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XY-to-Gaussian crossover for the Potts-model transition near the bicritical point of stressed $SrTiO_3$

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The trigonal-to-pseudotetragonal structural first-order transition in [111]-stressed $SrTiO_3$, realizing the three-state Potts model, is studied in the close vicinity of the bicritical point (BCP). The exponents describing the effects of fluctuations on this transition are shown to cross over from XY- to Gaussian-model values as the BCP is approached. The first-order line is shown to approach the BCP tangentially to the temperature axis.

The phase diagrams exhibiting the displacive phase transition of $SrTiO_3$ under uniaxial stress have been of great interest in recent years, providing the first experimental verification of many of the predictions of renormalization-group theory at multicritical points.[1–6] In particular, it has been shown[3,4] that stress p along the [100] axis leads to a bicritical point (BCP, with $p=0$ and $T=T_b \simeq 103$ K), at which the two critical lines separating the two ordered phases (with the order parameter along [100] or perpendicular to it) from the disordered phase approach the temperature axis *tangentially*, as $(T-T_b) \propto p^{1/\phi}$, where ϕ is the Heisenberg model crossover exponent ($\phi \simeq 1.25$ at three dimensions).[7] Stress p along [111] led to a more complicated phase diagram, shown schematically in Fig. 1.[1,2,5,6] At constant $p>0$ there appear two phase transitions, first a second-order (Ising-like) transition [at $T_1(p)$] from the "pseudocubic" (disordered) phase to the trigonal one, and then a *first-order* transition [at $T_2(p)$] into a "pseudotetragonal" (intermediate between trigonal and tetragonal) phase. The nature of this first-order transition remained a mystery for a long time, until it was realized[6] that it should be described by *the continuous version of the three-state Potts model.* The magnitude of the Potts symmetry-breaking term, w, was shown to be proportional to the trigonal order parameter M, and the prediction of earlier renormalization-group analyses[8,9] that the discontinuity should behave as $\Delta M \propto w^{\delta^*}$, with $\delta^* \simeq 0.6$ at three dimensions, was confirmed experimentally.[6] This was a clear indication that *critical fluctuations* (due to the underlying almost-second-order XY-model transition occurring at $w=0$) are important over a wide range of values of $T_2(p)$.

In spite of this success, details concerning this Potts-model transition *in the close vicinity of the BCP* remained unresolved. In this note we concentrate on studying this vicinity. Our most surprising result concerns the *nature of the critical fluctuations* affecting the Potts-model transition. We show, that although these fluctuations are governed by the XY-model exponents for a wide range of values of $T_2(p)$ (as confirmed experimentally in Ref. 6), they will undergo *a crossover to Gaussian- (or Landau-) model exponents in the close vicinity of the BCP.* The exponent δ^*, approximately equal to 0.6 along most of the line $T_2(p)$, will thus cross over to the value 1 (which it also has far away from the second-order transition, for sufficiently large w). This crossover, which results from the "irrelevance" of the cubic symmetry interactions, is rather slow, characterized by the *cubic* crossover exponent ϕ_v (Ref. 10) (which is negative and small). The same type of crossover (to Gaussian behavior) has previously been predicted for the *second*-order transition into the intermediate phase in the vicinity of a *tetracritical* point.[11] We emphasize here the generality of that result, and its consequences for the *Potts-model first-order transition.* Mea-

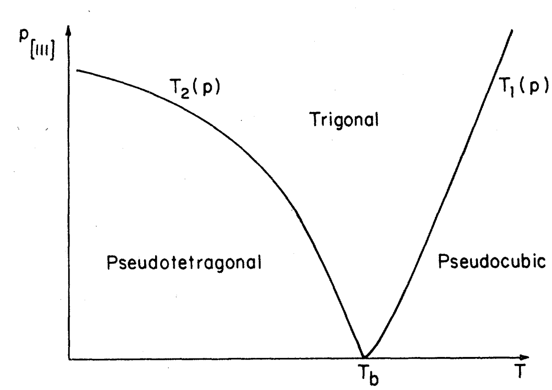

FIG. 1. Schematic phase diagram of $SrTiO_3$ for positive stress along the [111] diagonal.

surement of the exponent δ^* may be the easiest confirmation of this crossover.

