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Equations of state for the three-state Potts model with symmetry-breaking perturbations

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Abstract. Renormalisation-group recursion relations are used to construct equations of state for the critical region of the three-state Potts model with symmetry-breaking perturbations, to first-order in $\varepsilon = 4 - d$. Explicit scaling forms are obtained for the free energy and the longitudinal susceptibility above and below the critical point, as well as for the order-parameter discontinuity on the first-order phase boundary. Application to the trigonal-to-pseudotetragonal phase transition in $SrTiO_3$ under stress yields reasonable agreement with the experimental phase boundary.

1. Introduction

The statistical mechanics and the phase transitions of the q-state Potts model (1952) have already been studied for some while (Wu 1982). As a generalisation of the Ising model, the classical 'spins' on each side of a lattice can be in one of q states. In the case of an interaction between only nearest-neighbour sites, the interaction energy is ε_0 when two spins are in the same state and $\varepsilon_1 > \varepsilon_0$ when two spins are in different states.

The three-state Potts model is of particular interest, in view of the physical realisations described by this model. Indeed, it has been shown to describe, among other things: (i) the two-dimensional lattice-gas transition of He and other atoms adsorbed on Grafoil (Alexander 1975, Domany and Riedel 1978); (ii) the magnetic transition in a cubic ferromagnet with easy axes along the cube axes when placed in a magnetic field along the [1, 1, 1] diagonal (Mukamel *et al* 1976); (iii) the trigonal-to-pseudotetragonal structural phase transition in perovskites like $SrTiO_3$ under stress along the [1, 1, 1] direction (Aharony *et al* 1977).

Symmetry-breaking perturbations are crucial in determining the nature of a phase transition (Aharony 1976). Quite detailed results concerning the equations of state for bicritical points in the n-vector model are now available (Nelson and Domany 1976, Domany *et al* 1977, Amit 1984), while little is known about the Potts model.

The continuum version of the three-state Potts model in an external field has both critical and tricritical points (Straley and Fisher 1973, Blankschtein and Aharony 1980) which are of interest. Blankschtein and Aharony (1981) suggested that the model

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with linear and quadratic symmetry-breaking terms should describe the trigonal-to-pseudotetragonal phase transition of uniaxially stressed $SrTiO_3$ with *weak* off-diagonal stress along the $[1+\delta, 1+\delta, 1-2\delta]$ direction. Actually, the Hubbard–Stratonovich (1959, 1957) transformation on the discrete spin Hamiltonian for the three-state Potts model with spin anisotropy also generates trilinear and quartic symmetry-breaking terms in the effective Hamiltonian

$$\mathcal{H} = \int \mathrm{d}x \left(\tfrac{1}{2}[r\varphi^2 + g(\varphi_1^2 - \varphi_2^2) + (\nabla \cdot \boldsymbol{\varphi})^2] + w_1 \left(\varphi_1^3 - 3\frac{w_2}{w_1}\varphi_1\varphi_2^2 \right) \right.$$

$$\left. + u_1(\varphi^2)^2 + u_2(\varphi_1^4 + \varphi_1^2\varphi_2^2) - h_1\varphi_1 \right) + r_0 \tag{1.1}$$

where r_0 is a field-independent term, while higher powers of the field are neglected.

The trilinear and quartic symmetry-breaking terms have been shown in recent works to be relevant to mean-field theory (Fontanari and Theumann 1986) and to renormalisation-group (RG) calculations in $d = 4 - \varepsilon$ dimensions (Barbosa and Theumann 1988a, referred to as I). Indeed, the amplitude ratios t_c/t_t, h_c/h_t and M_c/M_t, between the reduced temperature t, external field h and magnetisation M of the underlying XY model at the critical and tricritical points of the Potts model were found to be *non*-universal in I, contrary to earlier conclusions by Blankschtein and Aharony (1980). The universality of these ratios is relevant to the ratio δ_c/δ_t for the phase transition in $SrTiO_3$.

Since non-universal ratios are of little use, it is of interest to determine further thermodynamic properties for the three-state Potts model with symmetry-breaking perturbations.

The importance of scaling forms for equations of state has been recognised for some time (Widom 1965, Domb and Hunter 1965). An explicit scaling form for the free energy for the three-state Potts model in an external field has been obtained by Rudnick (1975) to low order in $\varepsilon = 4 - d$. However, detailed RG (Wilson and Kogut 1974, Fisher 1974, Brézin *et al* 1976) results with further symmetry-breaking perturbations are not available.

In the present paper we calculate explicit RG scaling forms, to first order in $\varepsilon = 4 - d$, for the free energy and the equations of state (the magnetisation and the longitudinal susceptibility) for the three-state Potts model with symmetry-breaking perturbations. We also present renormalisation-group fluctuation corrections to the mean-field phase diagram with application to the Potts-model transition in $SrTiO_3$.

