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Critical behavior of an Ising model on a cubic compressible lattice

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Renormalization-group methods are applied to the critical behavior of an Ising-like system on an elastic solid of either cubic or isotropic symmetry. Except in the special case where $dT_c/dV = 0$, the bulk modulus is found to be negative very close to T_c, so that the phase transition at constant pressure must be at least weakly first order. In the isotropic case the solid may be stabilized by pinned boundary conditions, if crystal fracture can be avoided. A "Fisher-renormalized" critical point can then be observed. By contrast, the anisotropic cubic solid will develop a microscopic instability so that T_c cannot be reached, regardless of boundary conditions. Estimates of the size of these effects are given, and contact is made with the Baker-Essam model and a liquid, as limiting cases with a vanishing shear modulus.

I. INTRODUCTION AND SUMMARY

The role of elastic degrees of freedom in the behavior of systems near a critical point has long been a subject of debate. In particular, one may consider systems such as helium near its λ point, a ferromagnet near its Curie point, a binary alloy such as β-brass or a crystal such as NH_4Cl near its ordering temperature—all of them systems which undergo either a critical transition or a weak first-order transition from a disordered phase above a critical temperature T_c to an ordered phase of lower symmetry below T_c. In each case one may hypothesize an idealized model for the phase transition, such as the Ising model or Heisenberg model on a rigid lattice, for which the critical properties are known from series expansions or other techniques, and one may hope that the physical system shows the same behavior as the idealized model. In making such an assumption, one has to decide whether various properties obtained for the model correspond to properties of the physical system at constant volume V or at constant pressure P. As was pointed out by Rice,[1] Domb,[2] and Pippard,[3] and later by many others, this question is of particular importance if the specific heat of the ideal system diverges at T_c, as it does for the Ising model.

If one assumes that C_p diverges, i.e.,

$$C_p \sim |T - T_c(P)|^{-\alpha_I}, \tag{1.1}$$

where $\alpha_I > 0$ is the ideal exponent and $T_c(P)$ is a well-behaved function, one can then show that C_v must be finite at the transition, except when $dT_c/dP = 0$. More precisely, one can show that close to T_c, C_v is given by

$$C_v = \text{const} + \text{const}|T - T_c(V)|^{-\alpha_R}, \tag{1.2}$$

where

$$\alpha_R \equiv -\alpha_I/(1-\alpha_I) < 0 \tag{1.3}$$

is the "Fisher-renormalized" critical exponent.[4]

On the other hand, if one assumes that C_v diverges, i.e.,

$$C_v \sim |T - T_c(V)|^{-\alpha_I}, \tag{1.4}$$

where $T_c(V)$ is now well behaved, then one finds that, as long as $dT_c/dV \neq 0$, C_p as well as the isothermal modulus of bulk compressibility B both become negative close to T_c. In a fixed P experiment, one therefore expects to observe a first-order transition, accompanied by a volume discontinuity. The value of $T - T_c(V)$ would jump at the transition from a finite positive value to a finite negative value, and the regions of negative B and C_p would be avoided. Although a Maxwell construction must be made to find the exact location and other properties of the transition, some idea of the location as well as the size of the discontinuities can be obtained by estimating the reduced temperature t_v at which B vanishes above T_c. This estimate leads to

$$t_v \equiv \left| \frac{T - T_c(V)}{T_c(V)} \right| \cong \left[\frac{T_c C_{\text{sing}}}{B_0} \left(\frac{V}{T_c} \frac{dT_c}{dV} \right)^2 \right]^{1/\alpha_I} t_1, \tag{1.5}$$

where t_1 is a somewhat arbitrary value of t_v at the edge of the critical region, C_{sing} is the singular part of the Ising specific heat at t_1, and B_0 is the value of B at t_1, where B is still dominated by its fairly constant regular part. The associated volume jump is estimated by

$$\Delta V \cong \frac{2|T - T_c|}{dT_c/dV}. \tag{1.6}$$

If we examine further the consequences of assumption (1.4), we see that if an experiment is performed at fixed V, thermodynamics predicts that for $|T-T_c|$ sufficiently small, the system will break up into two coexisting phases of different densities. In the case of a solid, however, such a breakup may require fracturing of the solid. Thus, with appropriate boundary conditions, the possibility exists of entering the metastable region and even of exploring the region where B is negative.

The assumption of (1.4) and the conclusions which follow from it were named "magnetothermomechanics" by Mattis and Schultz,[5] a term we will continue to use in precisely that sense.

In order to decide between the alternative (1.1) and (1.4), a number of models were studied. Mattis and Schultz considered a compressible, nearest-neighbor Ising model with an exchange interaction which depended on bond length, but imposed the artificial constraint that all bond lengths be the same[5] (this may be thought of as a solid with infinite rigidity but finite compressibility). Upon minimizing the free energy with respect to the bond length, they indeed found that (1.4) was valid. But other models (e.g., various "decorated Ising models") suggested that in fact (1.1) might be correct.

More generally, Fisher as well as Lipa and Buckingham proposed that the ideal exponents be associated with transitions at constant values of the intensive variables or fields.[4] Thus, for example, in ^{3}He-^{4}He mixtures ideal behavior of the λ transition should be observed at fixed partial pressures of ^{3}He and ^{4}He but not at fixed concentration. Indeed, for a symmetry-breaking transition in a fluid, (1.1) is undoubtedly the correct assumption to make since at constant pressure there are only short-range forces in the liquid, whereas a constraint of constant volume introduces effective long-range forces (see also the discussion in Appendix D). However, in a solid the situation was less clear because of the long-range nature of the forces transmitted by the lattice both at fixed P and at fixed V. In particular, Wagner and Swift[6] have shown that if the elastic variables are integrated out in a nearest-neighbor compressible Ising Hamiltonian, where the interactions depend on the elastic displacements, the resulting pure spin Hamiltonian contains long-range, four-spin interactions.

One other model has received considerable attention: the Baker-Essam model (henceforth to be abbreviated as BE). That model was found to have an ideal transition at $P=0$, a first-order transition at $P<0$, and a Fisher-renormalized critical point at $P>0$,[7-9] i.e.,

$$C_p = \text{const} + \text{const}\,|T-T_c(P)|^{-\alpha_R}.$$

This model and some generalizations of it will be discussed in more detail below.

The above-mentioned models were either too intractable to yield definite results about the critical properties (e.g., Ref. 6), or did not accurately represent the elastic properties of a real solid—finite compressibility and rigidity moduli (e.g., Refs. 5 and 7–9). In 1969, however, Larkin and Pikin succeeded in analyzing a model with finite rigidity and compressibility and obtained results which strongly suggested that none of the above hypotheses is completely correct.[10] Their model, which had isotropic elastic properties, agreed with magnetothermomechanics in that a first-order transition is found at fixed P. However, the size of their transition is not given by (1.5), but by the usually smaller amount indicated in (4.26) below. Furthermore, if their model is examined at constant V, one finds that C_v does not have the ideal behavior of (1.4) very close to T_c, but rather the Fisher-renormalized behavior of (1.2). In addition, before the first-order transition occurs at constant P, there is usually a region of temperatures where the ideal, unrenormalized critical behavior can be observed. Therefore measurements at constant P may be better suited for observing ideal behavior than measurements at constant V. In the limit where the shear modulus tends to zero, the size of the Larkin-Pikin first-order transition vanishes, and pure ideal critical behavior is recovered for fixed P, as expected for a liquid.

These results for an Ising-like transition have been confirmed recently by Wegner[11] and by Sak[12] using modern renormalization-group techniques,[13-15] and are also supported by the present work. Specifically, we find for the case of an isotropic compressible solid: (a) For free boundary conditions (i.e., constant hydrostatic pressure), the solid will have a first-order transition except if $dT_c/dP=0$. (b) If we consider pinned boundary conditions (i.e., all displacements vanish at the surface), which may be realized by welding the sample to the inside of a rigid container, and if internal fracture can be avoided, then a critical-point transition with Fisher-renormalized Ising exponents will be observed. (c) The weaker constraint of constant volume (which could be realized by placing the sample in an incompressible liquid enclosed in a container of fixed volume) is not sufficient to stabilize the solid, and the critical point cannot be reached in this way. (d) When the first-order transition is very small, which is the usual case, one can observe critical behavior in a range of temperatures before the transition. We will call this situation pseudocritical behavior. At fixed

P we find pseudocritical behavior with ideal Ising exponents, while at fixed V there will be a crossover from ideal behavior to Fisher-renormalized behavior as T_c is approached.

Going beyond a purely isotropic solid, we have found that the critical behavior of the isotropic elastic Ising lattice is unstable with respect to the inclusion of any amount of cubic anisotropy in the elastic moduli. At constant pressure, the phase transition is still expected to be first order. However, in contrast with the isotropic case, it appears to be impossible to stabilize the solid even by imposing pinned boundary conditions, since the instability now involves microscopic normal modes of the system. At some temperature above the critical point (i.e., while the correlation length ξ is still finite), the crystal becomes very soft with respect to phonons along some of its symmetry directions. Before reaching this temperature, the solid will probably transform by a first-order transition to an inhomogeneous state.

In the special case when $dT_c/dP=0$, which corresponds to a maximum or minimum of T_c, the above discussions are inapplicable. One then finds that a critical point can occur for any boundary condition. C_v and C_p are then equivalent and diverge at T_c with the ideal exponent α_I. For small dT_c/dP, one can estimate the size of the first-order transition. This is done in Sec. IV below. The behavior of the latent heat in the vicinity of a maximum or minimum of $T_c(P)$ is shown schematically in Fig. 1.

A consequence of the universal appearance of a first-order transition at constant P is that an Ising-like tricritical point cannot occur in an elastic solid except when T_c is independent of P on the second-order side of P_t. (A tricritical point is defined as a pressure P_t where the nature of the transition between an ordered and a disordered phase changes from first order for, say, $P<P_t$ to second order for, say, $P>P_t$.) However, since the size of the first-order transition predicted by (4.26) is usually quite small, it is quite possible to have a pseudotricritical point at which the entropy jump ΔS changes from an appreciable fraction of k_B per particle to a much smaller amount, given by (4.33) (see Fig. 2). The tricritical points observed in[16-19] NH_4Cl and[20] ND_4Cl presumably are actually pseudotricritical points of this type. Because of the smallness of the jumps predicted by (4.32) and (4.33), it is not clear whether they are observable in practice. We find, however, that these jumps will be enhanced in the vicinity of a pseudotricritical point, as shown in (4.31). As the tricritical point is approached from its second-order side, the latent heat increases at first as $|P-P_t|^{2(1-\alpha_I)/\alpha_I}$, but later saturates at a finite but enhanced value inside the tricritical region.

The Larkin-Pikin model had the shortcoming that unphysical boundary conditions were employed. Although the over-all volume was permitted to vary, the shape of the boundary was constrained by imposing periodic boundary conditions.[10] In the treatment of Wegner,[11] free boundary conditions were assumed. An effective spin Hamiltonian was constructed in terms of the exact static elastic deformation modes associated with the free surface. The contribution of these surface modes was discussed explicitly using renormalization-group theory, at the price of a considerable complication of the analysis.

In the present paper, we separate the problem

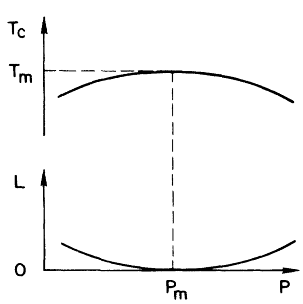

FIG. 1. Schematic diagram of latent heat L in the vicinity of a maximum (or minimum) of the transition temperature $T_c(P)$ for a transition that would have been an Ising-like critical point except for lattice-compressibility effects. The two curves are described by $T_c(P)-T_m \propto (P-P_m)^2$ and $L \propto (P-P_m)^{2(1-\alpha_I)/\alpha_I}$. The volume jump at the transition is proportional to $(P-P_t)L$.

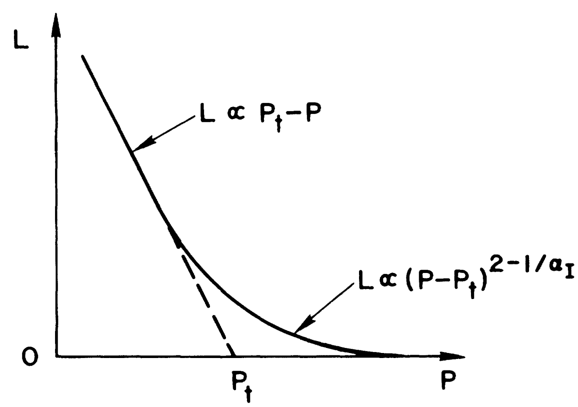

FIG. 2. Latent heat L in the vicinity of a tricritical point (schematic). Solid curve shows a pseudotricritical point, expected for real systems. Dashed curve shows a true tricritical point, which is possible for an Ising-like system on a cubic compressible lattice only if $dT_c/dP \equiv 0$ on the second-order side.

of boundary conditions from the renormalization-group analysis by the following approach: We assume that the standard results of 19th-century thermodynamic and elasticity theory describe macroscopic deformations of our sample at all temperatures other than the transition temperature. Thus we assume that the system has a proper thermodynamic limit, which is reached when the size of the sample is much greater than the correlation length ξ. The free energy per unit volume is then independent of the details of the boundary conditions, but depends only on the temperature T and the density ρ and on the local shearing strains $e_{\alpha\beta}$, if any. Changes in the free energy due to variations in the strains on a length scale large compared to ξ are determined by standard elasticity theory. Like the free-energy density, the elastic constants depend only on T, ρ, and $e_{\alpha\beta}$. We can now calculate these constants, as well as any other local properties of the system, using any convenient boundary conditions. The behavior of the system under other boundary conditions can then be deduced by using 19th-century physics. Periodic boundary conditions are normally the most convenient for calculations, and these will be utilized in the present paper.

In Sec. II of this paper we derive the renormalization-group equations of our model—a Larkin-Pikin–type continuum Hamiltonian but with cubic anisotropy in the elastic part. In Sec. III we analyze the solutions of these equations, finding their finite fixed points and their instabilities. In particular, we find that while the isotropic system only develops *macroscopic* instabilities (e.g., $B<0$) which do not prevent the Hamiltonian from reaching a fixed point, the anisotropic system develops a *microscopic* instability, as mentioned above, and the Hamiltonian is prevented from reaching a finite fixed point. In Sec. IV we discuss the physical properties of the system that arise from these mathematical properties of the renormalization-group equations. In particular, we estimate the location and size of the first-order transition under various assumptions, as well as determine what types of pseudocritical or pseudotricritical behavior can be expected. In Sec. V we outline some alternative ways of discussing the effect of different external or boundary conditions on the properties of the model. In Sec. VI we discuss a few models that lead to results which seem to contradict our general results. We show that these contradictions, which arise in some versions of the BE model as well as in a model recently proposed by Imry,[21] are the result of the particular pathologies of these models. More specifically, we show that these models, which exhibit a true tricritical point at constant P, manage to do so by having different elastic moduli for uniform strains and for finite-wavelength strains. These models also violate the rotational invariance of the free energy.

In Appendix A we develop some of the important properties of an elastic continuum with cubic anisotropy which are required for our discussion. In Appendix B we analyze the Baker-Essam model and some generalizations of it and show how they fall into the framework of our general discussion as a special case of a cubic system where one of the shear moduli vanishes. In Appendix C we give a more careful discussion of the solution of some of the renormalization-group equations. In Appendix D we develop a mathematical analogy between an Ising model in a compressible liquid and an Ising model in an isotropic elastic solid with periodic boundary conditions. In Appendix E we show how to apply a Maxwell construction for determining the exact properties of the first-order transition induced in an isotropic solid at fixed P.

II. DERIVATION OF RENORMALIZATION-GROUP EQUATIONS

We will consider a system of one-component Ising spins sitting on a harmonic elastic lattice with cubic anisotropy. The spins are coupled linearly and symmetrically to the elastic deformations. In the long-wavelength limit the bare Hamiltonian can be written in terms of continuum variables as follows:

$$\frac{H^0}{T} = \int d^d x \left(\tfrac{1}{2}\tilde{r}_0\psi^2 + \tfrac{1}{2}(\nabla\psi)^2 + \tilde{u}_0\psi^4 + \frac{g_0}{T^{1/2}}\psi^2(\nabla\cdot u)\right) + \frac{H_e^0}{T}, \tag{2.1a}$$

$$H_e^0 = \int d^d x \left(\tfrac{1}{2}C_{11}^0 \sum_{\alpha=1}^{d} e^2_{\alpha\alpha} + C_{12}^0 \sum_{\alpha<\beta} e_{\alpha\alpha}e_{\beta\beta} + \tfrac{1}{2}C_{44}^0 \sum_{\alpha<\beta} e^2_{\alpha\beta}\right), \tag{2.1b}$$

where $\psi(x)$ is the Ising-spin field variable and $e_{\alpha\beta}(x)$ are the components of the strain tensor, which are related to the displacement vector $u(x)$ by

$$e_{\alpha\beta}(x) = \tfrac{1}{2}\left(\frac{\partial u_\alpha}{\partial x_\beta} + \frac{\partial u_\beta}{\partial x_\alpha}\right). \tag{2.2}$$

It is understood that only fluctuations with wave vector less than some cutoff Λ (which we will take to be 1) are to be included. In (2.1a), g_0 is the bare coupling constant of the elastic and spin variables, while C_{11}^0, C_{12}^0, and C_{44}^0 represent bare values of the elastic moduli in ordinary units of energy per unit volume. (The notation C_{11}, C_{12}, and C_{44} corresponds to the usual Voigt notation at $d=3$, but we shall use the same symbols for all values of d.) The spatial variable x is measured in a coordinate system which deforms with the elastic solid, so that the integrations are over a fixed volume $V \equiv L^d$. The vector $u(x)$ is the difference between the actual position of a particle in the laboratory frame and its equilibrium position.

As explained in the Introduction, we will assume periodic boundary conditions for $\psi(x)$ and $u(x)$. It follows that the actual volume of the sample is the same as the original volume L^d, and the equilibrium expectation value of the strain $\langle e_{\alpha\beta}(x)\rangle$ must vanish. [This follows from a combination of the translational symmetry of the Hamiltonian and the periodicity of $u(x)$.]

We remark that, in principle, we could add arbitrary higher-order terms to (2.1), including anharmonic terms in the elastic energy, spin-elastic couplings quadratic in the strain, and couplings proportional to higher powers of the spin and of the gradients. All such terms turn out to be "irrelevant" in the renormalization-group sense (with certain qualifications discussed in Sec. IV B below), provided that they preserve the over-all cubic symmetry of the system.

Having assumed periodic boundary conditions, we can define Fourier components in the usual way:

$$u_\alpha(x) = \frac{1}{V^{1/2}} \sum_q u_{\alpha q} e^{iq\cdot x}, \qquad \psi(x) = \frac{1}{V^{1/2}} \sum_q \psi_q e^{iq\cdot x}, \tag{2.3}$$

where q, x, and u are d-dimensional vectors. In terms of ψ_q and u_q for $q \neq 0$, H^0 becomes

$$\frac{H^0}{T} = \sum_q \tfrac{1}{2}(\tilde{r}_0 + q^2)\psi_q\psi_{-q} + \frac{\tilde{u}_0}{V} \sum_{q_1q_2q_3} \psi_{q_1}\psi_{q_2}\psi_{q_3}\psi_{-q_1-q_2-q_3} + \sum_q \frac{1}{2T} u_q^* \cdot D^0 \cdot u_q + \frac{g_0}{(TV)^{1/2}} \sum_{qq_1} (iq\cdot u_q)\psi_{q_1}\psi_{-q-q_1}, \tag{2.4}$$

where $D^0_{\alpha\beta}(q)$ is the bare dynamical matrix, proportional to q^2, whose precise form is given in Appendix A. The $q=0$ component of $\psi(x)$ becomes important only below the critical point, while the $q=0$ component of $u(x)$ is absent from H^0 with our boundary conditions.