Our second new result concerns the *shape* of the line $T_2(p)$. We find that near the BCP one has $[T_b - T_2(p)] \propto p^{1/\psi}$ with $\psi = \phi - \phi_v > \phi > 1$. The line $T_2(p)$ should thus approach the T axis *tangentially*. The line $T_1(p)$ should also approach the T axis tangentially, as $p^{1/\phi}$.[3,5] Although conjectured in Ref. 5, this is the first *explicit* calculation of *the shape of a first-order line*. Both the early EPR experiments[1] and the more recent neutron scattering experiments[12] seem to disagree with these results, giving linear dependences of T_1 and T_2 on p. These experiments probably involved internal strains raising the BCP to finite values of p.[3,12] We hope that this paper will stimulate more detailed experiments in the closer vicinity of T_b.

The first few steps of our analysis are the same as in Ref. 6. Using the pseudocubic axial vector of the soft optic mode which lies at the [111] corner of the Brillouin zone, $\vec{Q}$, as the order parameter, and assuming stress p along [111], the reduced Ginzburg-Landau-Wilson Hamiltonian has (in addition to the usual $|\vec{Q}|^2$ and $|\vec{Q}|^4$ terms) a cubic term, $v(Q_1^4 + Q_2^4 + Q_3^4)$, and a stress term, $\frac{1}{3}pL_3(Q_1Q_2 + Q_2Q_3 + Q_3Q_1)$. The parameter v, measuring the cubic anisotropy, is negative and small.[1,2,6] We next define $S_1 = (Q_1 + Q_2 + Q_3)/\sqrt{3}$, $S_2 = (Q_1 - Q_2)/\sqrt{2}$, and $S_3 = (Q_1 + Q_2 - 2Q_3)/\sqrt{6}$, and find that for $p > 0$, the stress term will yield an ordering of $\langle S_1 \rangle = M$, i.e., $\vec{Q} \parallel [111]$ (trigonal phase). Replacing S_1 by $S_1 + M$ we finally obtain[6]

$$\begin{aligned}\bar{H} = \int d^dx \{ & \tfrac{1}{2}[\tilde{r}_1 S_1^2 + \tilde{r}_2(S_2^2 + S_3^2) + |\nabla \vec{S}|^2] + u|\vec{S}|^4 \\ & + v[\tfrac{1}{3}S_1^4 + 2S_1^2(S_2^2 + S_3^2) + 2\sqrt{2}S_1S_3(S_2^2 - \tfrac{1}{3}S_3^2) + \tfrac{1}{2}(S_2^2 + S_3^2)^2] \\ & + [r_1 + 4(u + \tfrac{1}{3}v)M^2]MS_1 + 4(u + v)MS_1(S_2^2 + S_3^2) \\ & + 4(u + \tfrac{1}{3}v)MS_1^3 + 2\sqrt{2}vMS_3(S_2^2 - \tfrac{1}{3}S_3^2) + \cdots \} ,\end{aligned} \tag{1}$$

where $\tilde{r}_1 = r_1 + 4(3u + v)M^2$, $\tilde{r}_2 = r_2 + 4(u + v)M^2$, $r_1 = r_0 + \frac{2}{3}L_3p$, $r_2 = r_0 - \frac{1}{3}L_3p$, r_0 is linear in T and p (vanishing at $p = 0$, $T = T_b$), and the dots represent higher-order terms (neglected in what follows).