A typical phase diagram for the three-state Potts model (Blankschtein and Aharony 1980, Fontanari and Theumann 1986), shown in figure 1, has three phase transitions involving one disordered and two ordered phases. In phase I, $\varphi_1 \neq 0$ and $\varphi_2 = 0$ but $\varphi_1 \to 0$ as $h_1 \to 0$; in phase II, $\varphi_1 \neq 0$ and $\varphi_2 = 0$ but $\varphi_1 \not\to 0$ as $h_1 \to 0$; in phase III, $\varphi_1 \neq 0$ and $\varphi_2 \neq 0$. The discontinuity in the order parameter φ_1 along the first-order transition I–II disappears at the critical point (CP) with a common non-zero magnetisation given by the thermal average $\langle \varphi_1 \rangle_c$. On the other hand, the first-order transition I–III changes over into a line of critical points at a tricritical point (TCP). For the reasons discussed below, we restrict the paper to the critical region of the phase transition I–II, and to the corresponding transition for $SrTiO_3$.

We make extensive use of the solutions to the RG recursion relations that were obtained in I. After making the usual shift $\varphi_1 = \tilde{\varphi}_1 + M$, while $\varphi_2 = \tilde{\varphi}_2$, in which $\tilde{\varphi}_1$ and $\tilde{\varphi}_2$ are the fluctuating parts with thermal averages $\langle \tilde{\varphi}_1 \rangle = \langle \tilde{\varphi}_2 \rangle = 0$ that are

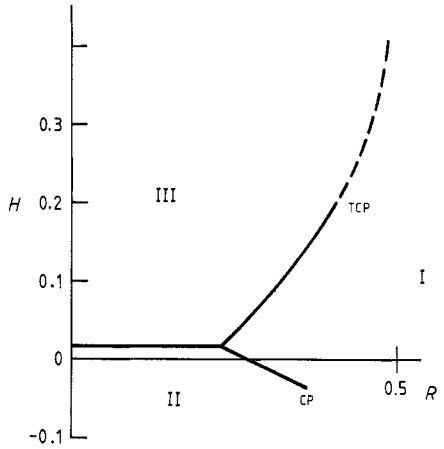

Figure 1. Typical mean-field phase diagram for the three-state Potts model with symmetry-breaking perturbations in terms of dimensionless temperature and field variables, $R = (4u_1/9w^2)r$ and $H = (16u_1^2/27w^3)h_1$, respectively. The solid lines represent first-order transitions ending at a critical point (CP) or at a tricritical point (TCP) and the broken line indicates a second-order transition.

appropriate for a study of the phase transition I–II, we obtain the new field-independent parameter

$$\tilde{r}_0 = r_0 + \tfrac{1}{2}r_1M^2 + w_1M^3 + (u_1 + u_2)M^4 - h_1M \tag{1.2}$$

in addition to the field-dependent effective Hamiltonian of equation (2.2) of I from which all the recursion relations used in I were derived. A study of the equation of state also requires a recursion relation for $\tilde{r}_0$, which will be derived below.

As in I we write the RG rescaling parameter as $b = e^l$ and denote by $v \equiv g_w$, $\tilde{v} \equiv \tilde{g}_w$, $y = g_{u_1}$ and $z = g_{u_2}$ the trilinear and quartic symmetry-breaking parameters used in I.

The outline of the paper is as follows. In § 2 we obtain scaling forms for the free energy and the longitudinal susceptibility both above and below the critical point in a finite field, as well as the discontinuity in the magnetisation just below the critical point. It is shown that, despite the trilinear and quartic symmetry-breaking terms in the effective Hamiltonian, the ratio χ^+/χ^- of the susceptibility above and below the critical point is universal. The fluctuation corrections to the phase diagram in $SrTiO_3$ are discussed in § 3 and we conclude with further remarks in § 4.

2. Critical scaling functions

2.1. Scaling ansatz

An *extended scaling ansatz* (Bruce and Aharony 1975, Fisher and Jasnow 1980) for the singular part of the free energy may be generalised in the form

$$F(t, w, \{s\}, h_1) = b^{-d}F(b^{\lambda_t}t, b^{\lambda_w}w, \{b^{\lambda_s}s\}, b^{\lambda_h}h_1) \tag{2.1}$$

where $t = (T - T_c)/T_c$ is the reduced critical temperature of the XY model, b is a rescale factor,

$$\begin{aligned} &\{s\} \equiv (g, v, y, z) \\ &\{b^{\lambda_s}s\} \equiv (b^{\lambda_g}g, b^{\lambda_v}v, b^{\lambda_y}y, b^{\lambda_z}z) \end{aligned} \tag{2.2}$$

and the basic assumption is that t, w, $\{s\}$, h_1 are all small. The trilinear coupling w and

the symmetry-breaking perturbations $\{s\}$ describe deviations from isotropic XY-model behaviour in an external field, given by $w = \{s\} = 0$.

