



**HAL**  
open science

## Critical behaviour of compressible Ising models at marginal dimensionalities

M. Vallade, J. Lajzerowicz

► **To cite this version:**

M. Vallade, J. Lajzerowicz. Critical behaviour of compressible Ising models at marginal dimensionalities. *Journal de Physique*, 1979, 40 (6), pp.589-595. 10.1051/jphys:01979004006058900 . jpa-00209143

**HAL Id: jpa-00209143**

**<https://hal.science/jpa-00209143>**

Submitted on 4 Feb 2008

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Classification  
 Physics Abstracts  
 75.40 — 77.80

## Critical behaviour of compressible Ising models at marginal dimensionalities

M. Vallade and J. Lajzerowicz

Université Scientifique et Médicale de Grenoble, Laboratoire de Spectrométrie Physique (\*),  
 B.P. 53, 38041 Grenoble Cedex, France

(Reçu le 8 décembre 1978, accepté le 25 février 1979)

**Résumé.** — Les méthodes du groupe de renormalisation sont appliquées à l'étude du comportement critique du modèle d'Ising compressible à  $n$  composantes avec interaction à courte distance à  $d = 4$  et du modèle d'Ising à une composante avec interactions dipolaires à  $d = 3$ .

Les équations de récurrence sont résolues exactement dans le cas d'un système élastique de symétrie sphérique ( $d = 4$ ) ou de symétrie cylindrique ( $d = 3$ ); de nouveaux types de corrections logarithmiques sont obtenus, correspondant à une renormalisation de Fisher pour la dimension marginale. On montre que le système présente une transition du premier ordre dans des conditions de pression extérieure constante ou quand l'anisotropie est prise en compte. On discute l'intérêt des présents calculs pour l'étude du comportement critique des ferro-électriques uniaxiaux.

**Abstract.** — Renormalization group methods are applied to study the critical behaviour of a compressible  $n$ -component Ising model with short range interactions at  $d = 4$  and a one component Ising model with dipolar interactions at  $d = 3$ .

The recursion equations are exactly solved in the case of an elastic system of spherical symmetry ( $d = 4$ ) or cylindrical symmetry ( $d = 3$ ); new types of logarithmic corrections, corresponding to a Fisher renormalization at marginal dimensions, are found. It is shown that the system exhibits a first-order transition for constant pressure external conditions or when anisotropy is taken into account. The relevance of the calculations to the critical behaviour of uniaxial ferroelectrics is discussed.

1. **Introduction.** — The role of the elastic degrees of freedom in the critical behaviour of the Ising model has been investigated by many authors during the last few years. Most of them agree with the fact that whenever the specific heat of the ideal incompressible system diverges ( $\alpha > 0$ ), the second order phase transition becomes first order when the magneto-elastic coupling is taken into account. This result was found in particular by Rice [1], Domb [2], Mattis and Schultz [3] using different kinds of approximations and by Larkin and Pikin [4] for a Ginzburg-Landau like free energy including the elastic and magneto-elastic energies. More recently, Sak [5] has used renormalization group theory to study the  $n$ -components Ising model coupled to an isotropic elastic continuum at  $d = 4 - \varepsilon$  dimension; he found also that none of the 4 possible fixed points can be reached when  $\alpha > 0$  and concluded that the transition is 1st order. This study was later extended to the case of anisotropic elastic models by de Moura *et al.* [6],

Khmel'nitskii and Shneerson [7] and Bergman and Halperin [8]. These last authors carefully analysed the critical behaviour of the elastic constants and the onset of the 1st order transition and they have shown that a 2nd order transition in a cubic system can be found only for some *pathological* models where the system is unstable under shear deformations (as in the Baker-Essam model [9]). They have shown also that their results remain unchanged whatever the external conditions: constant volume or constant pressure. Although they have thoroughly discussed the instability at  $d = 4 - \varepsilon$  dimension, they did not investigate the case of marginal dimensionalities, either  $d = 4$  for short range forces or  $d = 3$  for dipolar long range interactions. Khmel'nitskii *et al.* [7] considered the anisotropic  $d = 4$  case but without discussing the role of external conditions. As has been shown by Fisher [10], the role of magneto-elastic coupling is a special case of the more general problem of coupling of *hidden degrees of freedom* with the spin variables. This problem has been recently studied by Aharony for the case of dipolar Ising ferromagnets [11].