If fluctuations in S_1 are negligible [$\tilde{r}_1$ is sufficiently large, i.e., $T << T_1(p)$], we have $M^2 \simeq -r_1/4(u + \frac{1}{3}v)$, $\tilde{r}_1 \simeq -2r_1 > 1$, and we can integrate S_1 out of $\bar{H}$ to obtain

$$\begin{aligned}\bar{H}_{\text{eff}} = \int d^dx \{ & \tfrac{1}{2}[\tilde{r}_2(S_2^2 + S_3^2) + (\nabla S_2)^2 + (\nabla S_3)^2] \\ & + \tilde{u}_2(S_2^2 + S_3^2)^2 + wS_3(S_2^2 - \tfrac{1}{3}S_3^2)\} ,\end{aligned} \tag{2}$$

with

$$w \simeq 2\sqrt{2}vM, \quad \tilde{u}_2 \simeq -v(7u + 5v)/(6u + 2v) . \tag{3}$$

The second part of Eq. (3), i.e., $\tilde{u}_2 \propto -v$, is responsible for the new crossover predicted in this paper. As $v \to 0$, one expects the trigonal-to-pseudotetragonal phase transition to disappear (no more competition between symmetries), so that *all* the higher-order terms in $\bar{H}_{\text{eff}}$ should also vanish as $v \to 0$.[13] Note that similar effects occur at the boundaries of the intermediate phase near a tetracritical point, as discussed by Domany and Fisher.[11] In that case this will imply a *shrinking of the critical region* as the tetracritical point is approached along the boundaries of the intermediate phase.

If the parameter $\tilde{u}_2$ is not too far from its fixed-point value at the XY-model second-order transition, u_{XY}^*, then we may use the scaling properties near this fixed point to obtain the results of Ref. 6. The experimental observation of $\Delta M \propto w^{\delta^*} \propto M^{\delta^*}$ indeed justifies that analysis for *intermediate* values of $T_2(p)$.

When $T_2(p)$ approaches T_b it is no longer justified to ignore fluctuations in S_1. One must first carry out a finite number of iterations of the renormalization group, l_1, so that the renormalized value $\tilde{r}_1(l_1)$ becomes of order unity.[14,15] These iterations are performed in the vicinity of the *Heisenberg* multicritical point ($p = 0$, $T = T_b$), where v is believed to be *irrelevant*.[10,16] Thus, the renormalized variable $v(l_1) \simeq v\exp(\phi_v l_1/\nu)$ (ν is the correlation length exponent) *decreases* with increasing l_1, i.e., with decreasing $\tilde{r}_1$. To leading order in $\epsilon = 4 - d$ it turns out that after l_1 iterations Eq. (1) maintains the same form, with $\tilde{r}_1$, $\tilde{r}_2$, u, v, and M being replaced by their renormalized values.[15] As soon as $\tilde{r}_1(l_1) \simeq 1$ one can integrate S_1 out, and remain with (renormalized) Eqs. (2) and (3). Noting the fact that $|v(l_1)| << u(l_1) \simeq u_H^*$ (u_H^* is the Heisenberg fixed-point value), and using $M(l_1)^2 \simeq 1/(8u_H^*)$, we find that *both* $w = 2\sqrt{2}v(l_1)M(l_1) \simeq -v(l_1)/\sqrt{u(l_1)}$ and $\tilde{u}_2 \simeq -7v(l_1)/6$ become small for sufficiently large l_1. We are thus not very far from the *Gaussian* (two-component) fixed point, at which $w^* = \tilde{u}_2^* = 0$, and we must consider *crossovers from the Gaussian to both the XY and the first-order behavior.* Note that the higher-order terms [e.g., the coefficient of $(S_1^2+S_2^2)^3$] are quite small after l_1 iterations.