In place of the usual choice for b, as the temperature-dependent correlation length $\xi \simeq t^{-\nu}$, which yields an extended scaling form appropriate for the study of crossover (Fisher 1967) from isotropic XY-model behaviour, we take $b \simeq \xi \sim w^{-\nu_w}$. This identifies $\nu_w = \nu/\varphi_w$, and yields

$$F(t, w, \{s\}, h_1) \cong w^{(2-\alpha)/\varphi_w} \hat{F}(tw^{-1/\varphi_w}, \{sw^{-\varphi_s/\varphi_w}\}, h_1 w^{-\Delta/\varphi_w}) \tag{2.3}$$

appropriate for Potts-model asymptotic behaviour, where φ_w and φ_s are the crossover exponents of the isotropic XY-model to perturbations in w and in $\{s\}$, respectively. These may still be used here as long as tw^{-1/φ_w} and $sw^{-\varphi_s/\varphi_w}$, for each s, are not smaller than O(1). The usual exponents for the XY-model are known at least to order ε^2 (Wilson 1972, Brézin *et al* 1973, Rudnick 1975) while the new exponents

$$\varphi_v = \tfrac{1}{2}(1 - \tfrac{3}{10}\varepsilon) + O(\varepsilon^2) \qquad \varphi_y = -\tfrac{2}{5}\varepsilon + O(\varepsilon^2) \qquad \varphi_z = -\tfrac{1}{10}\varepsilon + O(\varepsilon^2) \tag{2.4}$$

follow from equations (2.18)–(2.21) of I and the relationships $\varphi_w = \nu\lambda_w$, $\varphi_v = \nu\lambda_v$, $\varphi_y = \nu\lambda_y$ and $\varphi_z = \nu\lambda_z$.

A similar argument can be used to write $b = e^l$ in a scaling form,

$$e^l \cong w^{-\nu/\varphi_w} \Psi(tw^{-1/\varphi_w}, \{sw^{-\varphi_s/\varphi_w}\}, h_1 w^{-\Delta/\varphi_w}). \tag{2.5}$$

Following Blankschtein and Aharony (1980), the critical region is obtained by integrating out the transverse component $\tilde{\varphi}_2$ until $T_2(l^*) = 1$ by means of the temperature variable $T_2(l)$ of equation (2.8) of I. This yields

$$\Psi(\{x_i\}) = u^{1/2}[x_1(1 - \tfrac{3}{10}x_4) - x_2 - \tfrac{11}{4} + \tfrac{11}{8}x_4 - \tfrac{43}{12}x_5]^{-1/2} \tag{2.6}$$

to zero-loop order, where

$$\begin{aligned} &x_1 \equiv u^* t w^{-1/\varphi_w} \qquad x_2 \equiv u^* g/w^2 \qquad x_3 \equiv v w^{-\varphi_v/\varphi_w - 1} \\ &x_4 \equiv (y/u^*) w^{-\varphi_y/\varphi_w} \qquad x_5 \equiv (z/u^*) w^{-\varphi_z/\varphi_w} \end{aligned} \tag{2.7}$$

are appropriate scaling variables and u^* is the fixed-point value of the symmetric quartic coupling. To zero-loop order they are dimensionless but their complete forms, as defined in (2.7) will be needed below.

2.2. *Free energy*

The free-energy density $F(\mathcal{H})$ follows from the RG relationship (Nelson 1975, Niemeijer and van Leeuwen 1976, Rudnick and Nelson 1976)

$$F(\mathcal{H}) = \int_0^l dl' \, e^{-dl'} G_0(l') + e^{-dl} F(\mathcal{H}(l)) \tag{2.8}$$

where the first term involves only the renormalisation with the spatial rescaling factor e^l of the spin-independent part $\tilde{r}_0$ in (1.2). The second term represents the contribution from renormalisations involving both the spatial and field rescaling factors (Wilson and Kogut 1974, Fisher 1974) and it is such that $F[\mathcal{H}(l)] = 0$ in the leading-order Landau theory.

The first term in (2.8) is calculated by integrating the recursion relation (Nelson 1975, Rudnick and Nelson 1976)

$$\mathrm{d}\tilde{r}_0(l)/\mathrm{d}l = (d-1)\tilde{r}_0(l) + \tfrac{1}{2}\ln[(1+\tilde{r}_1(l))(1+\tilde{r}_2(l))] \tag{2.9}$$

which yields

$$\int_0^l \mathrm{d}l'\, \mathrm{e}^{-dl'} G_0(l') = \mathrm{e}^{-dl}\left[\frac{1}{2}\left(t_1(l) - \frac{9}{2}\frac{w^2(l)}{u(l)}\right) M^2(l) + w_1(l)M^3(l) + (u_1(l)+u_2(l))M^4(l) - \hat{h}_1(l)M(l)\right] + F_0(l) \tag{2.10}$$

making use of equations (2.7) and (2.8) of I, where $\hat{h}_1$ is given by equation (2.10) of I and where $F_0(l)$ contains a singular part only in the XY-model limit, in addition to a regular part.