Using a Wilson-type approach,[15] we can now construct a renormalization-group transformation by integrating over intermediate wave vectors in the domain

$$b^{-1} < q < 1,$$

and making a change of scale

$$\begin{aligned} &x \to x' = x/b, && q \to q' = bq, \\ &\psi(x) \to \psi'(x') = b^a \psi(x), && \psi_q \to \psi'_{q'} = b^{a-d/2}\psi_q, \\ &u(x) \to u'(x') = b^{a_u} u(x), && u_q \to u'_{q'} = b^{a_u - d/2} u_q, \end{aligned} \tag{2.5}$$

where b is a constant greater than 1, and the scaling exponents a and a_u will be specified later. The equations are constructed by considering the $\tilde{u}$ and g terms as perturbations and making a diagrammatic expansion. The renormalization group constructed in this way is a simple generalization of the analogous renormalization group used by Halperin *et al.*[22] and by Achiam and Imry[23] to discuss coupling between an Ising-like field and a nonordering scalar field (e.g., a mass density or energy density).

Taking into account only the diagrams in Fig. 3(a), we get the following recursion equation for the inverse spin-spin propagator:

$$\tilde{r}_{l+1} + q'^2 = b^{d-2a}\left(\tilde{r}_l + q^2 + \frac{12\tilde{u}}{V}\sum_p \frac{1}{\tilde{r}_l + p^2} - \frac{4g_l^2}{V}\sum_p \frac{1}{\tilde{r}_l + p^2} \sum_{\alpha,\beta} [D_l^{-1}(p+q)]_{\alpha\beta}(p_\alpha + q_\alpha)(p_\beta + q_\beta)\right). \tag{2.6}$$

Even though we have included only the lowest-order terms here, i.e., those that will give rise to $O(\epsilon)$ terms in an expansion around $d=4$, we seem to have an extra q dependence in the last term on the right-hand side of (2.6). To investigate this further, we rewrite this term as an integral, and expand the integrand in powers of q:

$$-8\int \frac{d^dp}{(2\pi)^d} \frac{K_l(p+q)}{\tilde{r}_l + p^2} = -8\int \frac{d^dp}{(2\pi)^d} \frac{1}{\tilde{r}_l + p^2}\left(K_l(p) + q\cdot\frac{\partial K_l(p)}{\partial p} + \frac{1}{2}\sum_{\alpha,\beta} q_\alpha q_\beta \frac{\partial^2 K_l(p)}{\partial p_\alpha \partial p_\beta}\right), \tag{2.7}$$

where we have defined

$$K_l(q) \equiv \tfrac{1}{2} g_l^2 q \cdot D_l^{-1}(q) \cdot q. \tag{2.8}$$

Note that K_l really depends only on the direction of q. We will often emphasize this fact by writing the argument of K_l in the form of an appropriate unit vector, e.g., $\hat{q} \equiv q/|q|$. The integral in (2.7) is separated into an integral over the magnitude of p and an angular integral over the surface of the unit sphere described by $\hat{p}$. Because $K_l(-p) = K_l(p)$, the second term on the right-hand side vanishes. The last term includes the second-rank tensor $\partial^2 K_l/\partial p_\alpha \partial p_\beta$ which, when integrated over the angles, must yield a constant second-rank tensor. Because in cubic symmetry the only constant second-rank tensor is the unit tensor, we finally get

$$-8B_d \int_{b^{-1}}^{1} \frac{p^{d-1}dp}{\tilde{r}+p^2} \int \frac{d\Omega_d}{\Omega_d}\left(K_l(\hat{p}) + \frac{q^2}{2d}\nabla^2 K_l(\hat{p})\right), \tag{2.9}$$

where

$$B_d \equiv \Omega_d/(2\pi)^d, \tag{2.10}$$

and

$$\Omega_d \equiv 2\pi^{d/2}/\Gamma(\tfrac{1}{2}d) \tag{2.11}$$

is the surface area of the unit sphere in d dimensions. Since K_l is a homogeneous function of order 0 in the components of p, it can be expanded as a series of spherical harmonics with constant coefficients. The angular integral over $\nabla^2 K_l$ vanishes because the only spherical harmonic which could have survived it, i.e., Y_0, is made to vanish by ∇^2. Consequently there are no q^2 terms on the right-hand side of (2.6) other than the usual one. This leads to the usual ϵ-expansion results

$$\begin{aligned} \eta &= O(\epsilon^2), \\ d-2a &= 2+O(\epsilon^2), \\ d-4a &= \epsilon + O(\epsilon^2). \end{aligned} \tag{2.12}$$

The absence of extra q^2 terms on the right-hand side of (2.6) could also have been verified from the explicit form of $K_l(\hat{q})$ given below.

As a consequence of the above discussion, we can now write the recursion equation for $\tilde{r}_l$ in the form

$$\tilde{r}_{l+1} = b^{d-2a}\left(\tilde{r}_l + (12\tilde{u}_l - 8\langle K_l\rangle)B_d \times \int_{b^{-1}}^{1} \frac{p^{d-1}\,dp}{\tilde{r}_l+p^2}\right), \tag{2.13}$$

where the symbol $\langle K_l\rangle$ refers to an angular average:

$$\langle K_l\rangle \equiv \int \frac{d\Omega_d}{\Omega_d} K_l(\hat{p}). \tag{2.14}$$

Similarly we can derive recursion relations for the remaining parameters $\tilde{u}_{l+1}, g_{l+1}$, etc. For convenience, we will write all the recursion relations in the form of differential equations. To lowest order in $\epsilon = 4-d$ and in the coupling constants u_l and g_l, these equations can be obtained in a trivial way from the discrete relations by setting $\ln b = dl$. We thus find, using the diagrams of Fig. 3,

$$\frac{d\tilde{r}}{dl} = (d-2a)\tilde{r} + \frac{B_d}{1+\tilde{r}}(12\tilde{u} - 8\langle K\rangle), \tag{2.15}$$

$$\frac{d\tilde{u}}{dl} = (d-4a)\tilde{u} + \frac{B_d}{(1+\tilde{r})^2} \times (-36\tilde{u}^2 + 48\tilde{u}\langle K\rangle - 16\langle K^2\rangle), \tag{2.16}$$

$$\frac{dg}{dl} = \frac{g}{2}\left((d-4a) + (d-2a_u-2) + \frac{B_d}{(1+\tilde{r})^2}(-24\tilde{u} + 16\langle K\rangle)\right), \tag{2.17}$$

$$\frac{dD_{\alpha\beta}(q)}{dl} = (d-2a_u-2)D_{\alpha\beta}(q) - 2g^2 q_\alpha q_\beta \frac{B_d}{(1+\tilde{r})^2}, \tag{2.18}$$

$$\frac{dK(\hat{q})}{dl} = K(\hat{q})\left((d-4a) + \frac{B_d}{(1+\tilde{r})^2} \times [-24\tilde{u} + 16\langle K\rangle + 4K(\hat{q})]\right), \tag{2.19}$$

where we have suppressed the subscripts l, and where $\langle K^2\rangle$ is the angular average of $K^2(q)$. Note that (2.19) is not independent of the other equations—it was derived by combining (2.17) with an equation for D^{-1} obtained from (2.18).

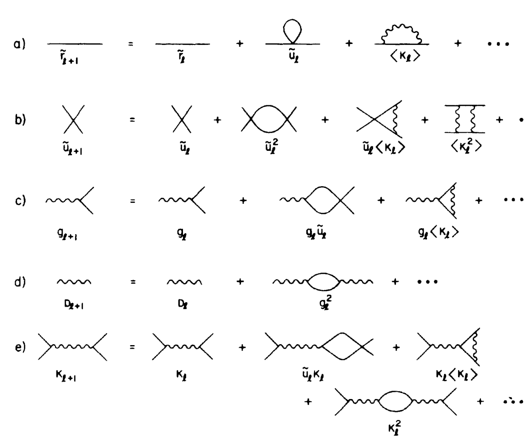

FIG. 3. Diagrams used to obtain the renormalization-group equations (2.15)–(2.19).

Using (2.18) and the explicit form of D [see (A7) in Appendix A] we can deduce the following equations for the renormalized elastic coefficients:

$$\frac{dC_{44}^l}{dl}=(d-2a_u-2)C_{44}^l, \tag{2.20}$$

$$\frac{d(C_{12}^l-C_{11}^l)}{dl}=(d-2a_u-2)(C_{12}^l-C_{11}^l), \tag{2.21}$$

$$\frac{dC_{11}^l}{dl}=(d-2a_u-2)C_{11}^l-2g_l^2\frac{B_d}{(1+\bar{r}_l)^2}\,. \tag{2.22}$$

In Appendix A we calculate K_l explicitly. Using Eqs. (A8) and (A13) we can write K_l in the form

$$K_l^{-1}(\hat{q})=\frac{2C_{11}^l}{g_l^2}+\frac{4(C_{12}^l-C_{11}^l+\frac{1}{2}C_{44}^l)}{g_l^2}Q(\hat{q}), \tag{2.23}$$

where Q is a ratio of polynomials symmetric in the components of $\hat{q}$. These polynomials have coefficients that depend only on the anisotropy parameter A, which is the ratio of the two principal shear moduli:

$$A\equiv\frac{\frac{1}{2}C_{44}}{C_{11}-C_{12}},\quad 0<A<\infty. \tag{2.24}$$

Note that $A=1$ for an isotropic system. The detailed form of Q, given in (A14), depends on d. For $d=3$, Q is given by

$$Q(\hat{q})=\frac{A(\hat{q}_x^2\hat{q}_y^2+\hat{q}_y^2\hat{q}_z^2+\hat{q}_z^2\hat{q}_x^2)+(1-A)(4-A)\hat{q}_x^2\hat{q}_y^2\hat{q}_z^2}{A^2+4A(1-A)(\hat{q}_x^2\hat{q}_y^2+\hat{q}_y^2\hat{q}_z^2+\hat{q}_z^2\hat{q}_x^2)+12(1-A)^2\hat{q}_x^2\hat{q}_y^2\hat{q}_z^2}\,. \tag{2.25}$$

We have not indicated any dependence on l in either A or Q, for the simple reason that they are independent of l, according to (2.20) and (2.21). As discussed in Appendix A, Q has the remarkable property that, for all allowed values of A, it satisfies

$$0\leq Q\leq(d-1)/2d, \tag{2.26}$$

the lower bound being attained when q is along a cubic axis (⟨100⟩ in three dimensions), while the upper bound is attained when q is along a body diagonal (⟨111⟩ in three dimensions).

One might wonder at this point how the matrix D and the vector u are to be generalized to nonintegral d. From the discussion leading up to (2.13) it is clear that the perturbation expansion only produces products of factors like $K(\hat{q})$ that have to be integrated over solid angles. While it is not clear how to generalize the functional form of K for nonintegral d, all that is really required for evaluating these integrals is the distribution of values of $K(\hat{q})$ and of products $\hat{q}\cdot\hat{p}K(\hat{q})K(\hat{p})$, etc. These distributions, which can be found for integral d, can presumably be continued analytically to nonintegral values of d. As we shall see in Sec. III, we will not even have to calculate these distributions explicitly because we will find that at a finite fixed point K has to be isotropic, in which case the distribution is trivial anyway.

The physical values of the elastic constants are given by

$$C(t)=e^{-(d-2a_u-2)l}C_l\big|_{l=\ln(\xi/\xi_0)}, \tag{2.27}$$

where C stands for C_{11}, C_{12}, C_{44}, or any linear combination of these constants, ξ is the spin-spin correlation length, and ξ_0 is the value of that length at $\bar{r}_0=1$, far from T_c. (See Appendix A for a derivation.) Consequently, it is clear from (2.20) and (2.21) that the physical values of C_{44} and $C_{11}-C_{12}$ are equal to the bare values C_{44}^0 and $C_{11}^0-C_{12}^0$. It is therefore convenient to choose the scaling exponent a_u to satisfy

$$d-2a_u-2=0, \tag{2.28}$$

since that choice ensures that these parameters also do not change under the renormalization group

$$C_{44}^l=C_{44}^0,\quad C_{11}^l-C_{12}^l=C_{11}^0-C_{12}^0. \tag{2.29}$$

We note that this remains true to any order of perturbation theory—this follows from the fact that the equation for D^l always has the form

$$\frac{dD_{\alpha\beta}^l}{dl}=(d-2a_u-2)D_{\alpha\beta}^l-2g_l^2F(\tilde{u}_l,K_l,q)q_\alpha q_\beta \tag{2.30}$$

to any order in K and $\tilde{u}$, where F has cubic symmetry in the components of q. From the explicit form of D [Eq. (A7)], it is now evident that the shear moduli are not renormalized when the choice of (2.28) is made.

The physical value of C_{11} will be given by

$$C_{11}(t)=C_{11}^l\big|_{l=\ln(\xi/\xi_0)}\,. \tag{2.31}$$

From (2.22) it is clear that unless $g\equiv0$, C_{11}^l is a monotonic decreasing function of l, and therefore that $C_{11}(t)$ is always less than the bare value. We shall see in Sec. III that sometimes the value of $C_{11}(t)$ turns out to be negative, even though C_{11}^0 is positive, and this will naturally have serious consequences for the stability of the system.

Returning to (2.30), we note that since $F(\tilde{u},K,q)$ in that equation is a regular function for small

q, $D^l_{\alpha\beta}(q)$ is analytic in the components of q near $q=0$. Similarly, g_l, $\tilde{u}_l$, and $\tilde{r}_l$ will depend on q in higher orders of perturbation theory, but this dependence will be completely regular in the components of q near $q=0$. Of all the quantities that appear in the equations, only K is nonanalytic when viewed as a function of q (rather than $\hat{q}$) near $q=0$. This does not cause any problems, however, since K only appears in connection with internal wavy lines (i.e., phonon propagators) in diagrams, and in that case it is only integrated over a shell in q space where $|q|>b^{-1}$.

By contrast, if we had tried to integrate over the elastic variables completely before setting up the renormalization-group equations, as has been done by others, and as we shall do in (5.2) below, we would have introduced singularities in the Hamiltonian at $q=0$. These singularities, which were ignored by Aharony and Bruce,[24] would presumably complicate the discussion in that approach.

III. FIXED POINTS AND CRITICAL BEHAVIOR–MICROSCOPIC AND MACROSCOPIC STABILITY

A. Fixed points

It is immediately clear from (2.19) that at any finite fixed point, $K(\hat{q})$ must be independent of $\hat{q}$. In that case $\langle K\rangle=K$ and $\langle K^2\rangle=K^2$. It is therefore useful to rewrite (2.15), (2.16), and (2.19) in terms of

$$u_l\equiv\tilde{u}_l-\langle K_l\rangle. \tag{3.1}$$

We write the resulting equations in their ϵ-expansion forms, using (2.12) and (2.28), and replacing B_d by B_4, and we note that it is quite easy to restore the more general form to any of the results. We thereby obtain

$$\frac{d\tilde{r}}{dl}=2\tilde{r}+\frac{B_4}{1+\tilde{r}}\,(12u+4\langle K\rangle), \tag{3.2}$$

$$\frac{du}{dl}=u(\epsilon-36B_4u)-20B_4(\langle K^2\rangle-\langle K\rangle^2), \tag{3.3}$$

$$\frac{dK(\hat{q})}{dl}=K(\hat{q})[\epsilon-B_4(24u+4\langle K\rangle)]+4B_4K(\hat{q})[K(\hat{q})-\langle K\rangle]. \tag{3.4}$$

The subscripts l have again been suppressed here.

These equations have four $O(\epsilon)$ fixed points, given by

$$G:\ \tilde{r}^*=u^*=K^*=0, \tag{3.5}$$

$$S:\ \tilde{r}^*=-\frac{\epsilon}{2},\quad u^*=0,\quad K^*=\frac{\epsilon}{4B_4}, \tag{3.6}$$

$$I:\ \tilde{r}^*=-\frac{\epsilon}{6},\quad u^*=\frac{\epsilon}{36B_4},\quad K^*=0, \tag{3.7}$$

$$R:\ \tilde{r}^*=-\frac{\epsilon}{3},\quad u^*=\frac{\epsilon}{36B_4},\quad K^*=\frac{\epsilon}{12B_4}. \tag{3.8}$$

These are, respectively, a Gaussian, a Fisher-renormalized Gaussian (i.e., a spherical), an Ising, and a Fisher-renormalized Ising fixed point. To verify the identification of the Fisher-renormalized fixed points, we can calculate from (3.2) the index ν that characterizes the critical behavior of the correlation length ξ:

$$\xi/\xi_0\equiv|\tilde{r}-\tilde{r}_c|^{-\nu}. \tag{3.9}$$

In this way we find

$$2\nu_S=\frac{1}{1-\epsilon/2}=\frac{2\nu_G}{1-\alpha_G}, \tag{3.10}$$

$$2\nu_R=1+\frac{\epsilon}{2}+O(\epsilon^2)=\frac{2\nu_I}{1-\alpha_I}, \tag{3.11}$$

where the subscripts clearly correspond to the fixed points.

These fixed points and their stability properties have been discussed by Rudnick *et al.*,[25] who discovered the point R (it was called L in Ref. 25) and found that it was the most stable of the four. In agreement with that discussion, we find from (3.3) and (3.4) the following regions of stability for the various points:

$$\begin{aligned} &G:\ u_0=K_0=0,\\ &S:\ u_0=0,\quad K_0>0,\\ &I:\ u_0>0,\quad K_0=0,\\ &R:\ u_0>0,\quad K_0>0. \end{aligned} \tag{3.12}$$

Outside of these regions, the system will have microscopic instabilities.

Thus, when $u_0<0$ the system is unstable against fluctuations of the local spin variable $\psi(x)$ and it will undergo a first-order transition. The points G and S characterize tricritical behavior of the spin Hamiltonian, as we shall discuss in Sec. IV B below.

Another region not included in (3.12) is $K_0<0$. We do not consider this possibility since it would mean that the bare Hamiltonian H^0 is elastically unstable: Some vibrational normal modes of the lattice then have negative energies independently of the spin states. We will not consider such instabilities of the elastic Hamiltonian since we are interested in the critical properties of the spin system. The elastic variables are assumed to have critical behavior only as a result of their interactions with the spin variables and not as a result of any intrinsic elastic instability.

The remaining possibility for being outside of the stable regions of (3.12) is for $K_0(\hat{q})$ to be anisotropic. We will return to discuss this case later.

B. Isotropic $K(\hat{q})$

When $u_0>0$ and K_0 is isotropic, the renormalized Hamiltonian H^l will ultimately tend towards either I or R depending on whether $g_0=0$ or $g_0\neq 0$, since by (2.8) that determines whether $K_0=0$ or $K_0>0$. The physical meaning of g_0 is established as follows. Suppose the sample is compressed or expanded, so that the volume is changed by the amount δV. The spin-lattice interaction present in (2.1) requires that H_0 be modified by the term

$$T^{1/2} g_0 \frac{\delta V}{V} \sum_q \psi_q \psi_{-q}. \tag{3.13}$$

Clearly, this term merely shifts the effective value of $\tilde{r}_0$ to

$$r_0 \equiv \tilde{r}_0 + \frac{2g_0}{T^{1/2}} \frac{\delta V}{V}. \tag{3.14}$$

Assuming that $\tilde{r}_0$ is the only parameter in (2.1) which depends on T [this is a good approximation for T very close to $T_c(V)$], we can write for the reduced temperature t,

$$t \equiv \frac{T - T_c(V)}{T_c(V)} \propto r_0 - r_c = \tilde{r}_0 - r_c + \frac{2g_0}{T_c^{1/2}} \frac{\delta V}{V}, \tag{3.15}$$

where r_c is the critical value of r_0. Consequently, since r_c is independent of V, we find

$$g_0 = -\frac{1}{2} \frac{d\tilde{r}_0}{dt} \frac{V}{T_c^{1/2}} \frac{dT_c}{dV}. \tag{3.16}$$

Thus, when $dT_c/dV=0$ we have $g_0=0$, and there is no coupling between the spins and the elastic variables. In that case H^l tends to I and the critical behavior is characterized by unrenormalized Ising exponents. When dT_c/dV is nonzero but small, so that $K_0 \ll u_0$, there will be crossover effects between I and R.

