + \frac{1}{2} G_{u_1} + \frac{1}{3} G_{u_2} \right) \epsilon + O(\epsilon^2). \quad (3.15)$$

Without the trilinear and quartic symmetry-breaking terms, λ_c is the ratio of exponents β/ϕ for the XY model that appears in the scaling form in Eq. (1.2).

Finally, Eq. (3.6) yields

$$h_c = - \frac{1}{16u^{*1/2}} \left(1 + 27G + \frac{17}{5} G_{u_1} - \frac{349}{3} G_{u_2} \right) f_c^{\mu_c - 3/2} \left(\frac{w^2}{u^*} \right)^{\mu_c} \quad (3.16)$$

for the field at the critical point, where

$$\mu_c = \frac{1}{2} \left[3 - \frac{\epsilon}{5} \right] + \frac{1}{5} \left(\frac{34}{5} G_{u_1} - \frac{349}{6} G_{u_2} \right) \epsilon + O(\epsilon^2), \quad (3.17)$$

with f_c defined in Eq. (3.11). Except for the first two terms, μ_c is not the ratio Δ/ϕ in BA-I.

B. The tricritical point

Assuming now that one starts with $\bar{r}_2 < \bar{r}_1$ and that the RG iterations are carried out until

$$T_1(l^*) = 1, \quad (3.18)$$

one may integrate φ_1 in the partition function to generate the reduced Hamiltonian

$$\mathcal{H}_{\text{eff}} = \int d\mathbf{x} \left\{ \frac{1}{2} [\bar{r}_{\text{eff}} \varphi_2^2 + (\nabla \varphi_2)^2] + \bar{u}_{\text{eff}} \varphi_2^4 + \bar{v}_{\text{eff}} \varphi_2^6 \right\} \quad (3.19)$$

for the tricritical point, where

$$\begin{aligned} \bar{r}_{\text{eff}} = & T_2 - 3(2\bar{u}_{\text{eff}} + 9\bar{w}_2^2) [1 - \bar{r}_2 \ln(1 + \bar{r}_2)] \\ & + 9\bar{w}_2^2 \left[1 + 2 \frac{\ln 2}{1 - \bar{r}_2} - \frac{(3 + \bar{r}_2)}{1 - \bar{r}_2} \bar{r}_2 \ln(1 + \bar{r}_2) \right. \\ & \left. + \bar{r}_2 \ln \bar{r}_2 \right], \end{aligned} \quad (3.20)$$

and $\bar{u}_{\text{eff}} = u_1(l^*) - 9\bar{w}_2^2(l^*)/2$, while the explicit form for \bar{v}_{eff} will not be needed here. The iterated external-field variable, $\tilde{h}(l^*)$, can be obtained in standard way from the equation of state, $\langle \varphi_1 \rangle = 0$, when use is made of Eq. (3.18) to fix a new l^* . Here, φ_1 denotes the fluctuating part of the field.

A new effective temperature-like variable \tilde{t}_{eff} is given by the same form as in Eq. (3.5), in terms of \bar{r}_{eff} and \bar{u}_{eff} . When combined with Eq. (2.5) this yields $\tilde{t}_{\text{eff}} = T_2(l^*) + O(\bar{w}^2)$. The Hamiltonian in Eq. (3.19) has then a tricritical point when

$$\tilde{t}_{\text{eff}} = \bar{u}_{\text{eff}} = 0, \quad (3.21)$$

and the first equation requires that, to leading order,

$$T_2(l^*) = 0. \quad (3.22)$$

With the tricritical temperature and magnetization, t_t and M_t , defined now as the amplitudes of $t(l^*)$ and $M(l^*)$ in Eqs. (2.11) and (2.16) that satisfy Eqs. (3.21), we first obtain from $T_1(l^*) = 1$ and $T_2(l^*) = 0$

$$t_t = \frac{9}{64} \left(39 + 10G - \frac{39}{8} G_{u_1} + \frac{73}{4} G_{u_2} \right) f_t^{1/\phi_t - 1} \left(\frac{w^2}{u^*} \right)^{1/\phi_t}, \quad (3.23)$$

where

$$\phi_t = 1 + \frac{\epsilon}{10} + \frac{1}{10} \left(\frac{1}{2} G_{u_1} - \frac{73}{156} G_{u_2} \right) \epsilon + O(\epsilon^2) \quad (3.24)$$

and

$$f_t = \frac{81}{32} \left(1 + \frac{2}{3} G + \frac{7}{40} G_{u_1} + \frac{13}{12} G_{u_2} \right). \quad (3.25)$$