The calculation of $F[\mathcal{H}(l)]$ in the second term of (2.8) yields the singular contribution

$$F[\mathcal{H}(l)]_{\mathrm{sing}} = -\frac{T_1^2(l)}{48(u_1(l)+u_2(l))}\left[\left(1+\frac{u_1(l)+u_2(l)}{u_1^*}\left(T_1(l)^{-\varepsilon/2}-1\right)\right)^{1/3} - 1\right] \tag{2.11}$$

in the Potts-model critical region, plus terms that become singular only in the XY-model limit. Here, $u_1^* = \varepsilon/36$ is the fixed-point coupling for the Ising model. A similar result appears in n-vector model calculations (Rudnick and Nelson 1976).

Collecting equations (2.10) and (2.11), the singular part of the free-energy density in the Potts-model critical region is given by

$$F(\mathcal{H})_{\mathrm{sing}} = \mathrm{e}^{-dl}\{\tfrac{1}{2}[t_1(l) - \tfrac{9}{2}(w^2(l)/u(l))]M^2(l) + w_1(l)M^3(l) + (u_1(l)+u_2(l))M^4(l) - \hat{h}_1(l)M(l)\} + \mathrm{e}^{-dl}F(\mathcal{H}(l))_{\mathrm{sing}}. \tag{2.12}$$

The singularity of each term in the first part of this equation lies in the dependence on $M(l)$ which indeed is singular on the coexistence curve, as will be seen below.

Next, we make a shift in the magnetisation,

$$M(l) = M_{\mathrm{c}}(l) + m(l). \tag{2.13}$$

where $M_{\mathrm{c}}(l)$ is the value at the critical point given by

$$M_{\mathrm{c}}(l) = -w_1(l)/4(u_1(l)+u_2(l)) \tag{2.14}$$

which follows from $w_{\mathrm{eff}} \cong \tilde{w}_1(l^*) = 0$ in equation (2.3) of I. Then $m(l)$ acts as an order parameter. The singular part of the free-energy density becomes now

$$F(\mathcal{H})_{\mathrm{sing}} = \mathrm{e}^{-dl}[\tfrac{1}{2}t_{\mathrm{eff}}(l)m^2(l) + (u_1(l)+u_2(l))m^4(l) - h_{\mathrm{eff}}(l)m(l)] + \mathrm{e}^{-dl}F(\mathcal{H}(l))_{\mathrm{sing}} \tag{2.15}$$

plus terms which are not singular in the Potts-model critical region, and where

$$t_{\mathrm{eff}}(l) \equiv t_1(l) - \tfrac{9}{2}(w^2(l)/u(l)) - \tfrac{3}{4}w_1^2(l)/(u_1(l)+u_2(l)) \tag{2.16}$$

$$h_{\mathrm{eff}}(l) = t_{\mathrm{eff}}(l)m(l) + 4(u_1(l)+u_2(l))m^3(l) + 6(u_1(l)+u_2(l))m(l)T_1(l)\ln T_1(l) \tag{2.17}$$

are effective temperature and external field variables, with the latter following from $\langle\tilde{\varphi}_1\rangle = 0$, in which

$$T_1(l) = t_{\text{eff}}(l) + 12(u_1(l) + u_2(l))m^2(l). \tag{2.18}$$

The equation $h_{\text{eff}}(l) = 0$ has a solution $m(l) = 0$ if $t_{\text{eff}}(l) > 0$. In analogy to a second-order transition, we refer to this in what follows as the 'disordered' phase. There are further solutions

$$m(l) = \pm\tfrac{1}{2}\{[|t_{\text{eff}}(l)|/(u_1(l)+u_2(l))][1-6(u_1(l)+u_2(l))\ln|2t_{\text{eff}}(l)|]\}^{1/2} \tag{2.19}$$

if $t_{\text{eff}}(l) < 0$, which we refer to as the 'ordered' phase. The separation between the two types of solutions takes place at the critical point where $t_{\text{eff}} = 0 = h_{\text{eff}}$. When $h_{\text{eff}} = 0$ and $t_{\text{eff}} < 0$ the coexistence curve is obtained between

$$\text{phase I} \qquad M(l) = M_c(l) + |m(l)| \tag{2.20a}$$

and

$$\text{phase II} \qquad M(l) = M_c(l) - |m(l)|. \tag{2.20b}$$

Thus, $2|m(l)|$ is the discontinuity in the magnetisation across the first-order phase boundary I–II. Note that the equality of the free-energy density on both sides of this boundary follows immediately from (2.15) when $h_{\text{eff}}(l) = 0$.