We now turn to a careful analysis of the stability of the system when $u_0>0$, $K_0>0$ and K_0 is isotropic. An isotropic K_0 can be expected in only two special cases of the cubic Hamiltonian of Eq. (2.1)[26]: $A=1$, corresponding to an isotropic system; $A=0$, corresponding to a generalized and slightly modified Baker-Essam model.

To investigate further the microscopic stability of the system in the isotropic case ($A=1$), we consider the explicit forms of $\det D^l$ and K_l for this case [see Eq. (A26)]:

$$\det D^l = q^{2d} C_{11}^l (\tfrac{1}{4} C_{44}^l)^{d-1}, \qquad K_l = g_l^2 / 2C_{11}^l. \tag{3.17}$$

From (3.3) and (3.4) it is clear that if u_0 and K_0 are small and positive, then u_l and K_l both remain positive and tend to their fixed-point values monotonically. From the explicit form of K_l we conclude that $C_{11}^l>0$. Together with the fact that $C_{44}^l = C_{44}^0 > 0$ (because C_{44} is proportional to the square of a sound velocity), this leads to the conclusion that $\det D^l>0$, so that no microscopic normal-mode frequency ever vanishes for $q\neq 0$.

The asymptotic behavior of C_{11}^l as H^l approaches R can now be found by noting that it must be the same as the asymptotic behavior of g_l^2. To find the latter, we use (2.17) with $\tilde{u} = u_R^* - K_R^*$, $\langle K \rangle = K_R^*$, $d-4a=\epsilon$, and $d-2a_u-2=0$ to get

$$\frac{dg_l^2}{dl} = -\frac{\epsilon}{3} g_l^2. \tag{3.18}$$

From the solution of this equation and using (3.17) we find

$$C_{11}^l \cong g_l^2 / 2K_R^* \propto e^{-\epsilon l/3}. \tag{3.19}$$

The physical value of C_{11} thus satisfies

$$C_{11} = C_{11}^l |_{e^l = \xi/\xi_0} \propto \xi_R^{-\epsilon/3} = \xi_R^{\alpha_R/\nu_R} \propto | T - T_c |^{\alpha_I/(1-\alpha_I)}, \tag{3.20}$$

where in the last two terms we have replaced $\epsilon/3$ by the critical exponent that it actually represents and used the fact that

$$\alpha_R = \frac{-\alpha_I}{1-\alpha_I} = -\frac{\epsilon}{6} + O(\epsilon^2). \tag{3.21}$$

We now turn to consider the bulk modulus of compressibility B:

$$B \equiv \frac{1}{d} C_{11} + \frac{d-1}{d} C_{12} = C_{11} - \frac{d-1}{d} \tfrac{1}{2} C_{44}, \tag{3.22}$$

where we have used the fact that for an isotropic system $C_{11} - C_{12} = \frac{1}{2} C_{44}$. As a result of Eqs. (2.29) and (3.19), we find that, as $l\to\infty$,

$$B_l = C_{11}^l - \frac{d-1}{d} \tfrac{1}{2} C_{44}^0 \to -\frac{d-1}{d} \tfrac{1}{2} C_{44}^0 < 0. \tag{3.23}$$

A negative value of B, no matter how small, implies however that under free boundary conditions (constant pressure P), the system will become macroscopically unstable. In fact, even if the total volume is constrained to be constant, the system will still be unstable. To see this, consider a distortion of the following type:

$$\vec{u}(\vec{x}) \propto (\vec{n} \cdot \vec{x}) \vec{x} - \tfrac{1}{2} x^2 \vec{n}, \tag{3.24}$$

where $\vec{n}$ is any constant vector. All the shear strains vanish for this mode of distortion, since

$$e_{\alpha\alpha} = (\vec{n} \cdot \vec{x}); \quad e_{\alpha\beta} = 0 \text{ for } \alpha \neq \beta. \tag{3.25}$$

Therefore the elastic energy associated with these "linear modes" is proportional to B, and they become unstable when $B\to 0$. It is easy to see that for a body whose shape has inversion symmetry around $X = 0$, the linear modes involve no change in the total volume to lowest order. For a body lacking this symmetry, we can find a linear combination of the "breathing mode" $u \propto \vec{x}$ and a linear mode that will not alter the volume and will become unstable when $B \rightarrow 0$.

Even if one manages to prevent both breathing- and linear-mode distortions by a judicious choice of boundary conditions, there is still a large number $[O(N^{2/3})]$ of surface normal modes of distortion whose effective elastic constants lie between B and C_{11}.[11] As the critical point is approached and $C_{11} \rightarrow 0$, all of these eventually become unstable. We conclude that in order to stabilize an isotropic solid completely in the vicinity of the critical point, we would have to prevent all of these surface distortions from occurring. That would require a complete pinning of all the surface atoms and not just fixing the volume and the shape. One could try to achieve such "pinned boundary conditions" in practice by welding the solid body to the inside of a very rigid container. For the case of pinned boundaries as well as the case of periodic boundary conditions in fixed volume, for which we have done our calculation, there is no first-order transition. The critical point can be reached, provided internal fracture does not occur. Furthermore, there exists a complete mathematical analogy between the isotropic solid at fixed V with periodic boundary conditions and the one-component fluid. This analogy, which is discussed in detail in Appendix D, enables one to deduce many of the results for the isotropic solid from the analogous results known to hold rigorously for the fluid.

In the BE case $(A = 0)$, $\det D^l$ and K_l are given by [see (A27)]

$$\det D^l = dB_l (C_{11}^l - C_{12}^l)^{d-1} \prod_{\alpha=1}^{d} q_\alpha^2 , \tag{3.26}$$

$$K_l = g_l^2 / 2B_l . \tag{3.27}$$

By an analysis similar to that of the isotropic case, we find that $B_l > 0$, $C_{11}^l - C_{12}^l = C_{11}^0 - C_{12}^0 > 0$, and hence $\det D^l > 0$ except along directions where a component of q vanishes and therefore $\det D^l \equiv 0$. Again, all the microscopic normal-mode frequencies are positive except along those directions, where some of them vanish identically. In this case there is no further trouble due to macroscopic instabilities, since B_l is kept positive by the microscopic renormalization-group equations.

The preceding discussion assumed periodic boundary conditions. The critical behavior found under that assumption is characteristic of the system at fixed V. The reduced temperature is then

$$t_v \equiv \frac{T - T_c(V)}{T_c(V)} . \tag{3.28}$$

The critical behavior at fixed P is described in terms of a different reduced temperature,

$$t_p \equiv \frac{T - T_c(P)}{T_c(P)} . \tag{3.29}$$

To determine the critical behavior at fixed P, we will first determine t_v as a function of t_p, and then substitute that dependence into the thermodynamic quantities whose behavior as functions of t_v is already known.

A simple calculation, which follows Bergman *et al.*,[27] yields

$$\frac{dt_v}{dt_p} = T_c(P) \left(\frac{\partial [T/T_c(V)]}{\partial T} \right)_P$$

$$= \frac{T_c(P)}{T_c(V)} + \frac{T T_c(P)}{[T_c(V)]^2} \frac{dT_c}{dV} \left(\frac{\partial P}{\partial T} \right)_V \left(\frac{\partial V}{\partial P} \right)_T . \tag{3.30}$$

In Sec. IV A we will show that if $C_{11} \gg C_{44}$, there will be a range of t_v where B is still positive and exhibits Fisher-renormalized Ising behavior,

$$B(t_v) \cong B_0 (t_v/t_2)^{\alpha_I/(1-\alpha_I)} \quad \text{for } t_3 \ll t_v \ll t_2 , \tag{3.31}$$

where t_2 defines the crossover from unrenormalized to renormalized Ising critical behavior, while t_3 defines the temperature at which $B \rightarrow 0$ [see Eq. (4.17) below]. In the region where (3.31) is valid, (3.30) becomes

$$\frac{d(t_v/t_2)}{d(t_p/t_2)} \cong 1 - \frac{V}{B_0} \frac{dT_c}{dV} \left(\frac{\partial P}{\partial T} \right)_V \left(\frac{t_v}{t_2} \right)^{-\alpha_I/(1-\alpha_I)}$$

$$\cong 1 + \left(\frac{t_v}{t_2} \right)^{-\alpha_I/(1-\alpha_I)} , \tag{3.32}$$

where we have used (4.35) as well as the fact that $(\partial P / \partial T)_V \cong dP_c/dT$ to get the last result. Since the second term on the right-hand side is much greater than 1, the solution of this equation is

$$\frac{t_v}{t_2} \cong \left(\frac{t_p}{t_2} \right)^{1-\alpha_I} . \tag{3.33}$$

As a result of this, all the behavior that was Fisher-renormalized-Ising-like as a function of t_v gets renormalized back again to ideal Ising behavior as a function of t_p for $t_p \gg t_3$. This is an example of Fisher renormalization at work even when the original specific heat is nondivergent at the critical point.[28]

Note that when $C_{44}=0$, the system exhibits exact unrenormalized Ising behavior at fixed P(i.e., for arbitrarily small values of t_p), since B never becomes negative and there is no instability.

Before closing this subsection, we would like to point out that the qualitative result that $K(\hat{q})$ must be independent of $\hat{q}$ at a nontrivial finite fixed point is valid to any order in $\bar{u}$ and g. From (2.23) it is clear that when $K_l(\hat{q})$ is anisotropic, its shape can only be preserved with changing l if $C_{11}^l \equiv C_{11}^0$. We already noted that in lowest order, this would require $g_l=0$. We now go further and argue that when all the elastic moduli do not get renormalized, and hence do not exhibit any critical behavior, then we must have rigorously $dT_c/dV = dT_c/dP = 0$. This follows from Pippard's relations.[3] Barring that eventuality [which is what we mean by a trivial fixed point for $K(\hat{q})$], C_{11}^l always depends on l. Therefore, unless $K_l(\hat{q})$ is isotropic, it will keep changing its shape with increasing l.

C. Anisotropic $K(\hat{q})$

When A is neither 0 nor 1 (and $g_0 \neq 0$, $u_0>0$), K_0 has a nontrivial dependence on $\hat{q}$. This will prevent the system from ever reaching the point R or any other of the finite fixed points, since (3.3) and (3.4) are clearly unstable against nonisotropic perturbations of $K_l(\hat{q})$ around any K^* such that $\langle K_l\rangle = K^*$: Wherever $K_l(\hat{q}) > K^*$, $K_l(\hat{q})$ will tend to grow whereas wherever $K_l(\hat{q}) < K^*$, it will tend to decrease. We will now show that in fact the maximum value of $K_l(\hat{q})$, defined by

$$K_{\max}^l \equiv \max_{\hat{q}} K_l(\hat{q}), \tag{3.34}$$

diverges at some finite value of l, and then changes sign and becomes negative.

In order to do this, we will focus attention on the ratio R_l of the two coefficients in the expression for K_l in terms of Q [Eq. (2.23)]:

$$R_l \equiv \frac{C_{44}^l - 2(C_{11}^l - C_{12}^l)}{C_{11}^l} = \frac{A-1}{A}\frac{C_{44}^l}{C_{11}^l}. \tag{3.35}$$

This can be either positive or negative, depending on whether $A>1$ or $A<1$. It is useful to write down the equation satisfied by R_l, derived from (2.20) and (2.22):

$$\frac{dR_l}{dl} = \frac{4B_d}{(1+\tilde{r}_l)^2}\frac{g_l^2}{2C_{11}^l}R_l \cong 4B_4\frac{g_l^2}{2C_{11}^l}R_l. \tag{3.36}$$

It is clear that as long as $g_l^2/2C_{11}^l > 0$, $|R_l|$ is a monotonically increasing function of l. That in itself already shows that the anisotropy of K_l will always grow with increasing l.

In the case when $A>1$, $K_{\max}^l$ always occurs when q is along a cubic axis, where $Q=0$, and its value is [see (A17)]

$$K_{\max}^l = \frac{g_l^2}{2C_{11}^l} \quad \text{for } A>1. \tag{3.37}$$

In order to determine the behavior of this $K_{\max}^l$ as $l\to\infty$, we consider all the conceivable alternatives: (a) If we assume that $g_l^2/2C_{11}^l$ remains bounded between two finite, positive values, then by (3.36), $R_l \to +\infty$. Consequently, the coefficient of Q in (2.23) will also tend to $+\infty$, while $K_l(\hat{q})\to 0$ for all q except along the cubic axes. This would lead H^l to the fixed point I, which is, however, unstable even against isotropic perturbations of K. Therefore this is not a possible alternative. (b) If we assume that $g_l^2/2C_{11}^l \to 0$ for some l (including $l=\infty$), then both coefficients in (2.23) must diverge to $+\infty$, and again $K_l\to 0$, which is unstable and hence impossible. (c) By elimination, we thus arrive at the conclusion that $g_l^2/2C_{11}^l = K_{\max}^l \to +\infty$ for some l (again including $l=\infty$).

We will show below that $K_{\max}^l$ always diverges to $+\infty$ at a finite value of l, denoted by l_∞, and then jumps to $-\infty$ and continues to increase with l. We will also show that g_l does not diverge at that point. Therefore, it is clear that $C_{11}^l \to 0$ and then becomes negative. This means that if ξ is large enough (i.e., if T is sufficiently close to T_c) so that $\xi/\xi_0 > e^{l_\infty}$, then the physical value of C_{11} will be negative. Consequently, the square of the isothermal sound velocity will be negative for longitudinal modes with q along or near a cubic axis, and these modes will be unstable.

Turning to the bulk modulus, we can write

$$B_l = C_{11}^l - \frac{d-1}{d}(C_{11}^l - C_{12}^l)$$

$$\to -\frac{d-1}{d}(C_{11}^0 - C_{12}^0) < 0 \quad \text{as } l \to l_\infty. \tag{3.38}$$

This means that even before $K_{\max}^l$ diverges, there is some $l<l_\infty$ at which B_l becomes negative, and we get into a macroscopic instability such as we already found in the isotropic system.

In the case when $0<A<1$, $K_{\max}^l$ always occurs when q is along a body diagonal, where Q also has its maximum, and its value is given by

$$K_{\max}^l = \frac{g_l^2}{2C_{11}^l + 2[(d-1)/d][\frac{1}{2}C_{44}^l - (C_{11}^l - C_{12}^l)]}$$

$$= \frac{g_l^2}{2\{B_l + [(d-1)/2d]C_{44}^l\}} \quad \text{for } A<1, \tag{3.39}$$

[see (A18) and the subsequent remarks on the case $A<1$]. We again consider all the conceivable alternatives for $g_l^2/2C_{11}^l$ as $l\to\infty$: (a) As before, if

$g_l^2/2C_{11}^l$ is bounded we find $|R_l|\to\infty$ and consequently, when

$$|R_l|Q_{\max}\equiv|R_l|\frac{d-1}{2d}=1, \tag{3.40}$$

$K_{\max}^l$ will diverge to $+\infty$ since now $R_l<0$. This will occur at some finite l. (b) If we assume that $g_l^2/2C_{11}^l\to 0$ for some l, then the coefficients in (2.23) diverge to $+\infty$ and $-\infty$, respectively. But because Q is anisotropic, the two terms cannot cancel each other except at some isolated q's. Consequently $K^l(\hat{q})\to 0$, which is unstable and impossible. (c) The last possibility is $g_l^2/2C_{11}^l\to+\infty$ for some l. Then, by (3.30), $|R_l|\to\infty$ too. Consequently, for some finite l before that point, (3.40) will hold and $K_{\max}^l\to+\infty$.

Using the above-quoted behavior of $K_{\max}^l$ and g_l near l_∞, where $K_{\max}^l$ diverges, it is now clear that the denominator in (3.39) vanishes at l_∞ and then becomes negative with further increase of l. Since the denominator is proportional to the squared velocity of the longitudinal mode with q along the body diagonal, it is clear that this mode becomes unstable when $\xi/\xi_0>e^{l_\infty}$. Moreover, the vanishing of this denominator means that

$$B_l\to-\frac{d-1}{d}\tfrac{1}{2}C_{44}^0<0 \quad\text{as } l\to l_\infty, \tag{3.41}$$

and therefore that again there is some $l<l_\infty$ at which B_l becomes negative, and we get into the associated macroscopic instability.

In order to determine more precisely when and how $K_{\max}^l$ diverges, we note that $K_l(\hat{q})$ becomes sharply peaked as $K_{\max}^l$ grows large. In particular, we expect that $K_{\max}^l$ will become large relative to the average $\overline{K}_l$. If we choose $\hat{q}$ in the direction $\hat{q}_{\max}$ which maximizes $K_l(\hat{q})$, then we should approximate (3.4) by

$$\frac{dK_{\max}^l}{dl}\cong 4B_4(K_{\max}^l)^2 . \tag{3.42}$$

The solution of this equation is

$$1/K_{\max}^l=C_0-4B_4 l, \tag{3.43}$$

where C_0 is a constant. We see that $K_{\max}^l\to\infty$ at

$$l_\infty=C_0/4B_4. \tag{3.44}$$

In order to determine the behavior of other quantities near $l=l_\infty$, we expand $K_l^{-1}(\hat{q})$ around l_∞ and $\hat{q}_{\max}$,

$$K_l^{-1}(\hat{q})\cong A_1(l_\infty-l)+A_2x^2,\quad A_1,A_2>0, \tag{3.45}$$

where x is a $(d-1)$-dimensional coordinate system on the surface of the unit sphere in q space with its origin at $\hat{q}_{\max}$. Consequently, for $l<l_\infty$ we find

$$\langle K_l\rangle\cong A_3\int\frac{x^{d-2}\,dx}{A_1(l_\infty-l)+A_2x^2}$$
$$\cong-\frac{A_3}{2A_2}\frac{2}{d-3}\left[\left(\frac{A_1}{A_2}(l_\infty-l)\right)^{(d-3)/2}-1\right], \tag{3.46}$$

where we introduced an arbitrary upper cutoff in the integral. Although the constant part of $\langle K_l\rangle$ will depend on this cutoff and will thus not be faithfully reproduced by (3.46), we are mainly interested in a possible divergence of $\langle K_l\rangle$ as $l\to l_\infty$, and this is well represented. An analogous calculation of $\langle K_l^2\rangle$ leads to

$$\langle K_l^2\rangle\cong A_3\int\frac{x^{d-2}\,dx}{[A_1(l_\infty-l)+A_2x^2]^2}$$
$$\cong-\frac{A_3}{2A_2^2}\frac{2}{d-5}\left[\left(\frac{A_1}{A_2}(l_\infty-l)\right)^{(d-5)/2}-1\right]. \tag{3.47}$$

Returning to (3.3) we see that, near $l=l_\infty$, we can try to approximate that equation by

$$\frac{du}{dl}\cong-\frac{20B_d}{(1+\tilde{r})^2}\langle K_l^2\rangle$$
$$\cong\frac{20B_dA_3}{(1+\tilde{r})^2A_2^2(5-d)}\left(\frac{A_1}{A_2}(l_\infty-l)\right)^{(d-5)/2} \quad\text{for } 1<d<5. \tag{3.48}$$

The solution of this equation has the form

$$u_l-u_0\propto\frac{2}{d-3}(l_\infty-l)^{(d-3)/2}\quad\text{for } d\neq 3,$$
$$u_l-u_0\propto\ln(l_\infty-l)\quad\text{for } d=3. \tag{3.49}$$

This means that while u_l^2 remains finite for $d>3$, it diverges like $\langle K_l\rangle^2$ for $d\leq 3$. In any case, this is weaker than the divergence of either $\langle K_l^2\rangle$ or $(K_{\max}^l)^2$, which completes the justification for using the Eqs. (3.42) and (3.48) as approximations to (3.4) and (3.3).

Finally, we can use (3.46) and (3.49) to substitute in (2.17) and investigate the behavior of g_l as $l\to l_\infty$. We see that although the right-hand side of (2.17) is singular, the solution of that equation for g_l does not diverge at l_∞ for $d>1$, and our earlier claim regarding this matter is thus proven.