(\*) Associé au C.N.R.S.

The interest of the marginal case study lies in the fact that the recursion equations can be integrated exactly and that the  $d = 3$  dipolar case corresponds to real physical systems namely uniaxial ferroelectric and ferromagnetic systems, for which the critical and tricritical behaviours have been studied experimentally.

In this paper we investigate the critical behaviour of the compressible Ising model at marginal dimensionalities by solving the recursion equations derived by de Moura *et al.* [6] from a Hamiltonian of the Sak-Larkin type. In part 2 we give an exact solution of these equations for  $d = 4$ , short range interactions and isotropic elastic symmetry. We discuss the influence of the external conditions imposed on the system.

In part 3 we investigate the  $n = 1$ , compressible dipolar Ising system with cylindrical elastic symmetry. In the final part, we conclude by comparing our results with the experimental critical behaviour of uniaxial ferroelectrics.

**2. Compressible Ising system at  $d = 4$ .** — Let us consider a  $n$ -component Ising system coupled to an elastic continuum. The Hamiltonian may be written in the form

$$\mathcal{H} = \mathcal{H}_m + \mathcal{H}_{e1} + \mathcal{H}_{int}$$

where

$$\beta \mathcal{H}_m = \int d^4x \left[ \frac{1}{2} (r |\mathbf{S}|^2 + |\nabla \mathbf{S}|^2) + \tilde{u} |\mathbf{S}|^4 + \dots \right]$$

$$\beta \mathcal{H}_{e1} = \frac{1}{2} \int d^4x \sum_{\alpha\beta\gamma\delta} c_{\alpha\beta\gamma\delta} e_{\alpha\beta}(x) e_{\gamma\delta}(x)$$

$$\beta \mathcal{H}_{int} = \int d^4x |\mathbf{S}(x)|^2 \sum_{\alpha\beta} f_{\alpha\beta} e_{\alpha\beta}(x).$$

The  $e_{\alpha\beta}(x)$  are the local strains,  $c_{\alpha\beta\gamma\delta}$  the elastic constants and  $f_{\alpha\beta}$  the magnetostrictive coefficients. Following de Moura *et al.* [6] one can eliminate the elastic degrees of freedom by integrating  $\mathcal{H}_{e1} + \mathcal{H}_{int}$  and this leads to an effective Hamiltonian :

$$\beta \mathcal{H}_{eff} = \frac{1}{2} \int_{\mathbf{q}} (r + q^2) (\mathbf{S}_{\mathbf{q}} \cdot \mathbf{S}_{-\mathbf{q}}) + \int_{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3, \mathbf{q}_4} \delta(\mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3 + \mathbf{q}_4) [u + v(\mathbf{q}_1 + \mathbf{q}_2)] (\mathbf{S}_{\mathbf{q}_1} \cdot \mathbf{S}_{\mathbf{q}_2}) (\mathbf{S}_{\mathbf{q}_3} \cdot \mathbf{S}_{\mathbf{q}_4}). \quad (1)$$

The values of the constants  $u$  and  $v(\mathbf{q})$  depend on the external conditions imposed on the system. If one takes all the macroscopic strains  $e_{\alpha\beta}^0 = 0$  i.e. if the sample keeps a constant volume and shape, then :

$$u = \tilde{u}$$

$$v(\mathbf{q}) = \begin{cases} -\Delta(\hat{q}) = -\frac{1}{2} \sum_{\alpha\beta\gamma\delta} f_{\alpha\gamma} q_\gamma [A^{-1}(\mathbf{q})]_{\alpha\beta} q_\delta f_{\beta\delta} & \text{if } \mathbf{q} \neq 0 \\ 0 & \text{if } \mathbf{q} = 0 \end{cases}$$

with

$$A_{\alpha\beta}(\mathbf{q}) = \sum_{\gamma\delta} c_{\alpha\gamma\beta\delta} q_\gamma q_\delta.$$