2.3. *Scaling forms*

We consider next the scaling forms for the singular part of the free-energy density when $h_{\text{eff}}(l) = 0$, in the ordered and disordered phases. In the disordered phase, where $m(l) = 0$, (2.18) becomes

$$T_1(l) = t_1(l) - t_c(l) = (x - x_c)(1 + \tfrac{3}{10}\hat{x}_4)\Psi^{-1}(\{x_i\})(1 + \varepsilon\Delta_1(\{x_i\})) \tag{2.21}$$

when use is made of (2.5) and (2.6) in the solutions to the RG equations discussed in I, and where

$$x \equiv x_1(1 + \tfrac{1}{10}\varepsilon \ln \Psi(\{x_i\}))u^{-1} \tag{2.22}$$

$$x_c \equiv [\tfrac{21}{4} - x_2 + \tfrac{21}{20}\hat{x}_4 - \tfrac{17}{4}x_5(1 + \tfrac{1}{10}\varepsilon \ln \Psi(\{x_i\}))]u^{-1} \tag{2.23}$$

$$\hat{x}_4 \equiv x_4(1 + \tfrac{2}{5}\varepsilon \ln \Psi(\{x_i\})) \tag{2.24}$$

and

$$\Delta_1(\{x_i\}) \equiv \tfrac{1}{10}[\ln(\tfrac{5}{2} - 2x_2 + \tfrac{17}{20}x_4 - \tfrac{47}{6}x_5)u^{-1} + \tfrac{21}{10} - \tfrac{19}{5}x_2 - \tfrac{609}{200}x_4 + \tfrac{329}{20}x_5]. \tag{2.25}$$

The scaling variables x_i are those defined in (2.7). Note that the critical point is approached as $x \to x_c$.

The singular part of the free-energy density in the disordered phase, that follows from (2.11) and (2.15), has then the scaling form

$$F^{+}(\mathcal{H})_{\text{sing}} = -\frac{w^{4-3\varepsilon/5}}{48(u_1+u_2)}(x-x_c)^{2-\varepsilon/6}B^2R_A^{1/3} \times\left(1+2\varepsilon\Delta_1(\{x_i\})-\frac{\varepsilon}{2}\ln\Psi(\{x_i\})+\frac{\varepsilon}{6}\frac{u_1+u_2}{u_I^* R_A}\ln\frac{\Psi(\{x_i\})}{B}\right) \tag{2.26}$$

in which

$$B \equiv 1+\tfrac{3}{10}\hat{x}_4 \tag{2.27}$$

$$R_A \equiv [(u_1+u_2)/u_I^*]-(x-x_c)^{\varepsilon/2}\{[(u_1+u_2)/u_I^*]-1\}. \tag{2.28}$$

When (2.26) is compared to the scaling *ansatz*, (2.3), with the power $w^{(2-\alpha)/\varphi_w}$, one can see that $\alpha=\varepsilon/10$ is the specific-heat exponent of the XY model, whereas the scaling function $\hat{F}^{+}$ carries the singularity in $(x-x_c)$ to the power $2-\alpha_I$, as $x\to x_c$, where $\alpha_I=\varepsilon/6$ is the specific-heat exponent for the Ising model.

In the ordered phase, where $h_{\text{eff}}=0$ but $m(l)\neq 0$ is given by (2.19), there is an exact cancellation of the $m(l)$-dependent terms in the first part of (2.15). The singular part of the free-energy density that follows from the remaining part then takes the scaling form

$$F^{-}(\mathcal{H})_{\text{sing}} = -\frac{w^{4-3\varepsilon/5}}{12(u_1+u_2)}(x-x_c)^{2-\varepsilon/6}B^2R_A^{1/3} \times\left(1+2\varepsilon\Delta_1(\{x_i\})-\frac{\varepsilon}{2}\ln\Psi(\{x_i\})+\frac{\varepsilon}{6}\frac{u_1+u_2}{u_I^* R_A}\ln\frac{\Psi(\{x_i\})}{2B}\right) \tag{2.29}$$

along the coexistence curve between phases I and II. The result for $F^{-}(\mathcal{H})_{\text{sing}}$ as well as that for $F^{+}(\mathcal{H})_{\text{sing}}$ is valid very close to the critical point. Note that the scaling function $\hat{F}^{-}$ in the scaling *ansatz* (2.3) is different from $\hat{F}^{+}$.