Returning to consider (3.49), we note that, while u_l is only weakly diverging for $d\leq 3$, it diverges to $-\infty$. Therefore, at some $l<l_\infty$ it will already have to become negative. This suggests that the system will in fact undergo a first-order transition before

l reaches l_∞. This transition, which should occur for pinned boundary conditions in fixed volume, would presumably be accompanied by inhomogeneities that resemble longitudinal sound waves along the soft directions. Of course for free boundary conditions, or free boundaries with constrained total volume, we expect that a first-order transition associated with a *macroscopic* instability will occur first. In Sec. IV we will estimate the sizes of some of the discontinuities, as well as discuss the question under what conditions is the critical behavior nevertheless observable.

IV. MAGNITUDES OF THE ELASTIC EFFECTS

The actual physical properties of any system near its critical point depend on the path that the Hamiltonian H^l follows when r_0 is very close to the critical value r_c. In particular, if $r_0 - r_c$ is too great, H^l will never come close to any of the fixed points and no simple critical behavior will be observed.

In this section we will attempt to analyze the behavior of the cubic magnetoelastic lattice along these lines. In particular, we will try to calculate where some of the instabilities discussed in Sec. III actually appear, as well as the size of the discontinuities that characterize the resulting first-order transitions. This will be done first for a nearly isotropic system ($A \cong 1$) both for the case when the system exhibits critical behavior governed by I or R, and for the case when the system exhibits tricritical behavior, governed by G or S. We will then analyze the transition in the case of the extremely anisotropic systems $A \gg 1$ and $A \ll 1$.

A. Pseudocritical behavior in a nearly isotropic system ($A \cong 1$)

When a system is nearly isotropic, i.e.,

$$|A-1| \ll 1, \tag{4.1}$$

then

$$B_0 = C_{11}^0 - \frac{d-1}{d}(C_{11}^0 - C_{12}^0)$$
$$\cong C_{11}^0 - \frac{d-1}{d}\,\tfrac{1}{2}C_{44}^0 > 0. \tag{4.2}$$

The ratio of the two coefficients in (2.23) satisfies

$$|R_0| \equiv \left|\frac{A-1}{A}\right| \frac{C_{44}^0}{C_{11}^0} \ll 1\,. \tag{4.3}$$

Consequently, K_0 is also nearly isotropic.[29] Therefore H^l will approach at least one of the fixed points very closely before the anisotropic instability is felt. Thus, we may expect that under ee boundary conditions of either fixed P or fixed the system will encounter a macroscopic instability in the same way as a precisely isotropic system. On the other hand, under pinned or periodic boundary conditions at fixed V, the anisotropy must become important sufficiently close to T_c, and then it will be the cause of an instability.

To proceed further, we will also assume that

$$0 < K_0 \ll u_0 \ll 1. \tag{4.4}$$

It is then clear from (3.3) and (3.4) that, at first, u_l (which is still nearly the same as $\bar{u}_l$) and K_l increase at the same rate $u_l \propto K_l \propto e^{-\epsilon l}$. This goes on until u_l tends asymptotically to its fixed-point value $u_I^* \cong \epsilon/36B_4$, which occurs at $l \cong l_1$, where

$$l_1 = \frac{1}{\epsilon}\ln\frac{u_I^*}{u_0} \cong \frac{1}{\epsilon}\ln\frac{\epsilon}{36B_4 u_0}\,. \tag{4.5}$$

As l increases beyond l_1, u_l remains equal to $u_I^* \cong u_R^*$ while K_l continues to increase but at a slower rate than before, namely, $K_l \cong K_{l_1} e^{\epsilon(l-l_1)/3}$. At this stage, K_l increases up to its fixed-point value $K_R^* \cong \epsilon/12B_4$. This takes place asymptotically over an interval $l_2 - l_1$ given by

$$l_2 - l_1 = \frac{3}{\epsilon}\ln\frac{K_R^*}{K_{l_1}} \cong \frac{3}{\epsilon}\ln\frac{3\bar{u}_0}{K_0}\,. \tag{4.6}$$

As l increases beyond l_2, both u_l and K_l remain at their fixed-point values $u_R^* \cong u_I^*$ and K_R^*, but C_{11}^l continues to decrease monotonically, as it did from the beginning [see (2.22)]. In order to determine its behavior, we need to know g_l^2. We therefore rewrite (2.17) in its ϵ-expansion form,

$$\frac{dg_l^2}{dl} = g_l^2(\epsilon - 24B_4 u_l - 8B_4\langle K_l\rangle)\,. \tag{4.7}$$

Assuming that u_l and K_l have appropriate fixed-point values in the various regions of l, we now find

$$g_l^2 \cong \begin{cases} g_0^2 e^{\epsilon l} & \text{for } 0 < l < l_1 \\ g_0^2 e^{\epsilon l_1} e^{\epsilon(l-l_1)/3} & \text{for } l_1 < l < l_2 \\ g_0^2 e^{\epsilon l_1} e^{\epsilon(l_2-l_1)/3} e^{-\epsilon(l-l_2)/3} & \text{for } l_2 < l\,. \end{cases} \tag{4.8}$$

We use these results to substitute on the right-hand side of (2.22), and then integrate that equ-tion to get C_{11}^l,

$$C_{11}^l = C_{11}^0 - 2B_4\int_0^l g_l^2\,dl$$
$$\cong \begin{cases} C_{11}^0[1-(K_0/K_S^*)e^{\epsilon l}] & \text{for } 0 < l < l_1 \\ C_{11}^0(1-e^{\epsilon(l-l_2)/3}) & \text{for } l_1 < l < l_2 \\ C_{11}^0 e^{-\epsilon(l-l_2)/3} & \text{for } l_2 < l\,. \end{cases} \tag{4.9}$$

A more careful treatment, given in Appendix C, yields an expression that is valid for any l,

$$C_{11}^l = \tfrac{1}{2}C_{11}^0\{1 - \tanh[(\epsilon/6)(l-l_2)]\}\,. \tag{4.10}$$

This reduces to (4.9) inside the various regions of l, but gives a more precise result at the edges; e.g., for $l = l_2$ (4.10) leads to

$$C_{11}^{l_2} = \tfrac{1}{2} C_{11}^0 \,. \qquad (4.10')$$

To calculate l_3, which is where $B_l \to 0$, we must make further assumptions about C_{44}^0 / C_{11}^0. The two interesting cases are

$$\text{(a)} \quad \frac{d-1}{d} \, \frac{\frac{1}{2} C_{44}^0}{C_{11}^0} \ll 1 \,,$$

where we find

$$l_3 - l_2 = \frac{3}{\epsilon} \ln\left(\frac{d}{d-1} \, \frac{C_{11}^0}{\frac{1}{2} C_{44}^0} \right), \quad l_3 \gg l_2 \,; \qquad (4.11)$$

$$\text{(b)} \quad \frac{B_0}{C_{11}^0} = 1 - \frac{d-1}{d} \, \frac{\frac{1}{2} C_{44}^0}{C_{11}^0} \ll 1 \,,$$

where we find

$$l_2 - l_3 = \frac{3}{\epsilon} \ln\left(\frac{C_{11}^0}{B_0} \right), \quad l_1 \ll l_3 \ll l_2 \,. \qquad (4.12)$$

In case (b), the instability occurs while the behavior of the system is still governed by I, whereas in case (a) the instability occurs while the behavior is governed by R.

The point $l = l_3$ is the limit of metastability of the disordered phase for a sample at constant pressure. The thermodynamic transition will occur at a slightly higher temperature, which should be calculated from the pressure-vs-volume curve via a "Maxwell construction" (see Fig. 4). We denote the value of l at the thermodynamic transition by l_T. In Appendix E we perform the Maxwell Construction and find that, for case (a),

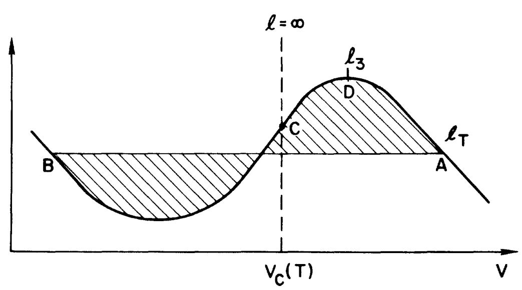

FIG. 4. Maxwell construction for the isotropic solid (schematic). When the equal pressure points A and B are chosen so that the shaded areas are equal, the first-order transition at fixed P takes place by a jump from A to B. The point C is where the Fisher-renormalized Ising transition would have occurred under pinned boundary conditions—it is an inflexion point where $\partial^2 P / \partial V^2$ passes through ∞ and changes sign, rather than simply vanishing, as it would at the inflexion point of an ordinary van der Waals loop. D is the limit of metastability for fixed P—where the bulk modulus vanishes. The curve $P(V)$ has been drawn to be asymmetric around C, so that in general $V_A - V_C \neq V_C - V_B$.

$$l_T = l_3 - O(\nu_I) \,, \qquad (4.13)$$

so that the difference between l_T and l_3 is small on the general scale of variation of l.

Thus far we have employed recursion relations valid only to lowest order in ϵ. It is not difficult to extend the renormalization-group arguments to arbitrary order in ϵ. This is aided by the fact, discussed in Appendix D, that there is a complete mathematical analogy between the Ising model in a liquid and in an isotropic solid with periodic boundary conditions and fixed V. Thus, the factor $3/\epsilon$ which appears in (4.6), (4.11), and (4.12) is related to the inverse of the crossover exponent which characterizes the growth of K_l and the specific heat. We can therefore make the replacement

$$\frac{3}{\epsilon} \to \frac{\nu_I}{\alpha_I} = \frac{\nu_R}{|\alpha_R|} = \left[\tfrac{1}{3}\epsilon - \tfrac{19}{81}\epsilon^2 + O(\epsilon^3) \right]^{-1} . \qquad (4.14)$$

Similarly, the factor $1/\epsilon$ appearing in (4.5) is related to the inverse of the crossover exponent that characterizes the growth of u_l. We can therefore make the replacement

$$\frac{1}{\epsilon} \to \frac{1}{d-4a} = \frac{1}{\epsilon - 2\eta_G} = \frac{1}{\epsilon} \,. \qquad (4.15)$$

In order to translate the above results on the behavior of H^l into conclusions about thermodynamic properties, we note that corresponding to every region of l there is a region of t where the correlation length $\xi(t)$ exhibits a simple behavior:

$$\xi(t) = \begin{cases} \xi_0 (t/t_0)^{-1/2} & \text{for } t_0 > t > t_1 \\ \xi_0 e^{l_1} (t/t_1)^{-\nu_I} & \text{for } t_1 > t > t_2 \\ \xi_0 e^{l_2} (t/t_2)^{-\nu_R} & \text{for } t_2 > t \,, \end{cases} \qquad (4.16)$$

where we have introduced the characteristic temperatures t_0, t_1, t_2, t_3, defined by

$$\xi(t_0) = \xi_0, \quad \xi(t_i) = \xi_0 e^{l_i}, \quad i = 1, 2, 3. \qquad (4.17)$$

We may choose t_0 to be any convenient temperature outside the critical region. From (4.16) and (4.17) we get the following results for t_1 and t_3:

$$t_1 = t_0 \left(\frac{u_0}{u_I^*} \right)^2 , \qquad (4.18)$$

$$t_3 = e^{-(l_3 - l_1)/\nu_I} t_1 = \left(\frac{C_{11}^0}{B_0} \, \frac{K_0}{K_R^*} \, \frac{u_I^*}{u_0} \right)^{1/\alpha_I} t_1 \quad \text{in case (b)}, \qquad (4.19)$$

$$t_3 = e^{-(l_3 - l_2)/\nu_R} e^{-(l_2 - l_1)/\nu_I} t_1 = \left(\frac{d-1}{d} \, \frac{\frac{1}{2} C_{44}^0}{C_{11}^0} \right)^{(1-\alpha_I)/\alpha_I} \left(\frac{K_0}{K_R^*} \, \frac{u_I^*}{u_0} \right)^{1/\alpha_I} t_1 \quad \text{in case (a)}. \qquad (4.20)$$

Note that t_1 is the reduced temperature at which deviations from Landau's classical theory become important, and that (4.18) can also be obtained from the Ginzburg criterion.[30,31] While there is some arbitrariness in the choice of t_0, the final result for either t_1 or t_3 must be unaffected by these different choices: This can come about because the initial values ξ_0, u_0, r_0, K_0, and, in principle, also C_{11}^0 and C_{44}^0 depend on t_0.

We can now identify C_{11}^0 and C_{44}^0 with the actual physical elastic constants at $t=t_0$. In order to similarly express K_0 in terms of measurable quantities we assume, as in Sec. III B, that $\tilde{r}_0$ is the only parameter in (2.1) which depends on t (this is a good approximation if $t_0 \ll 1$). Using (3.16) we find

$$K_0 = \frac{T_c}{4C_{11}^0}\left(\frac{d\tilde{r}_0}{dt}\right)^2\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2. \tag{4.21}$$

We now note that the mean-field approximation, which can be applied to (2.1) for $t>t_1$, predicts a jump in the constant-volume specific heat at T_c, given by

$$\Delta C_v^0 = \left(\frac{d\tilde{r}_0}{dt}\right)^2\frac{1}{8\tilde{u}_0}. \tag{4.22}$$

Therefore, if it is possible to estimate ΔC_v^0 by extrapolation of the observed specific heat from outside of the critical region, we can write

$$\frac{K_0}{\tilde{u}_0} = \frac{2T_c\Delta C_v^0}{C_{11}^0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2. \tag{4.23}$$

Finally, to estimate the factor u_I^*/K_R^*, which is equal to $\frac{1}{3}$ in the limit $\epsilon \to 0$, we note that since the initial rate of increase of K_l is characterized by α_I/ν_I, we can write $K_R^* \propto \alpha_I/\nu_I$. We can therefore make the following estimate (we assume $\alpha_I = \frac{1}{8}$, $\nu_I = 0.64$ for $d=3$):

$$\frac{u_I^*}{K_R^*} \cong \frac{\epsilon}{9}\,\frac{\nu_I}{\alpha_I} = \begin{cases}\frac{1}{3} & \text{for } d=4\\ 0.57 & \text{for } d=3.\end{cases} \tag{4.24}$$

Combining (4.23) and (4.24) with (4.19) and (4.20), we now get an estimate for t_3, where $B \to 0$ when T_c is approached from above (i.e., from the disordered side). We find, for $d=3$,[32] for case (b):

$$t_3 \cong \left[\frac{1.1T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_1, \qquad t_2 \ll t_3 \ll t_1; \tag{4.25}$$

for case (a):

$$t_3 \cong \left(\frac{C_{44}^0}{3C_{11}^0}\right)^{(1-\alpha_I)/\alpha_I}\left[\frac{1.1T_c\Delta C_v^0}{C_{11}^0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_1, \qquad t_3 \ll t_2, \tag{4.26}$$

with $\alpha_I \cong \frac{1}{8}$. Note that, since in case (a) $B_0 \cong C_{11}^0$, we can replace C_{11}^0 in the middle factor of (4.26) by B_0. Equation (4.25) then becomes just a special case of (4.26). The exact location of the first-order transition at fixed P when T_c is approached from the disordered side is denoted by the reduced temperature t_T. Throughout the rest of this section we will use t_3 as our estimate for t_T, based on the assertion of (4.13). In Appendix E, where we actually make a Maxwell construction for case (a), we find in fact that, for $d=3$, $t_T \cong 33t_3$.

An alternate approach for estimating t_3 is to choose t_0 inside the critical region, i.e., $t_2 < t_0 < t_1$, so that $u_0 \cong u_I^*$. In that case we should use t_0 instead of t_1 in (4.19) and (4.20). We can still identify C_{11}^0 and C_{44}^0 as the actual physical constants at $t=t_0$, and we can still use (4.21). Note, however, that the value of K_0 depends on t_0 through $\tilde{r}_0$. Since we can no longer use (4.22), we will try instead to relate the present value of K_0 to the previous value, obtained when $t_0 > t_1$. From (4.8), (4.9), (4.16), and (4.5) we find that the ratio between the two values of K_0/u_0 is given by

$$\frac{(K_0/u_0)_{\text{new}}}{(K_0/u_0)_{\text{old}}} = \frac{(u_0)_{\text{old}}}{u_I^*}\,e^{l_1}\,e^{\epsilon(l-l_1)/\epsilon} = \left(\frac{(t_0)_{\text{new}}}{t_1}\right)^{-\alpha_I} = \frac{C_{\text{sing}}^0}{\Delta C_v^0}, \tag{4.27}$$

where C_{sing}^0 is the singular part of the rigid Ising specific heat at the new t_0. We thus get, for $d=3$,[32]

$$t_3 \cong \left(\frac{C_{44}^0}{3C_{11}^0}\right)^{(1-\alpha_I)/\alpha_I}\left[\frac{1.1T_cC_{\text{sing}}^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_0, \tag{4.28}$$

where this expression applies to both cases (a) and (b).

Comparing these results with the result of magnetothermomechanics, Eq. (1.5), we see that our case (b) leads to essentially the same result. This is the case when the shear modulus $\frac{1}{4}C_{44}^0$ is much greater than the bulk modulus B_0. But in case (a) our result differs from (1.5) in that it includes the factor

$$(C_{44}^0/3C_{11}^0)^{(1-\alpha_I)/\alpha_I} \ll 1. \tag{4.29}$$

In practice, this factor is indeed often very small even though $C_{44}^0/3C_{11}^0$ is only moderately small—this is due to the rather large exponent

$$(1-\alpha_I)/\alpha_I \cong 7 \quad \text{for } d=3. \tag{4.30}$$

We conclude that whenever $C_{44}^0/3C_{11}^0 = 1-\delta$, where δ is not too small, our estimate for t_T will be considerably smaller than that of (1.5).

Note, however, that

$$t_3 \propto u_0^{2-1/\alpha_I} \cong u_0^{-6} \tag{4.31}$$

[see Eqs. (4.18)–(4.20)], which means that t_3 increases as one approaches a tricritical point, where $u_0=0$. In that case the treatment of this subsection breaks down, because (4.4) is violated. We shall see below that while t_3 increases, it does not in fact diverge when $u_0\to 0$, as one would be led to believe by (4.31).

Having calculated t_T, we can easily estimate the volume jump at the transition:

$$\Delta V = a_v t_T\left(\frac{1}{T_c}\frac{dT_c}{dV}\right)^{-1}, \tag{4.32}$$

where a_v is a number whose value depends on the ratio of the singular parts of B at the same value of $|t|$ above and below T_c. When that ratio is 1, $a_v=2$. In general $1<a_v<\infty$, and to determine its precise value requires a Maxwell construction. In Appendix E we find that $a_v\cong 9$ at $d=3$.

The latent heat may be calculated from the Clausius-Clapeyron relation:

$$L = T_c\Delta S = T_c\Delta V\left(\frac{dT_c}{dP}\right)^{-1}. \tag{4.33}$$

Furthermore, in our model the magnetic part of the free energy depends on temperature and volume only through the combination $(\bar{r}_0+g_0\delta V/V)$, so that along a line where this quantity is constant, we have

$$dP = d\left(\frac{dH_e^0}{dV}\right) = -B_0\frac{dV}{V}. \tag{4.34}$$

Thus we get

$$\frac{dT_c}{dP} = -\frac{V}{B_0}\frac{dT_c}{dV}. \tag{4.35}$$

At a pressure P_m where $dT_c/dP=0$, the above-calculated jumps will vanish. In the vicinity of P_m, we expect that dT_c/dP will be proportional to $P-P_m$, and hence $L\propto|P-P_m|^{2(1-\alpha_I)/\alpha_I}$. This is shown schematically in Fig. 1.

From (4.26) or (4.28) we can conclude that in practice t_3, and therefore also ΔV and L, will usually be very small. The actual transition temperature will thus be nearly the same as the critical temperature $T_c(V)$ or $T_c(P)$, and the important slope dT_c/dV can be simply determined from the observed line of transitions. Moreover, for $t>t_3$ there will be regions of temperature where the system will exhibit critical behavior characterized by a set of well-defined critical exponents. In the region $t_3<t<t_2$ [which only exists in case (a)], the behavior at fixed V, i.e., as a function of $T-T_c(V)$, is governed by R and one observes Fisher-renormalized Ising exponents. In the region $t_2<t<t_1$ the behavior is governed by I and one observes unrenormalized Ising exponents. In the region $t_1<t$, the behavior is governed by G and one oberves classical behavior, i.e., Gaussian exponents. The critical behavior as a function of $T-T_c(P)$, i.e., at fixed pressure, will however be characterized by unrenormalized Ising exponents even for $t<t_2$, as we showed in Sec. III B.