If the system is free to deform itself (zero external pressure), then the integration upon the  $e_{\alpha\beta}^0$  leads to [12] :

$$u = \tilde{u} - \Delta'$$

$$v(\mathbf{q}) = \begin{cases} \Delta' - \Delta(\hat{q}) & \text{if } \mathbf{q} \neq 0 \\ 0 & \text{if } \mathbf{q} = 0 \end{cases}$$

with

$$\Delta' = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} f_{\alpha\beta} [c^{-1}]_{\alpha\beta\gamma\delta} f_{\gamma\delta}.$$

One may note that  $\Delta(\hat{q})$  depends only on the orientation of the vector  $\mathbf{q}$  and that  $\Delta'$  and  $\Delta(\hat{q})$  are non negative.

Let us consider first the isotropic case discussed by Sak [5] for  $d < 4$ . There are only two independent elastic constants  $c_{11}$  and  $c_{44}$  related to the bulk modulus  $K = c_{11} - \frac{3}{4} c_{44}$  and to the shear rigidity

modulus  $\mu = c_{44}$ . The tensor  $f_{\alpha\beta}$  is reduced to its scalar part  $f\delta_{\alpha\beta}$ . Then  $v(\mathbf{q})$  is an angle independent constant  $v$  and the renormalization equations can be written in their differential form :

$$\frac{dr}{dl} \simeq 2r + 4K_4[(n+2)u + 2v](1-r) + \dots$$

$$\frac{du}{dl} \simeq -4K_4[(n+8)u^2 + 12uv + 4v^2] + \dots \quad (2)$$

$$\frac{dv}{dl} \simeq -4K_4[2(n+2)uv + (4+n)v^2] + \dots$$

with

$$K_d^{-1} = 2^{d-1} \pi^{d/2} \Gamma\left(\frac{d}{2}\right).$$

At  $d = 4 - \varepsilon$ , Sak [5] found 4 fixed points noted [13] G, I, R and S which are represented on the figure 1 in the  $(v, u)$  plane. When  $\varepsilon$  goes to zero the

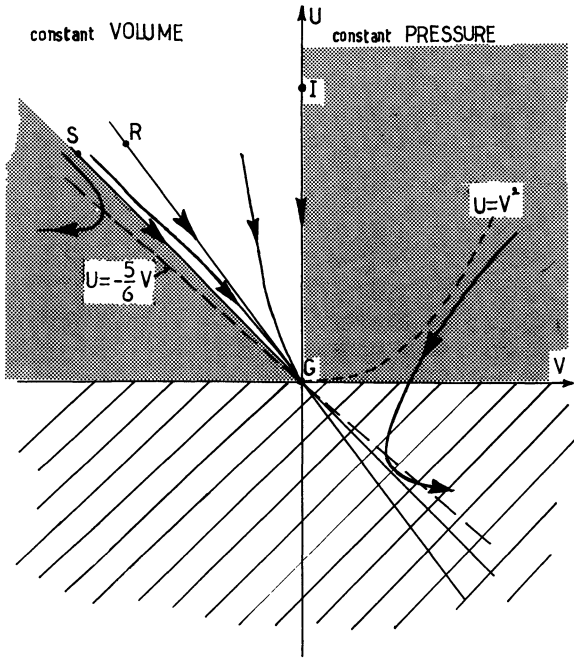


Fig. 1. — Schematic representation of the Hamiltonian flow for the compressible Ising model at  $d = 4, n = 1$  with isotropic elastic properties. (A similar diagram is obtained for the  $U$  and  $V$  parameters in the case of dipolar interactions at  $d = 3$ .) I, R, S and G denote the four fixed points found for  $d = 4 - \epsilon$ ; they merge together at the G point for  $d = 4$ , but the I, R and S lines characterize different critical behaviours. The line  $u = -\frac{5}{6}v$  corresponds to  $dv/du = 0$  (vertical tangents on the trajectories). The half plane  $u < 0$  corresponds to instability in the Landau mean field theory. The shaded areas are the regions for which a 1st order transition is due to the coupling between the fluctuations and the elastic degrees of freedom. The regions  $v < 0$  and  $v > 0$  correspond to a system at constant volume (*pinned boundary conditions*) and under constant pressure respectively. In the latter case a pseudocritical behaviour is expected if the initial values  $u_0$  and  $v_0$  lie near the parabola  $u_0 = v_0^2$  (see § 3 in the text).