Next, we find

$$\begin{aligned} M_t = & \frac{1}{16} \left(3 - 3G - 12G_w - \frac{783}{80} G_{u_1} - \frac{231}{8} G_{u_2} \right) \\ & \times \frac{1}{u^{*1/2}} f_t^{\lambda_t - 1/2} \left(\frac{w^2}{u^*} \right)^{\lambda_t}, \end{aligned} \quad (3.26)$$

where

$$\lambda_t = \frac{1}{2} - \frac{\epsilon}{5} - \frac{1}{5} \left(1 + 4G_w + \frac{261}{40} G_{u_1} + \frac{77}{16} G_{u_2} \right) \epsilon + O(\epsilon^2). \quad (3.27)$$

Since both $\phi_t \neq \phi_c$ and $\lambda_t \neq \lambda_c$, due to the quartic symmetry breaking terms, the dependence on w (which is the only system-dependent parameter) does *not* drop out in taking the ratios t_c/t_t and M_c/M_t which becomes thus *nonuniversal*.

Finally, the tricritical field that follows from the equa-

tion of state becomes

$$h_t = \frac{81}{256u^{*1/2}} \left(1 - \frac{14}{3}G - \frac{87}{120}G_{u_1} + \frac{887}{36}G_{u_2}\right) \times f_t^{\mu_t - 3/2} \left(\frac{w^2}{u^*}\right)^{\mu_t}, \quad (3.28)$$

where

$$\mu_t = \frac{1}{2} \left[3 - \frac{\epsilon}{5}\right] - \frac{1}{10} \left(1 + \frac{87}{30}G_{u_1} - \frac{887}{36}G_{u_2}\right) \epsilon + O(\epsilon^2). \quad (3.29)$$

Comparison of this with μ_c , Eq. (3.17) shows that also the ratio h_c/h_t is nonuniversal.

IV. APPLICATION TO STRONTIUM TITANATE

Although from the nonuniversality of h_c/h_t together with the work in BA-II one can infer that the ratio δ_c/δ_t is nonuniversal, our aim here is to estimate the order of magnitude of the effect to see if it is detectable experimentally.

A mean-field analysis¹⁹ shows that the free energy for the trigonal-to-pseudotetragonal phase transition in SrTiO₃ with uniaxial stress of pressure p along the $[1+\delta, 1+\delta, 1-2\delta]$ direction can be written as

$$F = \frac{1}{2}r(s_1^2 + s_2^2) + \frac{1}{2}g(s_1^2 - s_2^2) + w_1 \left[s_1^3 - 3\frac{w_2}{w_1}s_1s_2^2 \right] + u_1(s_1^2 + s_2^2)^2 + u_2(s_1^4 - 3s_1^2s_2^2) - h_1s_1 \quad (4.1)$$

to leading order in the symmetry-breaking parameter δ . The QSB parameter g and external "field" h_1 ,

$$g = -Cp\delta + O(\delta^2), \quad h_1 = -Dpm\delta \quad (4.2)$$

contain parameters C (>0) and D coupling elastic to order-parameter degrees of freedom that can be taken from the literature.²⁰ The trigonal order parameter

$$m = \left[\frac{-r_1}{4(u_0 + v_0/3)} \right]^{1/2} \quad (4.3)$$

depends on the temperature variable r_1 and on the isotropic (u_0) and anisotropic (v_0) quartic couplings in the free energy for the original pseudocubic phase of SrTiO₃.¹² Furthermore, the symmetric part of the trilinear term in Eq. (4.1) is given by $w = -(2\sqrt{2}/3)v_0m$.