Until now, we have discussed features in the behavior of the system for which the small anisotropy was unimportant. Under pinned boundary conditions, or periodic boundary conditions in a fixed volume, H^l develops without any instability until the anisotropy becomes important. Since K_l is already large (i.e., of order K_R^*) when this occurs, we can infer from the discussion in Sec. III C that $K_{\max}^l$ will diverge very soon after R_l becomes of order unity. We therefore estimate the point l_∞, where $K_{\max}^l$ diverges, by demanding $R_l=1$. With the help of (4.9), this leads to

$$l_\infty - l_2 = \frac{3}{\epsilon}\ln\left(\frac{C_{11}^0}{C_{44}^0}\frac{A}{A-1}\right) \gg \max(l_3-l_2,1), \tag{4.36}$$

and to a corresponding instability temperature[32]

$$\begin{aligned} t_\infty &= e^{-(l_\infty-l_2)/\nu_R} t_2 \\ &= \left|\frac{A-1}{A}\frac{C_{44}^0}{C_{11}^0}\right|^{(1-\alpha_I)/\alpha_I}\left[\frac{1.1T_c\Delta C_V^0}{C_{11}^0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_1 \\ &\cong \left|3(A-1)\right|^{(1-\alpha_I)/\alpha_I} t_3 \ll \text{both } t_3 \text{ and } t_2. \end{aligned} \tag{4.37}$$

These last results, which show that $l_\infty\gg l_3$ and $t_\infty\ll t_3$, also justify our total neglect of the small anisotropy in the discussion of the transition under conditions of fixed P or fixed V but with nonpinned boundaries.

B. Pseudotricritical behavior in a nearly isotropic system ($A\cong 1$)

We still assume that (4.1) and therefore also (4.3) are valid, but replace (4.4) by

$$0<u_0\ll K_0\ll 1. \tag{4.38}$$

As a result of this, it is clear that H^l will initially approach S rather than I. At this stage, K_l will tend asymptotically towards $K_S^*=\epsilon/4B_4$, and this will occur when $l>l_1$, where l_1 is now given by

$$l_1 = \frac{1}{\epsilon}\ln\frac{K_S^*}{K_0} \cong \frac{1}{\epsilon}\ln\frac{\epsilon}{4B_4K_0}. \tag{4.39}$$

In the next stage, u_l continues to increase until it eventually reaches u_R^* asymptotically. This occurs after l_2, where

$$l_2 = \frac{1}{\epsilon}\ln\frac{u_R^*}{u_0} \cong \frac{1}{\epsilon}\ln\frac{\epsilon}{36B_4u_0} \tag{4.40}$$

[this is the same as (4.5)]. At the same time, K_l decreases slowly towards K_R^*, but this only begins to happen after u_l has become sizable. As long as $l_1\ll l\ll l_2$, we can therefore assume that K_l is constant. Using the following approximation for

K_l:

$$K_l \cong \begin{cases} K_0 e^{\epsilon l} \ll K_S^* & \text{for } 0< l< l_1 \\ K_S^* & \text{for } l_1 < l < l_2, \end{cases} \quad (4.41)$$

we can solve (4.7) for g_l^2 to get

$$g_l^2 \cong \begin{cases} g_0^2 e^{\epsilon l} & \text{for } 0< l< l_1 \\ g_0^2 e^{\epsilon l_1} e^{-\epsilon(l-l_1)} & \text{for } l_1 < l < l_2. \end{cases} \quad (4.42)$$

Using this to solve for C_{11}^l as in (4.8), we get

$$C_{11}^l = C_{11}^0 - 2B_4 \int g_l^2\, dl$$

$$= \begin{cases} C_{11}^0 (1 - e^{\epsilon(l-l_1)}) & \text{for } 0< l< l_1 \\ C_{11}^0 e^{-\epsilon(l-l_1)} & \text{for } l_1 < l < l_2. \end{cases} \quad (4.43)$$

To calculate when $B_l \to 0$ we again have to make further assumptions, as in Sec. IV A:

(a) $\dfrac{9u_0}{K_0} \ll \dfrac{d-1}{d} \dfrac{\frac{1}{2}C_{44}^0}{C_{11}^0} \ll 1,$

then

$$l_3 - l_1 = \frac{1}{\epsilon} \ln\left(\frac{d}{d-1} \frac{C_{11}^0}{\frac{1}{2}C_{44}^0}\right), \quad l_1 \ll l_3 \ll l_2; \quad (4.44)$$

(b) $\dfrac{B_0}{C_{11}^0} \ll 1$, then

$$l_1 - l_3 = \frac{1}{\epsilon} \ln \frac{C_{11}^0}{B_0}, \quad l_3 \ll l_1. \quad (4.45)$$

Note that the left-hand-side inequality in case (a) is more restrictive than (4.38). In fact, if u_0/K_0 does not satisfy the more stringent inequality, then H^l will reach R before becoming unstable. In that case the system will exhibit critical (rather than tricritical) behavior just before the instability. A more precise solution of the renormalization-group equations, performed in Appendix C, confirms all of the above results and justifies the implicit assumption that K_l remains nearly isotropic until well beyond l_1.

The temperature corresponding to the actual first-order transition must again be found by a Maxwell construction, as described in Appendix E. The temperature t_3, at which $B(t)=0$, is found as in (4.19) and (4.20),

$$t_3 = e^{-l_3/\nu_G} t_0 = e^{2(l_1 - l_3)} e^{-2l_1} t_0$$

$$= \left(\frac{C_{11}^0}{B_0} \frac{K_0}{K_S^*}\right)^{2/\epsilon} t_0 \quad \text{in case (b)}, \quad (4.46)$$

$$t_3 = e^{-(l_3 - l_1)/\nu_S} e^{-2l_1} t_0$$

$$= \left(\frac{d-1}{d} \frac{\frac{1}{2}C_{44}^0}{C_{11}^0} \frac{K_0}{K_S^*}\right)^{2/\epsilon} t_0 \quad \text{in case (a)}, \quad (4.47)$$

where t_0 is defined as before in (4.17). Similarly, t_1 denotes the temperature at which control over the behavior of the system passes from G to S:

$$t_1 = \left(\frac{K_0}{K_S^*}\right)^{2/\epsilon} t_0. \quad (4.48)$$

We again identify C_{11}^0 and C_{44}^0 with the actual physical elastic constants at $t=t_0$. Except for anharmonic effects not included in (2.1), these constants should have the same values as in the previously discussed case (Sec. IV A). We can still use (4.21) for K_0, but we now relate $d\tilde{r}_0/dt$ to the latent heat L_0 and to the spontaneous value ψ_0 of the spin variable on the first-order side of the tricritical point, evaluated by mean-field theory. In order to do this, we must include a term $v_0\psi^6$ in the free energy of (2.1). Then for $u_0<0$ we find a first-order transition with

$$L_0 = \tfrac{1}{2} T_c \psi_0^2 \frac{d\tilde{r}_0}{dt}, \quad \psi_0^2 = \frac{1}{2} \frac{|u_0|}{v_0}. \quad (4.49)$$

The Landau theory is believed to be valid near the tricritical point for $d \geq 3$, except for logarithmic corrections at $d=3$.[33,34] These will be small if $v_0 \ll 1$. As an approximation, we may assume that v_0 is independent of T and V, that $\tilde{r}_0$ depends only on $T - T_c(V)$, and that u_0 depends only on V and varies as $V - V_t$, where V_t is the volume at the tricritical point.

We note that the inclusion of a ψ^6 term in H^0 and an explicit dependence of u_0 on the local density or dilatation ratio $\nabla \cdot u$ (this must be done for consistency once we allow u_0 to depend on V) will generate some new terms in the effective spin Hamiltonian H_{eff}, obtained if we integrate out the elastic variables in H^0. The density dependence of u_0 leads to a term

$$\int V \frac{du_0}{dV} (\nabla \cdot u)\psi^4 d^d x \quad (4.50)$$

in H^0, and this generates an effective spin-spin interaction proportional to ψ^8 in H_{eff}, which is however an irrelevant term even near the tricritical point. On the other hand, cross terms between (4.50) and the term $g_0 T^{-1/2}(\nabla \cdot u)\psi^2$ of (2.1) lead to an effective spin-spin term proportional to ψ^6. We can take this into account by an appropriate redefinition of v_0. Using (4.49) to substitute for $d\tilde{r}_0/dt$, we find, for $d=3$, for case (b):

$$t_3 \cong \left[\left(\frac{L_0}{T_c\psi_0^2}\right)^2 \frac{T_c}{B_0} \left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2 \frac{1}{K_S^*}\right]^2 t_0, \quad t_3 \gg t_1; \quad (4.51)$$

for case (a):

$$t_3 \cong \left(\frac{C_{44}^0}{3C_{11}^0}\right)^2 \left[\left(\frac{L_0}{T_c\psi_0^2}\right)^2 \frac{T_c}{B_0} \left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2 \frac{1}{K_S^*}\right]^2 t_0, \quad t_3 \ll t_1. \quad (4.52)$$

Here we have written B_0 instead of C_{11}^0 in the middle factor of (4.52) [see the remarks following (4.26)] so that (4.51) becomes just a special case of (4.52). This is the finite limit towards which t_3 of the Sec. IV A increases as the tricritical point is approached from the second-order side.

On the second-order side of the tricritical point (i.e., for $u_0 > 0$), the estimates for ΔV and L of (4.32) and (4.33) are still valid. Consequently, they too will become greater near the tricritical point, merging finally into the values one expects for the ideal (i.e., incompressible) model when $u_0 < 0$. Comparing our estimates of L for $u_0 > 0$, $u_0 \cong 0$, and $u_0 < 0$ [Eqs. (4.20), (4.49), and (4.52), respectively], we can make a crude interpolation for the variation of L throughout the tricritical region:

$$L = \begin{cases} a_1 |u_0| & \text{for } u_0 \ll -u_1 \\ a_2 & \text{for } u_0 \cong 0 \\ a_3 u_0^{2-1/\alpha_I} & \text{for } u_0 \gg u_2, \end{cases} \tag{4.53}$$

where, for $d = 3$,

$$u_1 = a_2/a_1,$$

$$u_2 = (a_3/a_2)^{\alpha_I/(1-2\alpha_I)},$$

$$a_1 = \frac{T_c}{2v_0}\left(\frac{L_0}{T_c\psi_0^2}\right),$$

$$a_2 = \left(\frac{C_{44}^0}{3C_{11}^0}\right)^2 \left[\left(\frac{L_0}{T_c\psi_0^2}\right)^2 \frac{T_c}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^2 \frac{t_0}{(K_S^*)^2},$$

$$a_3 = \left(\frac{C_{44}^0}{3C_{11}}\right)^{(1-\alpha_I)/\alpha_I} \left[\left(\frac{L_0}{T_c\psi_0^2}\right)^2 \frac{T_c}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} \frac{t_0}{(u_I^*)^2}. \tag{4.54}$$

This behavior is shown schematically in Fig. 2, which indicates that a first-order transition arising from the spin-lattice interactions might best be observed near the pseudotricritical point at $u_0 \cong 0$.

For $t_1 < t$, the system will exhibit the usual tricritical behavior, governed by G, that is a characteristic of the Ginzburg-Landau-Wilson Hamiltonian for a one-component spin variable.[33] At fixed V, this will change over to a Fisher-renormalized tricritical behavior governed by S for $t_3 < t < t_1$ in case (a). Using the arguments of Sec. III B, it can again be shown that for fixed P, this spherical-like behavior gets renormalized back to a simple Gaussian tricritical behavior.

C. An extremely anisotropic system with $A \gg 1$

We start by defining more precisely the kind of system we shall be discussing in this subsection. As shown in Appendix A, it is not enough to say that $A \gg 1$. One must make the more stringent demand [see (A24)]

$$A - 1 \gg \frac{d}{d-1}\frac{C_{11}^0}{C_{11}^0 - C_{12}^0} \tag{4.55}$$

in order to ensure that not only H^0 but also $K_0(\hat{q})$ is indeed extremely anisotropic. It follows that $C_{44}^0 \gg C_{11}^0$. We will also assume, similarly to (4.4), that

$$0 < K_{\max}^0 \ll u_0 \ll 1, \tag{4.56}$$

so that H^l does not come near to S.

Starting at $l = 0$, we find that u_l and $K_l(\hat{q})$ increase at the same rate, given by $e^{\epsilon l}$, up to $l = l_1$, given by (4.5) where $u_l \to u_I^*$. The shape of $K_l(\hat{q})$ is preserved at this stage. In the next stage saturation effects begin to appear in K_l which alter its shape, and we can thus no longer ignore the anistropy. Because of the extreme anisotropy of K_l, we can now ignore $\langle K_l \rangle$ as compared to $K_{\max}^l$, and the equation for $K_{\max}^l$ becomes

$$\frac{dK_{\max}^l}{dl} \cong \left(\frac{\epsilon}{3} + 4B_4K_{\max}^l\right)K_{\max}^l. \tag{4.57}$$

This can be solved exactly, yielding

$$\frac{K_R^*}{K_{\max}^l} = \frac{K_R^* + K_{\max}^{l_1}}{K_{\max}^{l_1}} e^{-\epsilon(l-l_1)/3} - 1 \quad \text{for } l_1 < l. \tag{4.58}$$

Clearly, $K_{\max}^l$ diverges at l_∞ where

$$l_\infty - l_1 = \frac{3}{\epsilon}\ln\left(\frac{K_R^*}{K_{\max}^{l_1}}\right) \cong \frac{3}{\epsilon}\ln\frac{3u_0}{K_{\max}^0}. \tag{4.59}$$

We can thus write

$$K_{\max}^l \begin{cases} K_{\max}^0\, e^{\epsilon l} & \text{for } 0 < l < l_1 \\ K_R^*(e^{-\epsilon(l-l_\infty)/3} - 1)^{-1} & \text{for } l_1 < l < l_\infty \end{cases} \tag{4.60}$$

and use this to substitute in the following equation for $\ln C_{11}^l$, obtained from (2.22) and (A17):

$$\frac{d\ln C_{11}^l}{dl} = -4B_4\frac{g_l^2}{2C_{11}^l} = -4B_4K_{\max}^l. \tag{4.61}$$

Solving this equation by a straightforward integration, and neglecting some small terms, we find

$$C_{11}^l \cong \begin{cases} C_{11}^0[1 - (K_{\max}^0/K_S^*)e^{\epsilon l}] & \text{for } 0 < l < l_1 \\ C_{11}^0(1 - e^{-\epsilon(l_\infty - l)/3}) & \text{for } l_1 < l < l_\infty. \end{cases} \tag{4.62}$$

Consequently, we can write

$$B_l = B_0 - C_{11}^0 e^{-\epsilon(l_\infty - l)/3} \quad \text{for } l_1 < l < l_\infty. \tag{4.63}$$

We see that $B_l \to 0$ at $l = l_3$, where, if we assume that $l_1 \ll l_3 < l_\infty$, we find

$$l_\infty - l_3 = \frac{3}{\epsilon}\ln\frac{C_{11}^0}{B_0}. \tag{4.64}$$

The temperature t_3, at which $B(t)=0$, is found to be

$$t_3 = e^{-(l_3-l_1)/\nu_I}t_1 = e^{(l_\infty-l_3)/\nu_I}e^{-(l_\infty-l_1)/\nu_I}t_1$$
$$= \left(\frac{C_{11}^0}{B_0}\frac{K_{\max}^0}{u_0}\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I}t_1, \qquad (4.65)$$

where t_1 is the size of the Ginzburg critical region and is again given by (4.18).

We can now use (4.23) as an estimate for $K_{\max}^0/u_0$, and (4.24) as an estimate for u_I^*/K_R^*. In this way, we obtain an estimate for the reduced temperature t_3 where $B\to 0$,[32]

$$t_3 \cong \left[\frac{1.1T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I}t_1, \quad \text{for } d=3, \qquad (4.66)$$

which is the same as (4.25). In order to ensure that $l_1 \ll l_3$, as assumed, we must require that

$$\frac{g^2}{2B_0} \ll u_0\frac{K_R^*}{u_I^*} \cong u_0, \qquad (4.67)$$

which is somewhat more stringent than (4.56). If (4.67) is not satisfied, we will find that the transition occurs for $l<l_1$, i.e., while the system is still governed by G. The jumps ΔV and L can be estimated as in (4.32) and (4.33).

Under pinned boundary conditions, a transition will still occur due to the microscopic instability encountered at l_∞. The temperature where that instability occurs is denoted by t_∞ and is given by[32]

$$t_\infty = e^{-(l_\infty-l_1)/\nu_I}t_1 = \left(\frac{K_{\max}^0}{u_0}\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I}t_1$$
$$= \left[\frac{1.1T_c\Delta C_v^0}{C_{11}^0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I}t_1$$
$$= \left(\frac{B_0}{C_{11}^0}\right)^{1/\alpha_I}t_3. \qquad (4.68)$$

The last form of this result shows that t_∞ can be much smaller than t_3 if B_0/C_{11}^0 is considerably less than 1. At t_∞, the longitudinal phonons along the cubic axes become soft, and a distortion of the lattice can be expected to appear in those directions. In practice, a first-order transition associated with this instability will probably occur somewhat before t_∞ is reached. One can find the detailed properties of this transition by means of a Maxwell construction, if one knows how to calculate the equation of state on the other side of the microscopic instability.

D. An extremely anisotropic system with $A \ll 1$

This is the kind of system that in the limit $A=0$ becomes a BE model with isotropic $K(\hat{q})$. For $A\neq 0$, K will still be nearly isotropic if (A23) is satisfied. Otherwise, K will be anisotropic, becoming extremely anisotropic if (A25) is satisfied. However, even if to begin with (at $l=0$) (A23) holds, (A25) will always become valid for sufficiently large l, if $A\neq 0$, and K_l will then become very anisotropic. As long as the anisotropy of K_l is negligible, H^l develops as in BE and there are no instabilities, microscopic or macroscopic. Instabilities appear only when the anisotropy of the K_l becomes appreciable. We will first discuss the case where K_0 already has considerable anisotropy, then we will discuss the case where K_0 is nearly isotropic.