3 non trivial fixed points merge into the Gaussian fixed point G but as we shall see later a memory persists of these 3 fixed points in the form of 3 different types of logarithmic corrections. The two last equations in (2) can be exactly integrated by considering the equation for the ratio  $k = u/v$  :

$$\frac{dk}{dl} = -\frac{4-n}{2\pi^2} v(k+1) \left( k + \frac{4}{4-n} \right) \quad (n \neq 4) \tag{3}$$

one can derive easily the relation :

$$\left( k + \frac{4}{4-n} \right)^{\frac{n+8}{4-n}} (k+1)^{-1} = Av \tag{4}$$

where  $A$  is a constant which depends only on initial conditions ( $u_0$  and  $v_0$ ). From (3) and (4) one obtains :

$$\left( k + \frac{4}{4-n} \right) = \left( \frac{u_0}{v_0} + \frac{4}{4-n} \right) \times \left[ 1 + (u_0 + v_0) \frac{n+8}{2\pi^2} l \right]^{-\frac{4-n}{n+8}} \tag{5}$$

From (3) or (5) one sees immediately that if  $v_0 = 0$ ,  $\frac{n-4}{4}u_0$  or  $-u_0$ ,  $k$  is constant and the trajectory in the  $(u, v)$  plane is a straight line. These 3 particular cases correspond to the I, R and S points in the  $\epsilon$  expansion. The dependence of  $u$  and  $v$  on the recursion parameter  $l$  take a simple form in these cases :

$$\begin{aligned} \text{I : } & v = 0, & u &= \frac{2\pi^2}{n+8} \frac{1}{l + \bar{l}_1} \\ \text{R : } & v = -\frac{2\pi^2(4-n)}{n(n+8)} \frac{1}{l + \bar{l}_2}, & u &= -\frac{4}{4-n} v \\ \text{S : } & v = -\frac{2\pi^2}{n} \frac{1}{l + \bar{l}_3}, & u &= -v. \end{aligned} \tag{6}$$

For other initial values of  $v_0$  and  $u_0$ , the explicit form of  $v$  is

$$v = \left[ -\frac{n(n+8)}{2\pi^2(4-n)} l + B \left( 1 + (u_0 + v_0) \frac{n+8}{2\pi^2} l \right)^{\frac{2(n+2)}{n+8}} - C \right]^{-1} \tag{7}$$

with :

$$\begin{aligned} B &= \left( \frac{u_0}{v_0} - \frac{4}{4-n} \right) (u_0 + v_0)^{-1} \\ C &= \frac{n}{4-n} (u_0 + v_0)^{-1}. \end{aligned}$$

The Hamiltonian flow which results from (5) and (7) is depicted schematically in figure 1.

For  $(u_0 + v_0) < 0$  or for  $v_0 > 0$  there is a runaway of the trajectories which corresponds to an instability of the system and to a first order transition.

For  $(u_0 + v_0) > 0$  and  $v_0 < 0$  the trajectories converge towards the R line if  $n < 4$ . One may consider that there is a Fisher renormalization of the critical behaviour [10] due to the coupling with elastic degrees of freedom. The I and S lines separate zones corresponding to 1st order and second order transitions and may thus be considered as characterizing some tricritical behaviour.

One may note that the R line was also found by Aharony for the random Ising model [14] at  $d = 4$  although the recursion equations were quite different. The common feature between the two problems is a modification of the quartic term in the Hamiltonian by some non-critical variables.

The integration of the eq. (2) for  $r(l)$  is easily made and one can deduce the logarithmic corrections for the critical behaviour of various thermodynamic quantities [15]. The results are summarized in table I. One can remark that the specific heat does not diverge in the cases R and S but has only a cusp at the transition point. These results are in agreement with the