There are three aspects in which Eq. (4.1) differs from the mean-field free energy for the three-state Potts model with symmetry-breaking perturbations, that follows from Eq. (1.3). These are (i) in the term $-3u_2s_1^2s_2^2$, (ii) in that u_1 is the quartic coupling for diagonal stress, and (iii) that the external-field term vanishes with the symmetry-breaking parameter. There is no such connection in the Potts model. As far as point (ii) is concerned, if one writes $u_1 = u - (g_{u_1} + \frac{1}{3}g_{u_2})$ for the Potts model, as in Eqs. (2.10), the condition

$$g_{u_1} + \frac{1}{3}g_{u_2} = 0 \quad (4.4)$$

has to be imposed in order to be applicable to the trigonal-to-pseudotetragonal phase transition in SrTiO₃. Then u_1 becomes the symmetric coupling u .

Knowing that¹² $u_0/v_0 = -\frac{1}{6}$ and taking the effective Hamiltonian of the original pseudocubic phase at the Heisenberg fixed point with $u_0 \sim u_H^*$, one finds that in the neighborhood of the bicritical point (Fig. 2),

$$w^2/u_{XY}^* \sim 0.003 \quad (4.5)$$

is the appropriate estimate for the parameter w^2/u^* , $u^* = u_{XY}^*$, in Eqs (3.16) and (3.28) for the critical and tricritical fields.

Next, we impose Eq. (4.4). From Eqs. (2.10) we also have $u_2 = -\frac{2}{3}g_{u_2}$, so that $u_2/u = -2G_{u_2}/3$ and $G_{u_1} = -G_{u_2}/3$, in terms of the amplitudes in Eqs. (2.20) and (2.21). With the relative quartic symmetry-breaking parameter $u_2/u \cong -2.6 \times 10^{-2}G$ for SrTiO₃ determined in a previous work in mean-field theory,¹⁹ which is sufficient for a calculation of the exponents μ_c and μ_t , Eqs. (3.17) and (3.29) to $O(\epsilon)$, we have thus $G_{u_1} = -1.3 \times 10^{-2}G$ and $G_{u_2} = 3.9 \times 10^{-2}G$, to be used at the critical and tricritical points where $G_c \cong 0.0298$ and $G_t \cong -0.158$, respectively. The mean-field results quoted here are based on Eq. (4.1) with the quartic symmetry-breaking term $-3u_2s_1^2s_2^2$ that constitutes the final difference with the three-state Potts model.

The values of G_{u_1} and G_{u_2} at the critical and tricritical points can now be used in the coefficients and the exponents in the expressions for h_c and h_t given by Eqs. (3.16), (3.17), (3.28), and (3.29).

The ratio δ_t/δ_c that follows from Eqs. (4.2),

$$\delta_t/\delta_c = (p_c m_c / p_t m_t) h_t / h_c \quad (4.6)$$

is basically determined, as in BA-II, by the ratio h_t/h_c

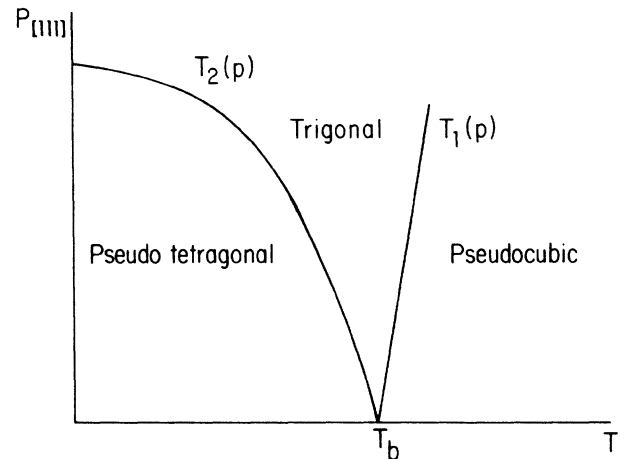


FIG. 2. Qualitative shape of the phase diagram in SrTiO₃ under diagonal stress, taken from Aharony *et al.*, Ref. 4. A first-order trigonal-to-pseudotetragonal transition and a second-order trigonal-to-pseudocubic transition meet at a bicritical point T_b .