We assume that the inequalities of (4.56) are valid when K_0 is already very anisotropic. Consequently, the system at first tends to I over an interval l_1 given by (4.5). At this stage, $K_l(\hat{q})$ increases according to $e^{\epsilon l}$ without any change of shape. After that, the rate of change of $K_{\max}^l$ is described by (4.57), and $K_{\max}^l$ is given by (4.60). The first deviation from the behavior described in Sec. IV C occurs when instead of (4.61) we write the following analogous but different equation:

$$\frac{d\ln\{B_l+[(d-1)/d]\frac{1}{2}C_{44}^0\}}{dl} = -4B_4\frac{g_l^2}{2\{B_l+[(d-1)/d]\frac{1}{2}C_{44}^0\}} = -4B_4K_{\max}^l. \qquad (4.69)$$

The solution of this is, like (4.62),

$$B_l+\frac{d-1}{d}\tfrac{1}{2}C_{44}^0 = \begin{cases}\left(B_0+\frac{d-1}{d}\tfrac{1}{2}C_{44}^0\right)\left(1-\frac{K_{\max}^0}{K_S^*}e^{\epsilon l}\right) & \text{for } 0<l<l_1\\ \left(B_0+\frac{d-1}{d}\tfrac{1}{2}C_{44}^0\right)\left(1-e^{-\epsilon(l_\infty-l)/3}\right) & \text{for } l_1<l<l_\infty,\end{cases}$$

(4.70)

where l_∞ is given by (4.59). We can therefore write for $l_1 < l < l_\infty$,

$$B_l = B_0(1 - e^{-\epsilon(l_\infty - l)/3}) - \frac{d-1}{d}\,\tfrac{1}{2}C_{44}^0 e^{-\epsilon(l_\infty - l)/3}. \tag{4.71}$$

We note that, according to (A25), we have in this case

$$\frac{d-1}{d}\,\frac{\frac{1}{2}C_{44}^0}{B^0} \gg 1\,. \tag{4.72}$$

To calculate l_3, where $B_l \sim 0$, we again assume $l_1 \ll l_3 \ll l_\infty$, and find

$$l_\infty - l_3 = \frac{3}{\epsilon}\ln\left(\frac{d-1}{d}\,\frac{\frac{1}{2}C_{44}^0}{B_0}\right), \quad l_3 \ll l_\infty\,. \tag{4.73}$$

The temperature t_3, at which $B(t)=0$, is found to be

$$t_3 = \left(\frac{d-1}{d}\,\frac{\frac{1}{2}C_{44}^0}{B_0}\,\frac{K_{\max}^0}{u_0}\,\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I} t_1\,, \tag{4.74}$$

where t_1 is again given by (4.18). To make contact with measurable quantities, we have to modify our expression for $K_{\max}^0$, since for $A<1$,

$$K_{\max}^0 = \frac{g_0^2}{2\{B_0 + [(d-1)/d]\frac{1}{2}C_{44}^0\}} \tag{4.75}$$

[see (A17), (A18), and the subsequent discussion]. Instead of (4.23) we now find, using (4.72),

$$\frac{K_{\max}^0}{u_0} = \frac{d}{d-1}\,\frac{2T_c\Delta C_v^0}{\frac{1}{2}C_{44}^0}\left(\frac{V}{T_c}\,\frac{dT_c}{dV}\right)^2. \tag{4.76}$$

Using this result, as well as (4.24), we find for $d=3$, under fixed P, that $B \to 0$ at[32]

$$t_3 \cong \left[\frac{1.1T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\,\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_1\,, \tag{4.77}$$

i.e., the same as (4.66) and (4.25). To ensure that $l_1 \ll l_3$ we have to require

$$1 \ll \frac{d-1}{d}\,\frac{\frac{1}{2}C_{44}^0}{B_0} \ll \frac{u_0}{K_{\max}^0}\,\frac{K_R^*}{u_I^*} \cong \frac{u_0}{K_{\max}^0}\,, \tag{4.78}$$

which, in view of (4.72), can be more stringent than (4.56).

Under pinned boundary conditions, a transition can only arise because of the microscopic instability, which occurs, for $d=3$, at[32]

$$t_\infty = e^{-(l_\infty - l_1)/\nu_I} t_1 = \left(\frac{K_{\max}^0}{u_0}\,\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I} t_1$$

$$= \left[\frac{1.1T_c\Delta C_v^0}{\frac{1}{3}C_{44}^0}\left(\frac{V}{T_c}\,\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_I} t_1 \ll t_3\,. \tag{4.79}$$

At that point, the longitudinal phonons along the body diagonals become soft and a distortion of the lattice is expected to appear in those directions. As in Sect. IV C, we expect that a first-order transition will occur somewhat above t_∞. The calculation of its detailed properties requires knowledge of the equation of state below t_∞ and use of a Maxwell construction.

Turning to the case where K_0 is nearly isotropic and assuming that (4.4) is valid, we find that H^l first develops similarly to the nearly isotropic case discussed in Sec. IV A. This continues up to l_2, given by (4.6). After that, H^l would remain near R except for the small anisotropy that now becomes important. For $l > l_2$, we can write the following approximate equation for $K_{\max}^l$, derived from (3.4) by assuming that $u_l = u_R^*$ and $\langle K_l\rangle = K_R^*$:

$$\frac{dK_{\max}^l}{dl} \cong 4B_4 K_{\max}^l (K_{\max}^l - K_R^*)\,. \tag{4.80}$$

The solution of this equation is given by

$$1 - \frac{K_R^*}{K_{\max}^l} = \left(1 - \frac{K_R^*}{K_{\max}^{l_2}}\right) e^{\epsilon(l-l_2)/3}\,, \tag{4.81}$$

which can be rewritten in a different form by noting that, because the shape of K_l remains unchanged up to l_2, we can write

$$\frac{K_{\max}^{l_2}}{\langle K_{l_2}\rangle} \equiv \frac{K_{\max}^0}{\langle K_0\rangle}\,, \tag{4.82}$$

and therefore that

$$1 - \frac{K_R^*}{K_{\max}^{l_2}} = \frac{K_{\max}^0 - \langle K_0\rangle}{K_{\max}^0}\,. \tag{4.83}$$

We can thus write, for $l > l_2$,

$$\frac{K_{\max}^l - K_R^*}{K_{\max}^l} = \frac{K_{\max}^0 - \langle K_0\rangle}{K_{\max}^0}\, e^{\epsilon(l-l_2)/3}\,, \tag{4.84}$$

and note that $K_{\max}^l$ diverges at $l = l_\infty$, where

$$l_\infty - l_2 = \frac{3}{\epsilon}\ln\frac{K_{\max}^0}{K_{\max}^0 - \langle K_0\rangle}\,. \tag{4.85}$$

We can summarize the results for $K_{\max}^l$ in the form

$$K_{\max}^l = \begin{cases} K_{\max}^0 e^{\epsilon l} & \text{for } 0 < l < l_1 \\ K_{\max}^0 e^{\epsilon l_1} e^{\epsilon(l-l_1)/3} & \text{for } l_1 < l < l_2 \\ K_R^*(1 - e^{\epsilon(l-l_\infty)/3})^{-1} & \text{for } l_2 < l < l_\infty\,. \end{cases} \tag{4.86}$$

We now substitute these results into (4.69) and integrate it to get

$$B_l + \frac{d-1}{d}\,\tfrac{1}{2}C_{44}^0 = \left(B_0 + \frac{d-1}{d}\,\tfrac{1}{2}C_{44}^0\right)(e^{\epsilon(l_\infty - l)/3} - 1) \times \frac{K_{\max}^0 - \langle K_0\rangle}{\langle K_0\rangle}\, e^{-K_{\max}^0/\langle K_0\rangle} \quad \text{for } l_2 < l < l_\infty\,. \tag{4.87}$$

In view of (A23), from which it follows that

$$\frac{d}{d-1}\frac{B_0}{\frac{1}{2}C_{44}^0} \gg 1, \tag{4.88}$$

we find that $B_l \to 0$ at l_3, where

$$l_\infty - l_3 \cong \frac{3}{\epsilon}\ln\left(\frac{d-1}{d}\frac{\frac{1}{2}C_{44}^0}{B_0}\frac{\langle K_0\rangle}{K_{\max}^0-\langle K_0\rangle}e^{K_{\max}^0/\langle K_0\rangle}+1\right). \tag{4.89}$$

With the help of (A17), (A18), and (A21) of Appendix A, we can show that in this case

$$\frac{K_{\max}^0-\langle K_0\rangle}{K_{\max}^0} = (a_0A)^{1/2}\frac{K_{\max}^0-K_{\min}^0}{K_{\max}^0} = \frac{d-1}{d}\frac{C_{11}^0-C_{12}^0}{C_{11}^0}(a_0A)^{1/2} < (a_0A)^{1/2}, \tag{4.90}$$

where a_0 is a number of order unity. Consequently, we find that

$$l_\infty - l_3 = \frac{3}{\epsilon}\ln\left[1+\frac{C_{11}^0}{B_0}\left(\frac{A}{a_0}\right)^{1/2}e\right], \tag{4.91}$$

where e is the base of natural logarithms. The temperature t_3 at which $B(t)=0$ is given by

$$t_3 = e^{(l_\infty-l_3)/\nu_R}e^{-(l_\infty-l_2)/\nu_R}e^{-(l_2-l_1)/\nu_I}t_1 = \left[1+\frac{C_{11}^0}{B_0}\left(\frac{A}{a_0}\right)^{1/2}e\right]^{(1-\alpha_I)/\alpha_I}\left(\frac{K_{\max}^0-\langle K_0\rangle}{K_{\max}^0}\right)^{(1-\alpha_I)/\alpha_I} \times\left(\frac{\langle K_0\rangle}{u_0}\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I}t_1, \tag{4.92}$$

where t_1 is given by (4.18).

To make contact with measurable quantities, we must modify our previous expression for $K_{\max}^0/u_0$. Although (4.75) remains true, we now have the inequality (4.88) instead of (4.72). Consequently, we find

$$\frac{\langle K_0\rangle}{u_0} \cong \frac{K_{\max}^0}{u_0} = \frac{2T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2. \tag{4.93}$$

Using this to substitute in (4.92), and using also (4.24) and (4.90), we find, for $d=3$,[32]

$$t_3 = \left[\frac{d-1}{d}\left(\frac{\frac{1}{2}C_{44}^0}{B_0}e+\frac{C_{11}^0-C_{12}^0}{C_{11}^0}(a_0A)^{1/2}\right)\right]^{(1-\alpha_I)/\alpha_I} \times\left[\frac{1.1T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_1}t_1. \tag{4.94}$$

The first factor is clearly much less than 1, going in fact to 0 when $A\to 0$ (and therefore also $C_{44}^0\to 0$).

Under pinned boundary conditions, no transition will occur as a result of the macroscopic instability at t_3, but a transition will still occur as a result of the microscopic instability at l_∞. The temperature where this instability is encountered is given by[32]

$$t_\infty = e^{-(l_\infty-l_2)/\nu_R}e^{-(l_2-l_1)/\nu_I}t_1 = \left(\frac{K_{\max}^0-\langle K_0\rangle}{K_{\max}^0}\right)^{(1-\alpha_I)/\alpha_I}\left(\frac{\langle K_0\rangle}{u_0}\frac{u_I^*}{K_R^*}\right)^{1/\alpha_I}t_1 = \left(\frac{d-1}{d}\frac{C_{11}^0-C_{12}^0}{C_{11}^0}(a_0A)^{1/2}\right)^{(1-\alpha_I)/\alpha_I} \times\left[\frac{1.1T_c\Delta C_v^0}{B_0}\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2\right]^{1/\alpha_1}t_1. \tag{4.95}$$

Again we see that the first factor is much less than 1. Comparing (4.95) with (4.92), we see that t_∞ is smaller than t_3, but not necessarily much smaller.

V. ALTERNATIVE DISCUSSION OF THE EFFECT OF EXTERNAL CONDITIONS

In order to discuss the effect of various types of external conditions on the critical properties of the system, we have taken the point of view that this can be determined from the macroscopic phenomenological equations of classical (i.e., 19th century) physics once all the phenomenological parameters are known. These parameters, of which the elastic moduli are typical examples, are entirely determined by the microscopic properties of the system and are independent of the external conditions. That is the reason why, although the microscopic calculations of the previous sections were performed for a system at fixed volume for reasons of convenience, the results we obtained sufficed to discuss the properties of the system under any external conditions.

It is instructive to compare the methods of the present paper with other treatments of compressible spin systems under various boundary conditions.

Thus, Larkin and Pikin,[10] and later Sak,[12] discussed the properties of an isotropic elastic spin system under constant pressure by including small uniform strains as well as strains that arise from a periodic displacement field $u(x)$ in the Hamiltonian of (2.1). The elastic variables are integrated over completely right at the beginning, leading to an effective spin Hamiltonian. In this integration, the uniform strains must be treated separately because they have $d(d-1)$ independent components as compared to the Fourier transform of the displacement field, which has only d independent components for every q. The effects due to small variations in the pressure can be found in this picture by adding the term

$$(P-P_0)(V-V_0) \cong (P-P_0)\int d^dx\sum_{\alpha=1}^{d}e_{\alpha\alpha} \tag{5.1}$$

to the Hamiltonian of (2.1). Here P_0, V_0 characterize the equilibrium state against which the displacements $u(x)$ are measured. Clearly this term will only affect the $q=0$ part of the Hamiltonian.

We note that since we will get $\langle e_{\alpha\alpha}\rangle \propto P-P_0$ in this picture, we are restricted to small values of $P-P_0$. (If large values are used, then $e_{\alpha\alpha}$ will typically include a large uniform dilatation, which can lead to unphysical results, as discussed in Sec. VI, below.)

Applying this method to our cubic system, we obtain the following effective spin Hamiltonian:

$$\frac{H_{\rm eff}}{T}=\sum_q \tfrac{1}{2}(r_0+q^2)\psi_q\psi_{-q}+\frac{\tilde{u}_0}{V}\sum_{q_1q_2q_3}\psi_{q_1}\psi_{q_2}\psi_{q_3}\psi_{-q_1-q_2-q_3} - \frac{1}{V}\sum_{\substack{qq_1q_2\\ q\neq 0}} K_0(q)\psi_{q_1}\psi_{-q_2}\psi_{-q-q_1}\psi_{q+q_2} - \frac{g_0^2}{2B_0}\frac{1}{V}\left(\sum_q \psi_q\psi_{-q}\right)^2, \qquad (5.2)$$

where

$$r_0\equiv\tilde{r}_0-2g_0(P-P_0)/B_0T^{1/2}\propto T-T_c(P). \qquad (5.3)$$

Obviously, this offers an alternative starting point for a discussion of the critical properties of the system. It is important to note, however, as we mentioned earlier in Sec. II, that the nonanalyticity of $K_0(q)$ at $q=0$ now appears directly in the Hamiltonian and one must be careful about taking limits of $q\to 0$. Holz[35] has recently discussed a discrete Ising system on a compressible bcc lattice by integrating separately over the macroscopic elastic normal coordinates, as we have done in this section. He has, however, ignored the above-mentioned singular behavior of the four-spin interaction term $K_0(q)$ as $q\to 0$, and has concluded, erroneously, that this term can be ignored to lowest order in q.

When K is isotropic this difficulty disappears, and $H_{\rm eff}$ can be rewritten in the form

$$\frac{H_{\rm eff}}{T}=\sum_q \tfrac{1}{2}(\tilde{r}_0+q^2)\psi_q\psi_{-q}+\frac{u_0}{V}\sum_{q_1q_2q_3}\psi_{q_1}\psi_{q_2}\psi_{q_3}\psi_{-q_1-q_2-q_3} + \left(K_0-\frac{g_0^2}{2B_0}\right)\frac{1}{V}\left(\sum_q \psi_q\psi_{-q}\right)^2, \qquad (5.4)$$

where, as before,

$$u_0\equiv\tilde{u}_0-K_0. \qquad (5.5)$$

For an isotropic system, this is just the form obtained by Sak.[12] In that case, the coefficient of the quartic pairing term [the last term in (5.4)] satisfies

$$K_0-\frac{g_0^2}{2B_0}=\frac{g_0^2}{2C_{11}^0}-\frac{g_0^2}{2B_0}<0, \qquad (5.6)$$

which is the cause of an instability in this approach leading, as expected, to a first-order transition.

For a BE system, the coefficient of the last term in (5.4) vanishes, and therefore at fixed P the system behaves exactly like a rigid Ising model and exhibits unrenormalized Ising exponents, as we saw before.

A different method was used by Wegner[11] to discuss an isotropic elastic spin system under fixed pressure: He first eliminates the elastic variables by minimizing the energy with respect to the displacement field $u(x)$ for a given spin configuration. The resulting static displacement is expanded in terms of exact static normal modes of the solid body. The resulting effective spin Hamiltonian separates rather naturally into a short-range part due to the microscopic modes, and a long-range part due to the macroscopic surface modes. A renormalization-group analysis is applied to this Hamiltonian. The actual calculation of these static surface modes, which is necessary in order to discuss the effective long-range forces in this approach, is in general very difficult. Furthermore, it must be repeated every time a new shape for the solid body or a new type of external condition is selected.

VI. PATHOLOGICAL MODELS

There have been various models proposed for Ising-type transitions in compressible systems. In some of these, features have been found which seem to be inconsistent with what we have observed in the previous sections. We will now analyze two of these models in order to understand how this comes about.

The first of these is the Baker-Essam model (denoted by BE), where a tricritical point has been found at $P=0$[8,9]: At $P>0$ there is a Fisher-renormalized Ising transition while at $P<0$ there is a first-order transition. At $P=0$ the system exhibits an unrenormalized Ising transition.

These results differ from our present results for the modified BE, where we always found an unrenormalized Ising transition at any constant P, because the two models are actually different: Whereas we defined the elastic moduli by expanding the elastic free-energy density around the equilibrium state of the elastic system (neglecting, however, the contribution of the spin-lattice interactions to the equilibrium state), and then assumed $C_{44}=0$, the original version of BE, henceforth to be called BE1, effectively assumes that $C_{44}=0$ only in the case that $P=0$. The same elastic harmonic Hamiltonian is then used to calculate the properties of the system under arbitrary external conditions.

For example, BE1 turned out to be rigorously reducible to a simple, nearest-neighbor, rigid Ising model with an effective exchange coefficient if the system is under fixed uniaxial stresses which have the same value P along all the cubic axes. Using our approach, this would correspond to adding the following term to the Hamiltonian of (2.1):

$$P\int d^dx \sum_\alpha e_{\alpha\alpha} = PV_0 \sum_\alpha e_{\alpha\alpha}. \tag{6.1}$$

This term clearly affects only the $q=0$ part of the Hamiltonian, but in a way which does not alter any of the elastic moduli. Therefore the critical behavior under fixed uniaxial stresses is exactly the same as at $P=0$; namely, one finds an unrenormalized Ising transition.

One could not seriously discuss the properties of BE1 under constant positive pressure as it is usually applied: Since $C_{44}=0$, any positive hydrostatic pressure, no matter how small, would cause the system to collapse to a line in the direction of the body diagonal. It was therefore necessary to restrict all the surface atoms on one half of all the faces of the crystal to lie upon given, mutually perpendicular planes. The volume was defined in the following way:

$$V \equiv V_0 \prod_{\alpha=1}^{d} (1+\langle e_{\alpha\alpha}\rangle). \tag{6.2}$$

Using this definition, and adding the following term to H^0:

$$P(V-V_0) = PV_0\Big(\sum_\alpha \langle e_{\alpha\alpha}\rangle + \sum_{\alpha<\beta} \langle e_{\alpha\alpha}\rangle\langle e_{\beta\beta}\rangle\Big), \tag{6.3}$$

we find that while the $q\neq 0$ part of H^0 remains unchanged, in the $q=0$ part C_{12} gets replaced by $C_{12}+P$. Consequently, if we now integrate over all the microscopic and macroscopic elastic variables as in Sak's method, we produce a quartic pairing term whose coefficient is

$$\frac{g^2}{2B} - \frac{g^2}{2(B+\frac{2}{3}P)}. \tag{6.4}$$

This coefficient will be positive or negative depending on whether $P>0$ or $P<0$, and the usual results of BE1 are reproduced. This is evidently a result of the pathological aspects of the model—the fact that it is not rotationally invariant[36] and that some of the elastic moduli for uniform strains differ from the elastic moduli for $q\neq 0$ strains. Note, however, that the fact that the shear modulus C_{44} vanishes in itself is not really pathological. It can in fact be quite useful to consider this as a limiting case of cubic anisotropy if it is discussed within the framework of a realistic physical approach, as was done in Secs. III and IV. The pathological BE1 model discussed above is interesting mainly as a solvable mathematical model with a non-Gaussian tricritical point.

The other model we shall briefly discuss has been proposed by Imry,[21] who used the isotropic version of (2.1) for the Hamiltonian at $P=0$, and added to it a $P(V-V_0)$ term as in (6.3). Integrating over the elastic variables he produced a quartic pairing term with the coefficient

$$\frac{g^2}{2C_{11}} - \frac{g^2}{2(B+\frac{2}{3}P)}, \tag{6.5}$$

which is positive or negative depending on whether

$$\tfrac{2}{3}P \gtrless \frac{d-1}{d}\,\tfrac{1}{2}C_{44}. \tag{6.6}$$

Obviously, this model suffers from the same pathologies as BE1. Furthermore, since in the $q=0$ part of H, C_{12} gets changed to $C_{12}+P$, it is clear that when the upper inequality of (6.6) is valid, i.e., when the transition should be second order, the system is in fact unstable against the uniform uniaxial shear strain $e_{xx}=-e_{yy}$. One should therefore constrain the system to have only dilatational strains in order to stabilize it.