Table I. — Critical behaviour of thermodynamics quantities near the Gaussian fixed point for different initial values of the parameters  $u_0$  and  $v_0$ . I ( $v_0 = 0, u_0 > 0$ , « incompressible Ising model »), R ( $0 > v_0 > -u_0, u_0 > 0$ , « Fisher renormalized behaviour ») and S ( $v_0 = -u_0, u_0 > 0$ , « spherical like behaviour »).  $\chi$  is the susceptibility,  $\xi$  the coherence length,  $C_{\text{sing}}$  the singular part of the specific heat,  $M$  the magnetization,  $f$  the magnetostrictive coefficient,  $c_{11}$  an elastic constant. The first 6 lines apply either to  $d = 4$  (short range interactions) or to  $d = 3$  ( $n = 1$  and dipolar interaction). The last 2 lines give relations between critical amplitudes respectively for the  $d = 4$  ( $n < 4$ ) and the  $d = 3$  ( $n = 1$ ) cases ( $t > 0$ ).

	I	R	S
$r(l)$	$e^{2l(l + \bar{l})} \frac{n+2}{n+8}$	$e^{2l(l + \bar{l})} \frac{6}{n+8}$	$e^{2l(l + \bar{l})}^{-1}$
$\chi \sim \xi^2$	$ t ^{-1} \left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{n+2}{n+8}}$	$ t ^{-1} \left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{6}{n+8}}$	$ t ^{-1} \left( \text{Ln} \left  \frac{t_0}{t} \right  \right)$
$C_{\text{sing}}$	$\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{4-n}{n+8}}$	$-\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{n-4}{n+8}}$	$-\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{-1}$
$M$	$ t ^{1/2} \left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{3}{(n+8)}}$	$ t ^{1/2} \left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{n+2}{2(n+8)}}$	$ t ^{1/2}$
$f$	0	$\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{-\frac{6}{n+8}}$	$\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{-1}$
$c_{11}$	constant	$\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{\frac{n-4}{n+8}}$	$\left( \text{Ln} \left  \frac{t_0}{t} \right  \right)^{-1}$
$\frac{\xi^4}{k} C_{\text{sing}} \frac{t^2}{ \text{Ln } t }$	$\frac{n(n+8)}{32 \pi^2 (4-n)}$	$\frac{-n(n+8)}{32 \pi^2 (4-n)}$	$-\frac{n}{32 \pi^2}$
$\xi^2 \xi_{\parallel} \frac{C_{\text{sing}}}{k} \frac{t^2}{ \text{Ln } t }$	$\frac{3}{32 \pi}$	$-\frac{3}{32 \pi}$	$-\frac{1}{32 \pi}$

general results for constrained systems at marginal dimensionality [11].

The behaviour of the coupling constant  $f$  and of the elastic constant  $c_{11}$  are derived from recursion equations similar to those written by Bergman and Halperin [8, 16]. Relations between critical amplitudes [17] of the correlation length and of the singular part of the specific heat are also given.

As has been noted above the initial value of  $u_0$  and  $v_0$  depend on the external conditions applied to the system. For pinned boundary conditions  $u_0 = \tilde{u}_0 > 0$  and  $v_0 = -f^2/2 c_{11} < 0$  so that a 2nd order transition arises for  $u_0 + v_0 \geq 0$  in this case. However, as  $c_{11}$  goes to zero at the transition, anharmonic terms would have to be taken into account. For constant pressure conditions one can show [12] that

$$u_0 = \tilde{u}_0 - \frac{f^2}{2K + 3P}$$

and

$$v_0 = f^2 \left( \frac{1}{2K + 3P} - \frac{1}{2c_{11}} \right)$$

and, for  $P < \mu$ ,  $v_0$  is positive. (For  $P > \mu$  the system is unstable [8].) In this case one expects a 1st order transition. These results are the same as for  $d < 4$  [5], but the reduced temperature  $t^*$  at which the instability

occurs is, in the present case, crucially dependent on the initial values  $u_0$  and  $v_0$ . Roughly speaking, the 1st order transition may be expected for  $l = l^*$  such that  $u(l^*) \sim 0$ , that is for  $|t^*|$  such that (see eq. (5)) :

$$\frac{1}{2} \text{Log} \left| \frac{t_0}{t^*} \right| \sim l^* \sim \frac{2 \pi^2}{(n+8)(u_0 + v_0)} \times \left[ \left( \frac{4-n}{4} \frac{u_0}{v_0} + 1 \right)^{\frac{n+8}{4-n}} - 1 \right] \quad (8)$$

and ( $t^*$ ) is vanishingly small as soon as the right hand side of (8) exceeds a few units, for example when  $v_0 < u_0$  and  $v_0 \lesssim 1$  ( $t_0$  is a non universal parameter  $\simeq 1$  [17]).