Since u_1+u_2 is the effective quartic coupling u_{eff} of the one-component Ising model that is left when the transverse component $\vec{\varphi}_2$ is integrated out (Blankschtein and Aharony 1980), one may take $u_1+u_2=u_I^*$ to be the Ising-model fixed point. The ratio of the free-energy densities. above and below the critical point, takes then the universal form

$$F^{+}_{\text{sing}}/F^{-}_{\text{sing}} = \tfrac{1}{4}(1+\tfrac{1}{6}\varepsilon\ln 2) \tag{2.30}$$

for the Ising model (Rudnick and Nelson 1976), independently of the symmetry-breaking parameters $\{x_i\}$ and consistent with the results of Domany *et al* (1977), due to the neglect of the singular XY-model behaviour in (2.11).

A scaling form for the discontinuity in the magnetisation across the first-order phase boundary can also be obtained from (2.19), in the form

$$m = \frac{w^{\beta/\varphi_w}}{2(u_1+u_2)^{1/2}}(x-x_c)^{1/2(1-\varepsilon/3)}B^{1/2}R_A^{1/3} \times\left(1+\frac{\varepsilon}{2}\Delta_1(\{x_i\})-\frac{\varepsilon}{4}\ln\Psi(\{x_i\})+\frac{\varepsilon}{6}\frac{u_1+u_2}{u_I^* R_A}\ln\frac{\Psi(\{x_i\})}{2B}\right) \tag{2.31}$$

with a singularity as $w\to 0$ that involves the exponent β for the XY-model, and a singularity as the Potts-model critical point is approached with the exponent $\beta=\frac{1}{2}$

$(1-\frac{1}{3}\varepsilon)$ for the Ising model. The dependence on w^{β/φ_w} is in accordance with (2.3) and the scaling relation $\alpha+\beta+\Delta=2$.

One may go ahead and consider the longitudinal susceptibility in zero-effective field that satisfies the relationship (Wilson and Kogut 1974)

$$\chi(\mathcal{H}) = e^{2l}\chi(\mathcal{H}(l)). \tag{2.32}$$

Explicit calculation yields

$$\chi(\mathcal{H}) = e^{2l}T_1^{-1}(l)[1-6(u_1+u_2)\ln T_1(l) - 9(\tilde{w}_1^2(l)/T_1(l))(1+\ln T_1(l)) - 9(\tilde{w}_2^2(l)/T_1(l))] \tag{2.33}$$

to one-loop order. The inverse susceptibility above the critical point,

$$(\chi^+)^{-1} = w^{2+\varepsilon/5}(x-x_c)^{1+\varepsilon/6}BR_A^{-1/3} \times [1+\varepsilon\Delta_1(\{x_i\}) - \frac{\varepsilon}{6}[(u_1+u_2)/u_1^* R_A]\ln(\Psi(\{x_i\})/B)] \tag{2.34}$$

that follows from (2.33) carries the XY-model singularity in the form w^{γ/φ_w}, in accordance with the scaling *ansatz* (2.3), and the singularity in $(x-x_c)\to 0$ with the Ising-model exponent $\gamma = 1+\varepsilon/6$. Similarly, on the coexistence curve below the critical point we find

$$(\chi^-)^{-1} = 2w^{2+\varepsilon/5}(x-x_c)^{1+\varepsilon/6}BR_A^{-1/3} \times \left(1+\varepsilon\Delta_1(\{x_i\}) + 4u(5+4x_4-\tfrac{1}{3}x_5) - \frac{\varepsilon}{6}\frac{u_1+u_2}{u_1^* R_A}\ln\frac{\Psi(\{x_i\})}{2B}\right) \tag{2.35}$$

Taking the isotropic XY-model quartic coupling u at its fixed-point value $u^* = \varepsilon/40$, and again $u_1+u_2 = u_1^*$, we find the universal ratio of inverse susceptibilities, above and below the critical point

$$(\chi^+)^{-1}/(\chi^-)^{-1} = \tfrac{1}{2}[1 - \tfrac{1}{10}\varepsilon(5+4x_4-\tfrac{1}{3}x_5) - \tfrac{1}{6}\varepsilon\ln 2]. \tag{2.36}$$

When the symmetry-breaking parameters are taken as $x_4 = x_5 = 0$ one recovers the universal ratio for the Ising model (Rudnick and Nelson 1976), as one would expect, consistent with Domany *et al* (1977).