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APPENDIX A: DYNAMICAL MATRIX AND RELATED FUNCTIONS FOR AN ELASTIC CONTINUUM WITH CUBIC ANISOTROPY

In Cartesian notation the free-energy density of a continuous elastic system is given by

$$F_e = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \lambda_{\alpha\beta\gamma\delta} e_{\alpha\beta} e_{\gamma\delta}. \tag{A1}$$

In a system with cubic anisotropy, there are only three different elastic moduli:

$$\lambda_{\alpha\alpha\alpha\alpha} \equiv C_{11}, \quad \lambda_{\alpha\alpha\beta\beta} \equiv C_{12}, \quad \lambda_{\alpha\beta\alpha\beta} \equiv \tfrac{1}{4}C_{44}, \quad \alpha\neq\beta, \tag{A2}$$

where C_{11}, C_{12}, C_{44} would correspond to the usual Voigt notation in three dimensions.

The dynamical matrix is defined in general by

$$D_{\beta\delta}(q) \equiv \sum_{\alpha\gamma} \lambda_{\alpha\beta\gamma\delta} q_\alpha q_\gamma. \tag{A3}$$

The physical values of the elements of the inverse matrix D^{-1} are related to the physical (i.e., the dressed) correlation functions of the Fourier components of the displacement vector u_q,

$$T[D^{-1}(q)]_{\alpha\beta} = \langle u_{\alpha q} u^*_{\beta q}\rangle_T = b^{d-2a_u}\langle u'_{\alpha q'} u'_{\beta q'}\rangle_T, \tag{A4}$$

where we used (2.5) to get the last result, and the brackets $\langle\,\rangle_T$ stand for a thermal average. The dressed correlation function can be approximated by the bare correlation function (i.e., calculated neglecting the spin-lattice interactions) when $b \equiv e^l = \xi/\xi_0$ or q^{-1}, whichever is smaller. Therefore, for ξ finite but large (i.e., $T \neq T_c$ but close to it) we find

$$\lim_{q=0} q^2[D^{-1}(q)]_{\alpha\beta} = e^{(d-2a_u-2)l} \times \lim_{q=0} q^2[D_l^{-1}(q)]_{\alpha\beta}\Big|_{l=\ln(\xi/\xi_0)}. \quad \text{(A5)}$$

Since D is linear in the elastic coefficients, we find that the physical value of any elastic coefficient, denoted generically by $C(t)$, satisfies

$$C(t) = e^{-(d-2a_u-2)l} C_l\Big|_{l=\ln(\xi/\xi_0)}. \quad \text{(A6)}$$

More generally, (A6) holds for any l satisfying $l \geq \ln(\xi/\xi_0)$. However, for $l > \ln(\xi/\xi_0)$ the renormalization-group equation for D, (2.18), reduces to a trivial change of scale, since $\tilde{r}_l > 1$ and thus only the first term on the right-hand side of that equation remains. The resulting dependence of C_l on l exactly cancels the exponential factor in (A6), so that $C(t)$ remains unchanged. Moreover, for $l < \ln(\xi/\xi_0)$, $\tilde{r}_l$ is small compared to 1, so that the renormalization-group equations can be evaluated as if we were at T_c. It follows that except for a finite correction of order ϵ, the quantity C_l entering (A6) may be evaluated at T_c, provided $l = \ln(\xi/\xi_0)$ as indicated.

In a cubic system, we find by an explicit calculation

$$D_{\alpha\alpha} = \mu q^2 + \mu_2 q_\alpha^2, \qquad D_{\alpha\beta} = \mu_1 q_\alpha q_\beta, \quad \alpha \neq \beta \quad \text{(A7)}$$

where

$$\mu \equiv \tfrac{1}{4}C_{44}, \quad \mu_1 \equiv C_{12} + \tfrac{1}{4}C_{44}, \quad \mu_2 \equiv C_{11} - \tfrac{1}{4}C_{44}. \quad \text{(A8)}$$

In what follows, we will give expressions for various symmetric functions of the components of the unit vector $\hat{q} \equiv q/|q|$. We will therefore define the following basic symmetric homogeneous polynomials:

$$F_1(\hat{q}) \equiv \sum_\alpha \hat{q}_\alpha^2 = 1, \qquad F_{1\beta\gamma}(\hat{q}) \equiv \sum_{\alpha\neq\beta,\gamma} \hat{q}_\alpha^2,$$
$$F_2(\hat{q}) \equiv \sum_{\alpha<\beta} \hat{q}_\alpha^2\hat{q}_\beta^2, \qquad F_{2\gamma\delta}(\hat{q}) \equiv \sum_{\substack{\alpha<\beta\\ \alpha,\beta\neq\gamma,\delta}} \hat{q}_\alpha^2\hat{q}_\beta^2,$$
$$F_3(\hat{q}) \equiv \sum_{\alpha<\beta<\gamma} \hat{q}_\alpha^2\hat{q}_\beta^2\hat{q}_\gamma^2, \quad F_{3\delta\theta}(\hat{q}) \equiv \sum_{\substack{\alpha<\beta<\gamma\\ \alpha,\beta,\gamma\neq\delta,\theta}} \hat{q}_\alpha^2\hat{q}_\beta^2\hat{q}_\gamma^2, \quad \text{etc.} \quad \text{(A9)}$$

Note that F_m and $F_{m\alpha\beta}$ can only be defined for $m \leq d$. We will use the convention that $F_m \equiv F_{m\alpha\beta} \equiv 0$ when $m > d$. In terms of these polynomials we find

$$\det D = [q^{2d}\mu^{d-1}(\mu+\mu_2) + \mu^{d-2}(\mu_2^2-\mu_1^2)F_2 + \mu^{d-3}(\mu_2-\mu_1)^2(\mu_2+2\mu_1)F_3 + \mu^{d-4}(\mu_2-\mu_1)^3(\mu_2+3\mu_1)F_4 + \cdots], \quad \text{(A10)}$$

$$(\det D)D^{-1}_{\alpha\alpha} = q^{2d-2}[\mu^{d-1} + \mu^{d-2}\mu_2 F_{1\alpha\alpha} + \mu^{d-3}(\mu_2^2-\mu_1^2)F_{2\alpha\alpha} + \mu^{d-4}(\mu_2-\mu_1)^2(\mu_2+2\mu_1)F_{3\alpha\alpha} + \cdots], \quad \text{(A11)}$$

$$(\det D)D^{-1}_{\alpha\beta} = -\mu_1 q^{2d-2}\hat{q}_\alpha\hat{q}_\beta[\mu^{d-2} + \mu^{d-3}(\mu_2-\mu_1)F_{1\alpha\beta} + \mu^{d-4}(\mu_2-\mu_1)^2F_{2\alpha\beta} + \cdots], \quad \alpha\neq\beta. \quad \text{(A12)}$$

From these expressions and (2.8) we can calculate an explicit expression for $K(\hat{q})$ and $Q(\hat{q})$,

$$\frac{1}{K(\hat{q})} = \frac{2(\mu+\mu_2)}{g^2} + \frac{4(\mu_1-\mu_2)}{g^2}Q(\hat{q}), \quad \text{(A13)}$$

$$Q(\hat{q}) = \frac{(1+A')F_2 + A'(3+4A')F_3 + 4A'^2(2+3A')F_4 + \cdots}{1+4A'F_2 + 12A'^2F_3 + 32A'^3F_4 + \cdots}, \quad \text{(A14)}$$

where we have used a slightly modified form for the anisotropy parameter

$$A' \equiv \frac{\mu_2-\mu_1}{2\mu} = \frac{1-A}{A}, \quad -1 < A' < \infty. \quad \text{(A15)}$$

We note that while it seems clear how the expansions in (A10)–(A14) should be continued to arbitrary order in F_m and $F_{m\alpha\beta}$, we have verified them by an explicit calculation only for $d = 2, 3, 4$. In this way we could only obtain the terms which are exhibited explicitly in these equations.

In both two and three dimensions, we found that Q reaches its maximum value, $\frac{1}{4}$ and $\frac{1}{3}$, respectively, when q is along the body diagonal (i.e., the ⟨11⟩ or ⟨111⟩ direction), while the minimum value, 0, is reached when q is along a cubic axis (i.e., the ⟨10⟩ or ⟨100⟩ direction). We conjecture that this is true for any d, and that consequently

$$0 \leq Q \leq (d-1)/2d. \quad \text{(A16)}$$

In order to prove this, one would have to show that

Q does not have its actual extrema in nonsymmetry directions.

We would like to note the remarkable fact that the extrema of Q are independent of the precise value of A'. Because of this, Q can never be rigorously independent of $\hat{q}$. However, when $A' \to \infty$ we find that $Q \to (d-1)/2d$, the maximum value, for every $\hat{q}$ outside of a small region around each of the hyperplanes $\hat{q}_x = 0$, $\hat{q}_y = 0$, etc., whose size shrinks to zero as $A' \to \infty$.

The extremum points and values of $K(\hat{q})$ are easily found from (A13), (A15), and (A16):

(a) For $A' < 0$ $(A > 1)$,

$$K_{\max} = \frac{g^2}{2(\mu + \mu_2)} = \frac{g^2}{2C_{11}}, \tag{A17}$$

with $\hat{q}_{\max}$ along the cubic axes, and

$$K_{\min} = \frac{g^2}{2\{\mu + \mu_2 + [(d-1)/d](\mu_1 - \mu_2)\}} = \frac{g^2}{2\{B + [(d-1)/d]\frac{1}{2}C_{44}\}}, \tag{A18}$$

with $\hat{q}_{\min}$ along the body diagonals.

(b) For $A' > 0$ $(A < 1)$, the roles of $K_{\max}$, $\hat{q}_{\max}$ and $K_{\min}, \hat{q}_{\min}$ are reversed as compared to (a).

The degree of anisotropy of $K(\hat{q})$ is not determined entirely by the anisotropy parameter of the system A (or A'), nor even by the ratio R of the two coefficients in (A13) [see (3.35) for the definition of R]. The reason for this is that K becomes approximately isotropic either when $|R|$ is very small, or when Q is nearly isotropic, which occurs when $A \ll 1$ (also when $A \gg 1$ for $d = 2$, see Ref. 26). In the latter case, $K(\hat{q})$ can be very nearly independent of $\hat{q}$ everywhere except in the vicinity of the lattice planes $q_x = 0, q_y = 0$, where K dips down rather drastically towards its minimum value. From the form of Q, we see that these dips occur when $\hat{q}$ is at a distance of the order of $A^{1/2}$ from one of these planes. Therefore, we can write the following estimate for $\langle K \rangle$:

$$\langle K \rangle = K_{\max} - O(A^{1/2})(K_{\max} - K_{\min}). \tag{A19}$$

A relevant measure for the anisotropy of K would be

$$(K_{\max} - \langle K \rangle)/K_{\max}, \tag{A20}$$

and we now find

$$\frac{K_{\max} - \langle K \rangle}{K_{\max}} = O(A^{1/2})\frac{K_{\max} - K_{\min}}{K_{\max}} \ll \frac{K_{\max} - K_{\min}}{K_{\max}}. \tag{A21}$$

Using (A20) to measure the anisotropy of K, we find that the qualitative features of the shape of K are determined by the following conditions:

(a) $K(\hat{q})$ is very nearly isotropic when

$$|A - 1| \ll \frac{d}{d-1}\frac{C_{11}}{C_{11} - C_{12}} \quad \text{for } A \geq O(1), \tag{A22}$$

or when

$$A \ll \frac{d}{d-1}\frac{B}{C_{11} - C_{12}} \quad \text{for } A \ll 1. \tag{A23}$$

(b) $K(\hat{q})$ is extremely anisotropic when

$$|A - 1| \gg \frac{d}{d-1}\frac{C_{11}}{C_{11} - C_{12}} \quad \text{for } A \geq O(1), \tag{A24}$$

or when

$$A \gg \frac{d}{d-1}\frac{B}{C_{11} - C_{12}} \quad \text{for } A \ll 1. \tag{A25}$$

Note that (A22) and (A24) allow $A < 1$ but not $A \ll 1$. Note also that if the elastic moduli in (A22)–(A25) are taken to have their renormalized values B_l, C_{11}^l, etc., then the right-hand side of these inequalities always decreases monotonically towards zero with increasing l. Consequently, for sufficiently large l, $K_l(\hat{q})$ always becomes very anisotropic unless $A = 1$ or $A = 0$ exactly.

An isotropic system is a cubic system in which $\mu_1 = \mu_2$, i.e., $A' = 0$ and $A = 1$. In that case we find

$$\begin{aligned} \det D &= q^{2d}\mu^{d-1}(\mu + \mu_2) = q^{2d}(\tfrac{1}{4}C_{44})^{d-1}C_{11}, \\ Q(\hat{q}) &= F_2(\hat{q}), \\ K(\hat{q}) &= g^2/2C_{11}. \end{aligned} \tag{A26}$$

A BE system is a cubic system in which $\mu = 0$, i.e., $A' = \infty$ and $A = 0$.[26] In that case we find

$$\begin{aligned} \det D &= q^{2d}(\mu_2 - \mu_1)^{d-1}[\mu_2 + (d-1)\mu_1]F_d(\hat{q}) \\ &= dq^{2d}(C_{11} - C_{12})^{d-1}BF_d, \\ Q(\hat{q}) &= (d-1)/2d \\ K(\hat{q}) &= \frac{g^2}{2\{\mu_2/d + [(d-1)/d]\mu_1\}} = \frac{g^2}{2B}, \end{aligned} \tag{A27}$$

where the last two equalities hold everywhere except in certain high-symmetry planes, and where

$$B \equiv \frac{1}{d}C_{11} + \frac{d-1}{d}C_{12} \tag{A28}$$

is the bulk modulus of compressibility. These are the only cases when K is isotropic.

A fluid is of course a system where both $\mu_1 = \mu_2$ and $\mu = 0$, i.e., an isotropic BE system. In that case $\det D \equiv 0$, since all but one of the eigenvalues (the longitudinal sound mode) vanish, $B = C_{11}$, and $K = g^2/2B$. In that case, the Hamiltonian depends only on one scalar elastic variable, $\nabla \cdot u$, and reduces completely to the form discussed in Refs. 22 and 23 (see Appendix D, below).

APPENDIX B: GENERALIZED BAKER-ESSAM MODEL

The Baker-Essam model was originally introduced as a system of Ising spins on a compressible, simple-cubic lattice with a rather special dependence of the Hamiltonian on the elastic variables[7]: Both the elastic energy and the exchange coefficient of a nearest-neighbor pair were assumed to depend only on the projection of the pair-separation vector onto its equilibrium direction, which was along one of the cubic axes, and all other interactions were taken to be zero. Assuming a quadratic elastic energy and a linear exchange coefficient, Baker and Essam were able to integrate over the elastic variables completely, thereby reducing the statistical mechanics of the model to that of an incompressible Ising model with only nearest-neighbor interactions and an effective exchange coefficient which could depend on the thermodynamic state of the system. This model was later generalized to include arbitrary nonquadratic elastic energies and nonlinear exchange coefficients.[9] Another generalization was that one could allow neighboring bonds to interact in the elastic energy and still be able to integrate out the elastic variables.[37] The resulting effective incompressible Ising model then includes next-nearest-neighbor interactions too. We will now derive the continuum limits of these models.

The Hamiltonian of the simple BE (no interactions between different bonds) in the uniaxial-stress ensemble (called the λ ensemble in Refs. 8 and 9) is

$$H=\sum_{(ij)}\{\tfrac{1}{2}\Phi_2(\xi_{ij}-\xi_0)^2+[J_0+J_1(\xi_{ij}-\xi_0)]\sigma_i\sigma_j+\lambda(\xi_{ij}-\xi_0)\},\qquad\text{(B1)}$$

where ξ_0 is the lattice parameter, λ/ξ_0^{d-1} is the external uniaxial stress, ξ_{ij} is the bond-vector projection described above, $\sigma_i=\pm1$ are the Ising spins, and the sum is over all nearest-neighbor pairs of sites on a simple-cubic lattice. In the continuum approximation, written explicitly for $d=3$, the components of strain become

$$e_{xx}=(\xi_x-\xi_0)/\xi_0,\ \text{etc.},\qquad\text{(B2)}$$

where ξ_x signifies the projection of a bond that normally lies in the x direction. We can thus approximate H by

$$\begin{aligned}H=\sum_i\{&\tfrac{1}{2}\Phi_2(e_{xx}^2+e_{yy}^2+e_{zz}^2)\xi_0^2\\&+[J_0+J_1e_{xx}\xi_0)\sigma_i\sigma_{i+\hat{x}}+(J_0+J_1e_{yy}\xi_0)\sigma_i\sigma_{i+\hat{y}}\\&+(J_0+J_1e_{zz}\xi_0)\sigma_i\sigma_{i+\hat{z}}]+\lambda\xi_0(e_{xx}+e_{yy}+e_{zz})\},\end{aligned}\qquad\text{(B3)}$$

where the sum is now over all the lattice sites, and $\hat{x},\hat{y},\hat{z}$ are the unit lattice vectors. In going over to the field-theory form of the long-wavelength part of H, we replace $e_{xx}\sigma_i\sigma_{i+\hat{x}}$ by $e_{xx}(x)\psi^2(x)$, and we thus obtain a Hamiltonian that has the form of (2.1) with $d=3$ and

$$C_{11}=\Phi_2/\xi_0,\quad C_{12}=C_{44}=0,\quad g=J_1/\xi_0^2.\qquad\text{(B4)}$$

The modified BE (including interactions between nearest-neighbor bonds) cannot be given as explicit a representation as (B1). We write it as follows:

$$\begin{aligned}H=V_2(\xi,\eta,\zeta)+\sum_i\{&[J_0+J_1(\xi_i-\xi_0)]\sigma_i\sigma_{i+\hat{x}}\\&+[J_0+J_1(\eta_i-\xi_0)]\sigma_i\sigma_{i+\hat{y}}\\&+[J_0+J_1(\zeta_i-\xi_0)]\sigma_i\sigma_{i+\hat{z}}\},\end{aligned}\qquad\text{(B5)}$$

where the sum is over all lattice sites and ξ_i,η_i,ζ_i stand for bond projections originating from the same site in the direction of x,y,z, respectively. V_2 is a quadratic function of the various bond projections with the property that every bond is correlated only with itself and its nearest-neighbor bonds; i.e., using $e^{-V_2/T}$ as a statistical distribution function, we require that

$$\xi_0=\langle\xi_i\rangle=\langle\eta_i\rangle=\langle\zeta_i\rangle,\qquad\text{(B6)}$$

$$A_2\equiv\langle(\xi_i-\xi_0)^2\rangle=\langle(\eta_i-\xi_0)^2\rangle=\langle(\zeta_i-\xi_0)^2\rangle,\qquad\text{(B7)}$$

$$\begin{aligned}B_2&\equiv\langle(\xi_i-\xi_0)(\eta_i-\xi_0)\rangle=\langle(\xi_i-\xi_0)(\eta_{i-\hat{y}}-\xi_0)\rangle\\&=\langle(\eta_i-\xi_0)(\zeta_i-\xi_0)\rangle=\langle(\eta_i-\xi_0)(\zeta_{i-\hat{z}}-\xi_0)\rangle\\&=\langle(\zeta_i-\xi_0)(\xi_i-\xi_0)\rangle=\langle(\zeta_i-\xi_0)(\xi_{i-\hat{x}}-\xi_0)\rangle,\end{aligned}\qquad\text{(B8)}$$

where $A_2>0$ and $B_2\neq0$, but $A_2>|B_2|$ (this is required for stability), and that all other correlations of the bond projections vanish. Note that stated in this form, we have made a simple assumption about the inverse matrix of the quadratic form V_2. V_2 itself must, however, be very complicated in order to lead to the simple results of (B6)–(B8).