In the anisotropic case  $v(\hat{q})$  depends on the direction of  $\mathbf{q}$  relative to the crystallographic axes, but one can show that the fixed point  $v$  must be independent of  $\hat{q}$  [6, 8]. Khmel'nitskii *et al.* [7] discussed the stability of this fixed point at  $d = 4$  and they found that it is never stable since  $\Delta v(\hat{q}) = v(\hat{q}) - \langle v \rangle$  decreases more slowly than  $\langle v \rangle$  for  $n < 4$  (in their notations  $\Gamma(\hat{q})$  corresponds to our  $u + v(\hat{q})$ ). As a criterion for the onset of the instability they give  $|\Delta v_{\text{max}}(\hat{q})| \simeq u_l + \langle v_l \rangle$ . When all  $v(\hat{q})$  are negative (constant volume) this condition is always fulfilled for a finite  $l = l^*$ . However when all  $v_0(\hat{q})$  are positive

(this is probably the case for constant pressure) the recursion equation for  $v(\hat{q})$  :

$$\frac{dv(\hat{q})}{dl} = -4 K_4 v(\hat{q}) [2(n+2)u + 4\langle v \rangle + nv(\hat{q})] \quad (9)$$

indicates that all  $v_i(\hat{q})$  decrease towards zero as long as  $u_i > 0$  so that an instability occurs first for  $u_i \simeq 0$ . If this condition arises for

$$\langle v_i \rangle^2 \gg \langle \Delta v_i^2 \rangle \quad (\text{i.e. for } \langle v^2 \rangle \simeq \langle v \rangle^2)$$

the criterion for the instability is the same as in the isotropic case (eq. (8)) (with  $\langle v_0 \rangle$  in the place of  $v_0$ ). This may happen for large  $\langle v_0 \rangle/u_0$  and small anisotropy.

In the other cases, anisotropy is important for determining the temperature of the first-order transition.

**3. Compressible Ising model with dipolar interactions at  $d = 3$ .** — We investigate only the case  $n = 1$ . The effective Hamiltonian is essentially the same as in the  $d = 4$  case except that  $(r + q^2)$  is changed into  $(r + q^2 + g \frac{q_z^2}{q^2})$ .

In order to be consistent with the uniaxial character of the dipolar coupling, we consider a system with cylindrical anisotropy for  $v(\hat{q})$ , that is  $v$  depends only on the variable  $\cos \theta = q_z/q$ . In practice, crystals of hexagonal symmetry are of this type. The renormalization equations are in this case :

$$\begin{aligned} \frac{dr}{dl} &\simeq 2r + 4K_3[3uI_{01}(r, g) + 2I_{11}(r, g)] \\ \frac{dg}{dl} &\simeq 2g \\ \frac{du}{dl} &\simeq u - 4K_3[9u^2I_{02}(0, g) + 12uI_{12}(0, g) + 4I_{22}(0, g)] \\ \frac{dv(\theta)}{dl} &\simeq v(\theta) - 4K_3[6uv(\theta)I_{02}(0, g) + 4v(\theta)I_{12}(0, g) + v^2(\theta)I_{02}(0, g)] \quad (10) \end{aligned}$$

where

$$I_{nm}(r, g) = \int_0^\pi \frac{\sin \theta v^n(\theta)}{(1+r+g \cos^2 \theta)^m} d\theta \cdot 2\pi$$

and

$$K_3 = \frac{1}{2\pi^2}.$$

As  $g \sim e^{2l}$  becomes very large when  $l$  grows, one

may easily see that  $\theta = \pi/2$  gives the largest contribution in  $I_{nm}(r, g)$  and one gets

$$I_{nm}(0, g) \simeq v^n\left(\frac{\pi}{2}\right) \cdot \frac{\pi}{2mg^{1/2}} + o(g^{-1}) \quad m = 1, 2.$$

As usual [18], we define new parameters  $U = u/\sqrt{g}$  and  $V = v/\sqrt{g}$ , and the recursion equations for  $U$  and  $V(\pi/2)$  are exactly the same as for  $u$  and  $v$  in the  $d = 4$  case (except for the change  $K_4 \rightarrow K_3 \frac{\pi}{4\sqrt{g_0}}$ ).