3. Coexistence surface and application to strontium titanate

We consider first the effect of fluctuations on the coexistence surface between phases I and II for the three-state Potts model and, for simplicity, we restrict the results to linear and quadratic symmetry-breaking perturbations. The solution of $h_{\text{eff}} = 0$ for $t_{\text{eff}} < 0$ yields a first-order coexistence surface given by

$$H_1 = \tfrac{1}{27}[2-9(G+R)] - \tfrac{2}{135}(5-9G)\ln\tfrac{1}{4}[9(R-G)+7]w^2/u \tag{3.1}$$

to one-loop order, in terms of the dimensionless parameters

$$H_1 \equiv \tfrac{16}{27}h_1u^2/w^3 \qquad R \equiv \tfrac{4}{9}ru/w^2 \qquad G \equiv \tfrac{4}{9}gu/w^2. \tag{3.2}$$

The zero-loop order term has been obtained before (Blankschtein and Aharony 1980), and it yields a straight line in the (R, H_1) plane. Note that the one-loop order correction

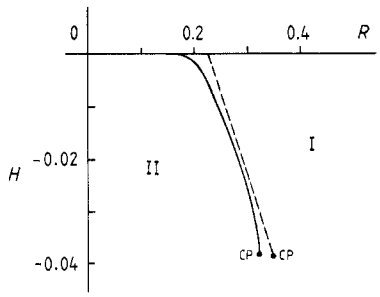

Figure 2. The coexistence surface between phases I and II (cf figure 1) for the three-state Potts model with fluctuation corrections (left curve) on the mean-field result.

becomes dimensional through the dependence on w^2/u and the new curved coexistence surface is shown in figure 2.

We consider next the trigonal-to-pseudotetragonal phase transition in $SrTiO_3$ that may be described by the effective Hamiltonian of (1.1) if we continue to neglect here trilinear and quartic symmetry-breaking terms. The couplings r, g, w, u and h_1 in there can be related to known parameters for $SrTiO_3$, as discussed by Blankschtein and Aharony (1981). Equation (3.1) may then be used to provide an explicit expression for the coexistence surface in terms of p, T and the off-diagonal stress parameter δ through the relationships

$$\begin{aligned} H_1 &= -6.24\times 10^{16} p\delta/f(K,p) \qquad & R &= (1.45\,K + 2.3\times 10^{16} p)/f(K,p) \\ G &= -5.35\times 10^{16}\, p\delta/f(K,p) \qquad & w^2/u &= 0.6\times 10^{-29} f(K,p) \end{aligned} \tag{3.3}$$

in which

$$f(K,p) = 1.32\times 10^{15}\, p - K \tag{3.4}$$

where K is a temperature-dependent parameter. Although this dependence does not appear explicitly in the literature, an estimate can be inferred as follows.

The 'high'-temperature pseudocubic phase in $SrTiO_3$ under diagonal stress can be described by an effective Hamiltonian with a three-component order parameter $\boldsymbol{\varphi} = (\varphi_0, \varphi_1, \varphi_2)$ that has a quadratic part (Aharony *et al* 1977)

$$\mathcal{H}_{02} = \tfrac{1}{2}\int \mathrm{d}\boldsymbol{x}\left[\sum_{i=0}^{2} r_i \varphi_i^2 + (\boldsymbol{\nabla}\cdot\boldsymbol{\varphi})^2\right] \tag{3.5}$$

plus isotropic quartic and cubic terms in the field components which do *not* depend on pressure and temperature. Here,

$$r_0 = K + \tfrac{2}{3} b_t p \tag{3.6}$$

where b_t (<0) is temperature independent. Neglecting fluctuations, i.e., in the Landau theory, the pseudocubic-to-trigonal phase boundary is given by $r_0 = 0$. From the fit of the experimental phase boundary (Müller *et al* 1970) to a straight line it follows then that $K \cong 3.14\times 10^{23}\,(T - T_b)$, in which T_b is the bicritical temperature (figure 3). Since the quartic and cubic terms in the Hamiltonian do not depend on pressure and temperature, it is reasonable to expect that this relationship remains basically unchanged by fluctuations.

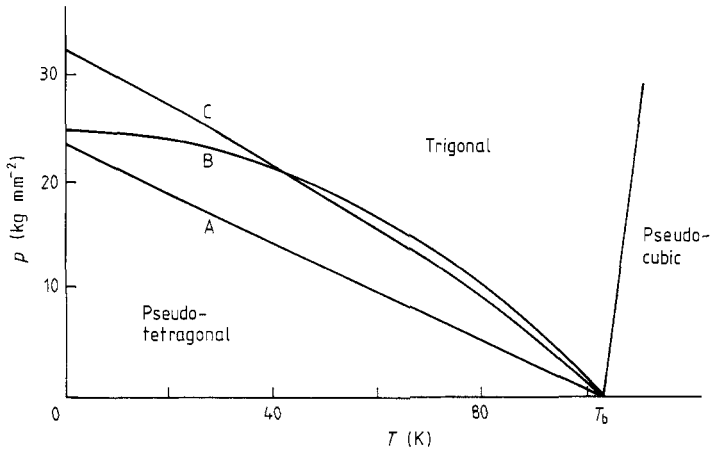

Figure 3. Pressure–temperature phase diagram for $SrTiO_3$ under diagonal ($\delta = 0$) stress. The first-order trigonal-to-pseudotetragonal phase boundary is shown in mean-field theory (A) and with fluctuation corrections to one-loop order (C), compared to the experimental curve (B) (Müller *et al* 1970).