since $p_c m_c / p_t m_t = O(1)$. The nonuniversality of the ratio h_t / h_c implies thus that δ_t / δ_c is nonuniversal. Since p and m are parameters of the original cubic system, there is no reason to believe that the possible nonuniversality of the ratio $p_c m_c / p_t m_t$ will cancel that in h_t / h_c to yield a universal δ_t / δ_c .

Our result may be written as

$$\delta_t / \delta_c = (\delta_t / \delta_c)_{\text{BA}} \left[\left(\frac{81}{32} \right)^{-0.016} \left(\frac{2}{3} \right)^{-0.013} \right] \left[\frac{w^2}{u_{XY}^*} \right]^{-0.003}, \quad (4.7)$$

when $\epsilon = 1$ (or $d = 3$), where $(\delta_t / \delta_c)_{\text{BA}}$ is the result of BA-II which contains a 0.02% universal fluctuation correction on their mean-field result with QSB. The terms in square brackets are our universal fluctuation corrections with quartic symmetry breaking; both together give a further 0.3% correction. Finally, making use of Eq. (4.5), the last factor yields a nonuniversal correction of about 2%, which follows from the quartic symmetry-breaking terms in the exponents μ_c and μ_t , for the critical and tricritical fields. Although this correction is 1 order of magnitude beyond present experimental accuracy it is 2 orders of magnitude larger than the fluctuation correction to the mean-field result in $(\delta_t / \delta_c)_{\text{BA}}$. We conclude, therefore, that the ratio δ_t / δ_c for SrTiO₃ is nonuniversal (the universality of quantities for the Potts-model transition in SrTiO₃ refer to the independence on the Hamiltonian parameters of the initial cubic systems), although the nonuniversality will be difficult to detect experimentally. Nevertheless, the nonuniversality should be taken seriously since it arises as a fluctuation effect in the structural phase transition in SrTiO₃ which has been found experimentally to have nonclassical (non-Landau-like) behavior.²¹

V. SUMMARY AND CONCLUDING REMARKS

In this paper we carried out RG calculations to one-loop order in $d = 4 - \epsilon$ dimensions, for the three-state Potts model in an external field with quadratic, very weak trilinear and full quartic symmetry-breaking perturba-

tions to show that the ratios t_c / t_t , h_c / h_t , and M_c / M_t between the reduced temperature t , external field h , and magnetization M of the underlying XY model at the critical and tricritical points of the Potts model are nonuniversal, in distinction to earlier work by Blankshtein and Aharony. The nonuniversality is due to the trilinear and quartic symmetry-breaking perturbations. The latter is the crucial one for all three ratios; the former one enters only in the magnetization ratio.

An estimate of the ratio δ_t / δ_c for SrTiO₃ was found to be nonuniversal, due to fluctuation corrections on the mean-field theory ($\epsilon = 0$) result which are 2 orders of magnitude larger than previous universal fluctuation corrections due to Blankshtein and Aharony. Since the parameters for SrTiO₃ are not known with sufficient accuracy, the nonclassical region for δ_t / δ_c in which nonuniversality is expected to appear may be difficult to reach. This applies even more so to the much smaller nonclassical region of BA-II. Nevertheless, the considerable interest over the past in structural phase transitions in perovskites²² calls for the calculation of further properties once it becomes clear that ratios of critical-to-tricritical parameters in SrTiO₃ are nonuniversal.