Thus, the conclusions are identical to those derived in paragraph 2. Nevertheless one must check that an instability does not occur because of a divergence of  $V(\theta)$  for a  $\theta \neq \pi/2$ . The differential equation for  $V(\theta)$  is for large  $l$  :

$$\frac{dV(\theta)}{dl} = -\frac{V(\theta)}{2\pi\sqrt{g_0}} \left(6U + 4V\left(\frac{\pi}{2}\right) + V(\theta)\right). \quad (11)$$

This equation can be integrated exactly knowing the asymptotic form of  $U_l$  and  $V_l(\pi/2)$  and one arrives at the conclusion that  $|V_l(\theta)|$  goes to zero only if :

$$V_0\left(\frac{\pi}{2}\right) < V_0(\theta) < 0. \quad (12)$$

As in the isotropic case, one can show that the sign of  $V_0(\theta)$  depends on external conditions (see appendix I). For constant volume conditions,

$$v_0(\theta) = -\Delta_0(\theta) < 0.$$

The condition (12) can be fulfilled if  $\Delta_0(\theta)$  is maximum for  $\theta = \pi/2$  and a second order transition is then possible.

This result seems to contradict the general statement relative to the anisotropy [6, 7]. It is a consequence of the large anisotropy in the Green function for large  $l$  ( $g_l \cos^2 \theta \gg 1$ , when  $\theta \neq \pi/2$ ).

For constant pressure conditions,  $v_0(\theta) = \Delta'_0 - \Delta_0(\theta)$  is positive. An analysis similar to that of paragraph 2 (eq. (8)) shows that a first order transition occurs for :

$$l^* \simeq \frac{2\pi\sqrt{g_0}}{9(u_0 + v_0(\pi/2))} \left[ \left( \frac{3}{4} \frac{u_0}{v_0(\pi/2)} + 1 \right)^3 - 1 \right]. \quad (13)$$

The discussion about the role of the anisotropy in the  $(x, y)$  plane is similar to that developed in the case  $d = 4$  (§ 2).

**4. Discussion.** — The principal motivation of the above calculations was to compare the predictions of renormalization group theory with the observed critical and tricritical behaviour of uniaxial ferroelectric (or ferromagnetic) crystals. It is well known that 2nd order phase transitions are found in some of these

compounds either at room pressure (TGS [19], RbDP [20], LiTbF<sub>4</sub> [21]) or under high pressure (KDP [22], SbSI [23]). The experiments being generally performed at constant external pressure, this seems to contradict the above theoretical results. One might argue that the 1st order discontinuity is unobservable because the compressibility of these materials is weak. This point has to be examined more carefully : actually, if one attempts to evaluate the importance of the electrostrictive coupling through the ratio  $\langle v_0(\pi/2) \rangle / u_0$  (where the brackets mean an average in the plane perpendicular to the ferroelectric axis), one gets [24, 25]

$$\frac{\langle v_0(\pi/2) \rangle}{u_0} = \frac{\Delta'_0 - \langle \Delta_0(\pi/2) \rangle}{u_0} \sim 0.4$$

for TGS,  $\sim -2$  for KDP and  $\sim -10$  for SbSI (at ambient pressure). In the two last cases the ratio is negative since the transition is first order and  $u_0$ , which is taken proportional to the quartic term of the Landau free energy, is negative ; under pressure this coefficient becomes positive, so that a point exists where  $\langle v_0(\pi/2) \rangle / u_0$  diverges. Considering these orders of magnitude one can conclude that the influence of compressibility is not negligible, especially in the vicinity of a tricritical point, since it greatly affects the  $S^4$  terms in the Hamiltonian.