We now proceed to iterate the renormalization-group recursion relations for the effective Hamiltonian (2). The results, to order $\epsilon=4-d$, may be written[15]

$$t_2(l)=t_2(0)e^{2l}/Q(l)^{2/5},\quad t_2(0)=\tilde{r}_2(0)+O(\epsilon)\ ,$$
$$\tilde{u}_2(l)=\tilde{u}_2e^{\epsilon l}/Q(l),\quad w(l)=w\exp[(1+\epsilon/2)l]/Q(l)^{3/5}\ , \tag{4}$$

where the factor $Q(l)=1+(e^{\epsilon l}-1)\tilde{u}_2/u_{XY}^*$ reflects the Gaussian to XY crossover. If Eqs. (4) are iterated until $t_2(l_2)\simeq 1$, and Landau theory is then used,[15] one finds the first-order Potts transition at $\tilde{r}_2(l_2)\simeq w(l_2)^2/2\tilde{u}_2(l_2)=O(1)$. Thus, $e^{\epsilon l_2}\propto(w^2/\tilde{u}_2)^{-\epsilon/2}\propto|v(l_1)/u_H^*|^{-\epsilon/2}$, and we have $Q(l_2)-1\propto|v(l_1)|^{1-\epsilon/2}\propto(T_b-T_2)^\lambda$, where $\lambda=|\phi_v|(1-\omega\nu)$, $\omega=\epsilon+O(\epsilon^2)$ being the exponent associated with $\tilde{u}_2$. For T approaching T_b this becomes small, $Q(l_2)$ becomes of order unity and Eqs. (4) reduce to *Gaussian* scaling, i.e., to Landau exponents. As $T_2(p)$ decreases, l_1 will decrease, and we may have a range of $T_2(p)$ for which $Q(l_2)>>1$, yielding XY-like exponents. One should note that $|\phi_v|$ is rather small [probably smaller than 0.1 (Ref. 10)], so that the range over which $Q(l_2)\simeq 1$ may be small. The experiments analyzed in Ref. 6, which had $T_b-T_2(p)\gtrsim 1.5$ K, must have been outside of this range.

The result concerning the shape of $T_1(p)$ follows in the same way. After l_1 iterations, $\tilde{r}_2(l_1)$ is also a combination of $t(l_1)\propto(T_b-T)e^{l_1/\nu}$ and $p(l_1)\propto pe^{l_1\phi/\nu}$. Combining the conditions of $\tilde{r}_1(l_1)\simeq 1$ and $\tilde{r}_2(l_1)\simeq w^2/2\tilde{u}_2\propto v(l_1)$ we finally find that at $T_2(p)$ one has $p(l_1)\propto v(l_1)$, yielding $T_b-T_2(p)\propto p^{1/\psi}$.[5]

It should be noted that combining the parameters used in the Landau-theory calculations[1,2,17] with the coefficients of the gradient terms[12] (ignoring all higher-order terms), one finds (dimensionless) values of u and v which are too small to yield *any* regime of nonclassical exponents (even at $p=0$).[15] In fact there are many *transient irrelevant variables* [e.g., the coefficient f of $-\sum_\alpha(\nabla_\alpha Q_\alpha)^2$, see Refs. 18 and 19], which cause an *increase* in u and v in the *first few iterations.* This initial growth in v may be responsible for the observed intermediate XY-like regime.

Because of these conflicting transient effects, there is no theoretical quantitative way to estimate the size of the crossover region below which the new Gaussian behavior will be observed. Since the earlier experiments had $t=(T_b-T_2)/T_b\gtrsim 10^{-2}$, further studies with smaller values of t may yield upper bounds on this region, or begin to show the new behavior. We hope this paper will stimulate such experiments.

In addition to the present calculation we have also calculated the tricritical and critical points into which the Potts transition turns under stress along $[(1+\delta)(1+\delta)(1-2\delta)]$. The universal ratio of the values of δ_t and δ_c at these points also exhibits an XY-to-Gaussian crossover as T_b is approached.[15]

Finally, it should be noted that similar results apply to all the other cases in which the phase diagram of Fig. 1 applies, e.g., a cubic ferromagnet in a magnetic field along [111].[20]

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