If we now view the function $e^{-V_2/T}$ as a statistical distribution function for the components of strain treated as statistically independent quantities, and make the identification

$$e_{xx}(i)=\frac{\xi_i-\xi_0}{\xi_0},\quad e_{yy}(i)=\frac{\eta_i-\xi_0}{\xi_0},\quad e_{zz}(i)=\frac{\zeta_i-\xi_0}{\xi_0},\qquad\text{(B9)}$$

we find that

$$\begin{aligned}&\langle e_{\alpha\alpha}^2\rangle=A_2\xi_0^2,\\&\langle e_{\alpha\alpha}e_{\beta\beta}\rangle=B_2\xi_0^2\quad\text{for }\alpha\neq\beta.\end{aligned}\qquad\text{(B10)}$$

Using (2.1b) for a similar calculation, we find

$$\begin{aligned}&\langle e_{\alpha\alpha}^2\rangle=\frac{(C_{11}+C_{12})T}{(C_{11}-C_{12})(2C_{12}+C_{11})},\\&\langle e_{\alpha\alpha}e_{\beta\beta}\rangle=\frac{C_{12}T}{(C_{12}-C_{11})(2C_{12}+C_{11})}\quad\text{for }\alpha\neq\beta.\end{aligned}\qquad\text{(B11)}$$

A comparison of the two results (B10) and (B11) enables us to determine C_{11} and C_{12} in terms of A_2 and B_2. Since the Hamiltonian of (B5) still has no dependence on the other strains, e_{xy}, e_{yz}, e_{zx}, we still get $C_{44}=0$.

This generalization of the BE model is a very natural one from the point of view of renormalization-group theory: Even if we started out with $C_{12}=0$, as in (B4), the renormalization-group transformation would generate a nonzero value of C_{12}. From (2.21) and (2.22) we can get an equation for C_{12},

$$\frac{dC_{12}^l}{dl}=(d-2a_u-2)C_{12}^l-2g_l^2\frac{B_d}{(1+\tilde{r})^2}, \tag{B12}$$

which clearly demonstrates this fact. There is thus no fundamental significance to the fact that $C_{12}=0$ in the original version of BE, since this property is not conserved by the equations. On the other hand, the fact that $C_{44}=0$ is significant, because it is responsible for the fact that Q and hence K are independent of $\hat{q}$, and that property is conserved by the equations [see (2.20)].

APPENDIX C: SOLUTION OF THE EQUATIONS FOR C_{11}^l and K_l

In order to obtain the asymptotic behavior of C_{11}^l for the situation described in Sec. IV A, we start out by solving the equation for K_l more carefully. Assuming that K_l is isotropic and that $l>l_1$, (3.4) becomes

$$\frac{dK_l}{dl}\cong K_l(\epsilon/3-4B_4K_l)\quad\text{for } l>l_1. \tag{C1}$$

Its solution is

$$K_l\cong\frac{K_R^* e^{\epsilon(l-l_1)/3}}{3\tilde{u}_0/\langle K_0\rangle+e^{\epsilon(l-l_1)/3}}, \tag{C2}$$

where we used the fact that

$$\frac{K_R^*}{\langle K_{l_1}\rangle}=\frac{3\tilde{u}_0}{\langle K_0\rangle}\gg 1. \tag{C3}$$

Using this result, (4.7) can be written as

$$\frac{dg_l^2}{dl}=-g_l^2\frac{\epsilon}{3}\tanh\left(\frac{\epsilon}{6}(l-l_1)-\tfrac{1}{2}\ln\frac{3\tilde{u}_0}{\langle K_0\rangle}\right)\quad\text{for } l>l_1. \tag{C4}$$

The solution of this equation is

$$\frac{g_l}{g_{l_1}}=\frac{\cosh[\frac{1}{2}\ln(3\tilde{u}_0/\langle K_0\rangle)]}{\cosh[\frac{1}{2}\ln(3\tilde{u}_0/\langle K_0\rangle)-(\epsilon/6)(l-l_1)]}. \tag{C5}$$

For most values of l this has the same form as (4.8). However, as $l\to l_2$ we find

$$g_{l_2}^2=\tfrac{1}{4}g_l^2\,3\tilde{u}_0/\langle K_0\rangle, \tag{C6}$$

which differs from (4.8) by the extra factor $\frac{1}{4}$.

Using (C5) to subsitute for g_l^2 in (2.22), we can integrate that equation to get C_{11}. We thus find

$$\begin{aligned}C_{11}^l&=C_{11}^0-2B_4\int_0^l g_l^2\,dl\\&=C_{11}^0-2B_4g_0^2\left\{\frac{e^{\epsilon l_1}-1}{\epsilon}+e^{\epsilon l_1}\cosh^2\left(\tfrac{1}{2}\ln\frac{3\tilde{u}_0}{\langle K_0\rangle}\right)\right.\\&\qquad\left.\times\frac{6}{\epsilon}\left[1-\tanh\left(\tfrac{1}{2}\ln\frac{3\tilde{u}_0}{\langle K_0\rangle}-\frac{\epsilon}{6}(l-l_1)\right)\right]\right\}\\&\cong\tfrac{1}{2}C_{11}^0\left(1-\tanh\frac{\epsilon}{6}(l-l_2)-\frac{\langle K_0\rangle}{9\tilde{u}_0}\right).\end{aligned} \tag{C7}$$

Turning to the situation discussed in Sec. IV B, we first note that when K_l is isotropic, the equation for u_l, (3.3), is independent of K_l. Its exact solution is then given by

$$\frac{u_l^*}{u_l}=1+\frac{u_l^*-u_0}{u_0}e^{-\epsilon l}. \tag{C8}$$

Under the assumptions of that subsection [see (4.36)], u_l remains very small nearly up to l_2, so that we can neglect it in solving (3.4) for K_l. We thus get

$$\frac{K_l}{K_S^*}=\frac{1}{1+(K_S^*/K_0)e^{-\epsilon l}}\quad\text{for } 0<l<l_2. \tag{C9}$$

Using this result in (4.7) and neglecting u_l, we get the following equation for g_l^2:

$$\frac{dg_l^2}{dl}=\epsilon g_l^2\tanh\left(\tfrac{1}{2}\ln\frac{K_S^*}{K_0}-\frac{\epsilon l}{2}\right). \tag{C10}$$

The solution of this equation is

$$\frac{g_l}{g_0}=\frac{\cosh\frac{1}{2}\ln(K_S^*/K_0)}{\cosh[\frac{1}{2}\ln(K_S^*/K_0)-\epsilon l/2]}, \tag{C11}$$

which leads to the following result for C_{11}^l:

$$\begin{aligned}C_{11}^l&=C_{11}^0-2B_4\int_0^l g_l^2\,dl\\&=C_{11}^0\left[1+\tfrac{1}{2}\tanh\left(\tfrac{1}{2}\ln\frac{K_S^*}{K_0}-\frac{\epsilon l}{2}\right)\right.\\&\qquad\left.-\tfrac{1}{2}\tanh\left(\tfrac{1}{2}\ln\frac{K_S^*}{K_0}\right)\right].\end{aligned} \tag{C12}$$

Evaluating this expression in various limits leads to

$$C_{11}^l=\begin{cases}C_{11}^0 & \text{for } 0<l\ll l_1\\ \tfrac{1}{2}C_{11}^0 & \text{for } l=l_1\\ C_{11}^0e^{-\epsilon(l-l_1)} & \text{for } l_1\ll l\ll l_2.\end{cases} \tag{C13}$$

APPENDIX D: RELATION BETWEEN THE ELASTIC SOLID AND A COMPRESSIBLE LIQUID—EXPONENTS TO ALL ORDERS IN ϵ

As was mentioned in the Introduction, if a symmetry-breaking transition occurs in a one-component liquid, ideal exponents are expected for the system at constant pressure. This is most easily appreciated if one considers a fixed, finite volume, in which N, the total number of atoms, is permitted to vary with temperature so as to keep the total pressure constant. One may then represent the effective Hamiltonian entering the partition function as

$$\frac{(H-\mu N)_0}{T}=\int d^dx\left(\tfrac{1}{2}\tilde{r}_0\psi^2+\tfrac{1}{2}|\nabla\psi|^2+\tilde{u}_0\psi^4+\tfrac{1}{2}g_0\psi^2\tilde{\rho}-\frac{\mu_0}{T}\tilde{\rho}+\frac{B_0\tilde{\rho}^2}{2T}\right), \tag{D1}$$

where $\tilde{\rho}(x)$ is the deviation of the liquid density at point x from some specified value, B_0 is a bare value of the bulk modulus, μ_0 is a constant, and the other symbols are the same as in (2.1). We shall assume periodic boundary conditions. Since $\tilde{\rho}$ enters only quadratically, the associated degrees of freedom lead only to Gaussian integrals in the partition function, which can be performed explicitly. The resulting effective Hamiltonian for ψ has the Ginzburg-Landau-Wilson form, and leads immediately to ideal exponents for the transition (see Refs. 13–15).

The model (D1) can be modified to represent a liquid with a constant number of atoms in a fixed volume, simply by imposing the constraint

$$\int\tilde{\rho}\,d^dx=0. \tag{D2}$$

Such a constraint must then lead to Fisher-renormalized exponents, if $\alpha_I>0$ and $g_0\neq0$, as was shown in Ref. 4. The model described by (D1) and (D2) is mathematically equivalent, however, to our model (2.1) for the elastic solid with periodic boundary conditions in a fixed volume, in the isotropic case. We see that the transverse components of the displacement field u do not couple to the order parameter ψ, while the longitudinal part can be replaced by a scalar field

$$\tilde{\rho}=\nabla\cdot u. \tag{D3}$$

The constraint (D2) is automatically satisfied, since u is periodic. The elastic energy associated with a longitudinal displacement field is simply

$$\tfrac{1}{2}C_{11}^0(\nabla\cdot u)^2=\tfrac{1}{2}C_{11}^0\tilde{\rho}^2. \tag{D4}$$

It is clear then that the critical properties of the isotropic solid and the one-component liquid are identical when considered at fixed volume and periodic boundary conditions, except that the bulk modulus of the liquid is replaced by C_{11} in the solid. In principle, a solid with periodic boundary conditions can show ideal behavior (e.g., ideal temperature dependence of the magnetic susceptibility) if the volume is constrained to vary as

$$\frac{1}{V}\frac{dV}{dT}=\frac{1}{C_{11}}\left(\frac{dP}{dT}\right)_V. \tag{D5}$$

This constraint leads to variation in pressure given by

$$\frac{dP}{dT}=\left(1-\frac{B}{C_{11}}\right)\left(\frac{dP}{dT}\right)_V. \tag{D6}$$

We now use the equivalence of the liquid-Ising and the isotropic-solid-Ising models to derive the critical behavior of the bulk compressibility of the solid B_{sol} from the specific heat of an incompressible Ising model. We begin by noting that the bulk compressibility of the liquid B_{liq} satisfies the following relationship near T_c (this is one of Pippard's relations[3]):

$$B_{\text{liq}}\cong\frac{T_c}{C_p}\left(\frac{dT_c}{dP}\right)^{-2}, \tag{D7}$$

where the singular part of C_p is the same as the specific heat of an incompressible Ising model,

$$C_p=A_\pm|t_p|^{-\alpha_I}+A_r. \tag{D8}$$

Here and later, the notation $A_\pm$ refers to $t\gtrless0$. Writing a similar expression for B_{liq},

$$\frac{1}{B_{\text{liq}}}=\frac{1}{B_r}+\frac{|t_p|^{-\alpha_I}}{B_\pm},\quad B_r\text{ and }B_\pm>0 \tag{D9}$$

we find, using (D7),

$$\frac{B_+}{B_-}=\frac{A_-}{A_+}. \tag{D10}$$

The equation connecting t_p and t_v is, following (3.30) and (D9),

$$\frac{dt_v}{dt_p}=\frac{B_r}{B_\pm}|t_p|^{-\alpha_I} \tag{D11}$$

when the right-hand side is much greater than 1. Consequently,

$$t_v=\frac{B_r}{B_\pm}\frac{|t_p|^{-\alpha_I}}{1-\alpha_I}, \tag{D12}$$

and when this is substituted into (D9) we get

$$\frac{1}{B_{\text{liq}}} = \frac{1}{B_r} + \left(\frac{B_r}{1-\alpha_I}\right)^{\alpha_I/(1-\alpha_I)} \frac{|t_v|^{-\alpha_I(1-\alpha_I)}}{B_\pm^{1/(1-\alpha_I)}} . \tag{D13}$$

Invoking the above-mentioned equivalence, the same type of equation also describes the behavior of C_{11} in the isotropic solid. Since B_{sol} only differs from C_{11} by the nonsingular term $-(d-1)\frac{1}{2}C_{44}/d$, (D13) also describes correctly the singular part of B_{sol}. More precisely, we can write

$$B_{\text{sol}} = -b_0 + b_\pm |t_v|^{\alpha_I/(1-\alpha_I)}, \quad b_0 \text{ and } b_\pm > 0 \tag{D14}$$

where

$$b_0 = \frac{d-1}{d}\,\tfrac{1}{2}C_{44} ,$$
$$b_\pm = B_\pm^{1/(1-\alpha_I)}\left(\frac{1-\alpha_I}{B_r}\right)^{\alpha_I/(1-\alpha_I)} . \tag{D15}$$

Note that by (D10), the ratio b_+/b_- is simply connected to the specific-heat ratio A_+/A_- of the incompressible Ising model,

$$\frac{b_\pm}{b_-} = \left(\frac{A_-}{A_+}\right)^{1/(1-\alpha_I)} . \tag{D16}$$

Equation (D14) is valid when the singular part of $1/C_{11}$ is greater than the regular part, which requires $t \ll t_2$, i.e., that the system be governed by R under periodic boundary conditions and fixed V. This is the range of t where Fisher-renormalized Ising exponents are observed.

APPENDIX E: MAXWELL CONSTRUCTION FOR THE FIRST-ORDER TRANSITION IN AN ISOTROPIC SYSTEM

In Sec. IV we calculated a temperature t_3 where $B(t)=0$, as well as a temperature t_∞ where a longitudinal phonon became soft. Both of these are limits of metastability at which the system becomes unstable with regard to arbitrarily small fluctuations. We will now try to estimate where the first-order transition really occurs at fixed P by means of a Maxwell construction applied to the equation of state $P(V)$ in the vicinity of $V_c(T)$ for an isotropic system.

This is a fairly straightforward procedure, since we know how to calculate $B(t)$ down to $t=0$ for the isotropic system by assuming periodic boundary conditions. This calculation could have been extended to the other side of T_c by a technique similar to the one used to obtain the equation of state of the rigid Ising model below T_c.[38] Instead of doing that, we will use the correspondence, established in Appendix D, between the isotropic-solid- and the liquid-Ising models.

We will consider specifically the case of an isotropic system in which the transition takes place in a region of t where Fisher-renormalized behavior is observed [this was called case (a) in Sec. IV A]. The bulk compressibility then has the form

$$B(t) = -b_0 + b_\pm |t_v|^{\alpha_I/(1-\alpha_I)}, \quad b_0 \text{ and } b_\pm > 0 \tag{E1}$$

for sufficiently small t of either sign, where the notation $b_\pm$ here and later refers to $t \gtrless 0$. The values of b_0 and b_+ can be determined from calculations for $t>0$, while the ratio b_+/b_- is related to the specific-heat ratio A_+/A_- of the incompressible Ising model by (D16). That ratio can be determined from various calculations, but we have chosen to take it from experimental data on C_v at the gas-liquid critical point. (Note that C_v and not C_p of the gas-liquid system corresponds to the ideal Ising specific heat.)

The equation of state $P(T,V)$ near $T_c(V)$ can be found by integrating over $B(t)$,

$$P(t) - P(t_0) = -\int_{V_0}^{V} \frac{dV}{V} B \cong -\frac{T_c}{V_c}\frac{dV_c}{dT}\int_{t_0}^{t(V)} B(t)\,dt . \tag{E2}$$

The resulting function $P(V)$ has the characteristic shape shown schematically in Fig. 4. The equal-area rule for the Maxwell construction is

$$0 = \int_{P(t_-)}^{P(t_+)} \frac{V-V_c}{V_c}\,dP \cong -\left(\frac{V}{T_c}\frac{dT_c}{dV}\right)^2 \int_{t_-}^{t_+} B(t)t\,dt , \tag{E3}$$

where t_+ and t_- are a pair of reduced temperatures above and below T_c such that

$$P(t_+) - P(t_-) \propto \int_{t_-}^{t_+} B(t)\,dt = 0. \tag{E4}$$

Equations (E3) and (E4) must be solved to find t_+ and t_-, which characterize the first-order transition.

By carrying out the integrations in (E3) and (E4), we get

$$\tfrac{1}{2}b_0 t_+^2 - \frac{1-\alpha}{2-\alpha} b_+ t_+^{(2-\alpha)/(1-\alpha)} = \tfrac{1}{2}b_0 t_-^2 - \frac{1-\alpha}{2-\alpha} b_- |t_-|^{(2-\alpha)/(1-\alpha)}, \tag{E5}$$

$$b_0 t_+ - (1-\alpha) b_+ t_+^{1/(1-\alpha)} = -\left[b_0 |t_-| - (1-\alpha) b_- |t_-|^{1/(1-\alpha)} \right], \tag{E6}$$

where we have suppressed the index I on α, and will continue to do so in this appendix. By considering the way in which the equal-area rule is applied, it is clear that both sides of (E5) must be negative, and hence that

$$|t_\pm|^{\alpha/(1-\alpha)} > \frac{b_0}{b_\pm}\frac{1-\alpha/2}{1-\alpha}. \tag{E7}$$

Depending on whether $b_+ > b_-$ or $b_+ < b_-$, we also deduce from (E5) that $t_+ < t_-$ or $t_+ > t_-$, and that both sides of (E6) are negative or positive, respectively.

To facilitate the solution of (E5) and (E6), we make the following substitution, which is especially suitable for the case $b_- < b_+$ encountered in practice:

$$|t_\pm|^{\alpha/(1-\alpha)} = \frac{b_0}{b_-}\frac{1-\alpha/2}{1-\alpha}a_\pm. \tag{E8}$$

We thus obtain equations for a_+ and a_-:

$$\left(\frac{a_-}{a_+}\right)^{2(1-\alpha)/\alpha}(1-a_-) = 1 - \frac{b_+}{b_-}a_+, \tag{E9}$$

$$\left(\frac{a_-}{a_+}\right)^{(1-\alpha)/\alpha}\left[1-\left(1-\frac{\alpha}{2}\right)a_-\right] = -\left[1-\left(1-\frac{\alpha}{2}\right)\frac{b_+}{b_-}a_+\right], \tag{E10}$$

which can be solved numerically rather easily by an iterative procedure once it is noted that $(a_-/a_+)^{2(1-\alpha)/\alpha}$ is a very large number even when a_-/a_+ is only moderately large. Using $\alpha = \frac{1}{8}$ and $b_+/b_- = 2.053$ [the last result was obtained from experimental data on the specific heat at the gas-liquid critical point of CO_2, Ref. 39, with the aid of (D16)], we find, for $d=3$,

$$a_- = 1.008, \quad a_+ = 0.749. \tag{E11}$$

These values satisfy (E7) as well as all the other inequalities mentioned after (E7), and lead to the following result:

$$|t_-| \cong 8.05 t_+. \tag{E12}$$

The constant a_ν in (4.32) is therefore given by

$$a_\nu = (t_+ + |t_-|)/t_+ \cong 9. \tag{E13}$$

The reduced temperature t_3 was defined as the positive value of t for which $B(t)=0$. From (E1) and (E8) we see that

$$t_+ = t_3\left(\frac{a_+ b_+}{b_-}\frac{1-\alpha/2}{1-\alpha}\right)^{(1-\alpha)/\alpha} \cong 33 t_3. \tag{E14}$$

Identifying t_+ with the upper transition temperature t_T of Sec. IV A for case (a), we can now calculate the difference between l_T and l_3 for $d=3$,

$$l_T - l_3 = \nu_R \ln\frac{t_3}{t_+} = -\nu_I\frac{1}{\alpha}\ln\left(\frac{a_+ b_+}{b_-}\frac{1-\alpha/2}{1-\alpha}\right) \cong -4\nu_I. \tag{E15}$$

This confirms the assertion made in (4.13).

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