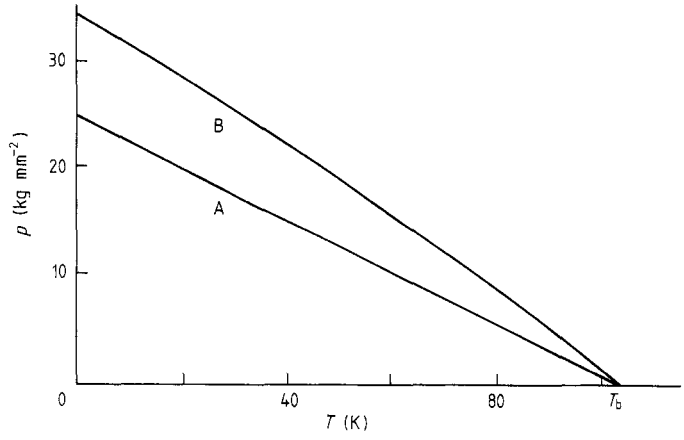

Figure 4. Trigonal-to-pseudotetragonal phase boundary for $SrTiO_3$ under off-diagonal ($\delta = 0.005$) stress, in mean-field theory (A) and with fluctuation corrections to one-loop order (B).

Equations (3.1), (3.3) and (3.4) yield then, for the first order trigonal-to-pseudotetragonal phase boundary, not too close to the bicritical point,

$$p = [2.317/(1 - 10.598\delta)]10^7(T_b - T)^{1-a\varepsilon} \times [\![1 - a\varepsilon \ln\{10^{-6}[(4.65 + 46.91\delta/(1 - 10.598\delta)]\}]\!] \tag{3.7}$$

$$a = (0.145 - 2.35\delta)/(1 - 10.598\delta)$$

The results for $\delta = 0$ and $\delta = 0.005$ are shown in figures 3 and 4. Although there is a considerable improvement of the one-loop order result for $T \gtrsim 40$ K, as can be seen from the rather good agreement with experiment in that region, we do not obtain the flattening of the experimental curve at lower T. It is possible that higher-loop order

corrections may account for this. Since the off-diagonal stress parameter at the critical point is $\delta_c \cong 0.008$ (Blankschtein and Aharony 1981), there is only a small range of δ where the effects of the symmetry-breaking perturbations take place. They are therefore hardly observable, as far as the phase boundary is concerned, except at low T, in view of the weak dependence of our results on δ.

4. Summary and concluding remarks

We have obtained explicit scaling forms for the singular part of the free energy and for the longitudinal susceptibility of the three-state Potts model with symmetry-breaking perturbations, both above and below the critical point in non-zero external field, to one-loop order in $4 - \varepsilon$ dimensions. These scaling forms exhibit Ising singularities and they have a specific dependence on the Potts-model couplings and on the symmetry-breaking terms through appropriate scaling variables. However, as one would expect, both the ratios of the free energy and of the susceptibility above and below the critical point turn out to be universal. We have also obtained a scaling form for the order-parameter discontinuity along the first-order phase boundary.

Our results are restricted to the critical region of the phase boundary I–II. The reason for this is calculational limitations. Indeed, the renormalisation-group results discussed in I apply only to the phase transition I–II and to the *continuous* part of the phase transition I–III, i.e., to the second-order phase boundary and to the tricritical point. The field component φ_2 now orders discontinuously along the first-order part of the phase boundary, requiring the derivation of new RG equations. Although this is feasible, the difficulty that one has to meet is that this phase boundary can only be determined numerically, as can already be seen in the Landau theory (Blankschtein and Aharony 1980). Thus, it does not seem possible to obtain scaling forms *below* the tricritical point.

We have also shown that the results for the critical region of the three-state Potts model can be applied to the trigonal-to-pseudotetragonal phase transition in $SrTiO_3$ with an off-diagonal δ (*positive*) stress parameter. We found that the one-loop order fluctuation corrections to the mean-field phase boundary go in the correct direction over most of the temperature interval to explain the experimental results assumed to be performed for $\delta = 0$. The small change of our results with δ suggests that even for non-zero δ the one-loop order fluctuation corrections should be quite satisfactory.

By adapting the Potts-model calculations with symmetry-breaking perturbations to the trigonal-to-pseudotetragonal phase transition in $SrTiO_3$, as discussed in I, one can also predict the jump in the order parameter across the first-order phase boundary, as an application of (2.31). We omit this here since the critical region in $SrTiO_3$, to which such a prediction would be restricted, has not yet been determined.

Finally, we point out that the magnetic transition in cubic ferromagnets in an *off*-diagonal magnetic field is a further realisation of the three-state Potts model with symmetry-breaking perturbations (Barbosa and Theumann 1988b).

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