It should be of interest to look for universal amplitude ratios above and below the critical or tricritical point for the three-state Potts model. Indeed, in further work to be presented elsewhere we found universal amplitude ratios for the susceptibility at the critical point, as well as specific scaling forms for the equation of state, with application to SrTiO₃.¹⁴

ACKNOWLEDGMENTS

One of us (W.K.T.) thanks A. Aharony, D. Blankshtein, and M. A. Gusmão for discussions, and E. Pytte for a short visit to IBM Thomas J. Watson Research Laboratories Yorktown Heights, NY. A travel grant to one of us (W.K.T.), sponsored by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Brazil, is gratefully acknowledged. This work was supported in part by CNPq and Financiadora de Estudos e Projetos (FINEP), Brazil.

¹F. Y. Wu, *Rev. Mod. Phys.* **54**, 235 (1982).

²S. Alexander, *Phys. Lett.* **54A**, 353 (1975); E. Domany and E. K. Riedel, *J. Appl. Phys.* **49**, 1315 (1978).

³D. Mukamel, M. E. Fisher, and E. Domany, *Phys. Rev. Lett.* **37**, 565 (1976).

⁴A. Aharony, K. A. Müller, and W. Berlinger, *Phys. Rev. Lett.* **38**, 33 (1977).

⁵A. Theumann (unpublished).

⁶A. Aharony, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.

⁷D. Blankshtein and A. Aharony, *J. Phys. C* **13**, 4635 (1980), referred to in the text as BA-I.

⁸L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, Oxford, 1958).

⁹J. P. Straley and M. E. Fisher, *J. Phys. A* **6**, 1310 (1973).

¹⁰P. C. Hohenberg, A. Aharony, B. I. Halperin, and E. D. Siggia, *Phys. Rev. B* **13**, 2986 (1976); C. Bervillier, *ibid.* **13**, 4964 (1976); M. C.-Chang and A. Houghton, *Phys. Rev. Lett.* **44**, 785 (1980); *Phys. Rev. B* **21**, 1881 (1980); C. Bagnuls and C. Bervillier, *Phys. Lett.* **107A**, 299 (1985); J. F. Nicoll and P. C. Albright, *Phys. Rev. B* **31**, 4576 (1985).

¹¹K. G. Wilson and J. Kogut, *Phys. Rep.* **12C**, 76 (1974); M. E. Fisher, *Rev. Mod. Phys.* **46**, 597 (1974).

¹²D. Blankshtein and A. Aharony, *J. Phys. C* **14**, 1919 (1981), referred to in the text as BA-II.

¹³D. J. Amit, *Field Theory, the Renormalization Group and Critical Phenomena* (McGraw-Hill, New York, 1978).

¹⁴Marcia G. Barbosa and W. K. Theumann (unpublished).

¹⁵J. Hubbard, *Phys. Rev. Lett.* **3**, 77 (1959); R. L. Stratonovich, *Dokl. Akad. Nauk SSSR* **115**, 1097 (1957) [*Sov. Phys. Dokl.* **2**, 416 (1957)].

- ¹⁶F. J. Wegner and A. Houghton, *Phys. Rev. A* **8**, 401 (1973); F. J. Wegner, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, New York, 1976), Vol. 6.
- ¹⁷J. Rudnick and D. R. Nelson, *Phys. Rev. B* **13**, 2208 (1976).
- ¹⁸M. E. Fisher, Proceedings of the Temple University Conference on *The Renormalization Group in Critical Phenomena and Quantum Field Theory*, edited by J. D. Gunton and M. S. Green (Temple University Press, Philadelphia, PA, 1974), p. 65.
- ¹⁹J. F. Fontanari and W. K. Theumann, *Phys. Rev. B* **33**, 3530 (1986).
- ²⁰K. A. Müller, W. Berlinger, and J. C. Slonczewski, *Phys. Rev. Lett.* **25**, 734 (1970); J. C. Slonczewski, *Phys. Rev. B* **2**, 4646 (1970).
- ²¹P. A. Fleury and K. Lyons, in *Structural Phase Transitions I*, edited by K. A. Müller and H. Thomas (Springer-Verlag, Berlin, 1981).
- ²²See the other review articles in Ref. 21.