Nevertheless eq. (13) indicates that even if anisotropy is small  $\langle v_0(\pi/2) \rangle / u_0$  is not the only relevant parameters in determining the first order transition temperature, but that  $(u_0 + \langle v_0(\pi/2) \rangle) / \sqrt{g_0}$  must also be taken into account. The coefficient  $g_0$  can be estimated from the following expression of the susceptibility :

$$\chi^{-1}(T, \mathbf{q}) = \frac{4\pi}{C} \left[ (T - T_c) + \left( \frac{J}{k} \right) (qa)^2 + \frac{C}{\varepsilon_L} \frac{q_z^2}{q^2} \right] \sim \sim \left( r_0 + q^2 + g_0 \frac{q_z^2}{q^2} \right),$$

where  $C$  is the Curie constant,  $J$  the interaction energy and  $\varepsilon_L$  the non-divergent « lattice » contribution to the dielectric constant.  $J/k$  can be obtained from X-ray or neutron critical scattering data and is found to be  $\simeq 120$  K in TGS [26] and  $\simeq 10$  K in KD<sub>2</sub>PO<sub>4</sub> [27]. Hence one gets

$$g_0 = \frac{C}{\varepsilon_L} \frac{k}{J} \sim 4$$

for TGS and  $\simeq 34$  for KH<sub>2</sub>PO<sub>4</sub> (taking the value of  $J$  relative to KD<sub>2</sub>PO<sub>4</sub>).  $u_0$  is given approximately by [18]  $(bP_s^4 v / 4 k T_c) (k T_c / J)^2$  where  $bP_s^4 / 4$  is the usual quartic term in the Landau expansion of the free energy, and  $v$  is the volume of the unit cell. Using published values [24], one gets  $u_0 \simeq 0.2$  for TGS so that, using eq. (13)

$$\frac{1}{2} \text{Log} \left| \frac{t_0}{t^*} \right| \sim l^* \sim 30.$$

This would explain why the observed critical behaviour [28] in this crystal looks like that of an incompressible dipolar Ising system and would justify the hypothesis recently made by Nattermann [29]. However the anisotropy in  $v_0(\pi/2, \varphi)$  is not small in this material since

$$\frac{f_3^2}{c_{33}} \simeq 5 \frac{f_1^2}{c_{11}}$$

and it is possible that it leads to a  $t^*/t_0$  significantly larger than the preceding value. More accurate data would be necessary for a detailed numerical comparison. In the case of KDP,  $u_0$  becomes very small under pressure and eq. (13) leads then to :

$$l^* \sim \frac{\pi}{4} \frac{\sqrt{g_0} u_0}{\langle v_0(\pi/2) \rangle^2} = \frac{\pi}{4} \frac{U_0}{\langle V_0(\pi/2) \rangle^2}.$$

One expects that the 1st order character begins to become *unobservable* when  $l^* \gtrsim 1$  that is for values of  $U_0$  and  $\langle V_0(\pi/2) \rangle$  near the parabola  $U_0 = \langle V_0(\pi/2) \rangle^2$  (see Fig. 1).

For KDP one thus expects that a *pseudo-tricritical* transition will arise for  $u_0 \simeq 0.3$  and not for  $u_0 = 0$  as in mean field theory.

Nevertheless, the pseudo-tricritical behaviour will be well described by mean field theory since the transition takes place for small  $l$  values. For higher  $u_0$  (i.e. higher pressure), a 2nd order-like transition characteristic of the incompressible model is again expected [20]. Recent experiments [31] indeed seem to confirm that the tricritical-like behaviour is well described by a classical Landau expansion with the coefficient of the quartic term varying linearly with temperature and pressure.

It would be interesting to compare these constant pressure experiments with the behaviour of a sample with *pinned boundary conditions* ; unfortunately, such a situation can be achieved only with a crystal embodied in a perfectly rigid matrix, and in this case it is probably difficult to perform accurate experiments.

To conclude we have solved exactly the renormalization group equations for the Sak-Larkin-Pikin model Hamiltonian in the case of an isotropic elastic system at  $d = 4$  and of the dipolar Ising model with cylindrical anisotropy at  $d = 3$ . The results are essentially the same as those obtained in the  $d = 4 - \varepsilon$  case. A *Fisher renormalized* behaviour with logarithmic corrections different from those of the incompressible system is found for certain initial values of the parameter  $v_0$  ( $0 > v_0 > -u_0$ ) which can be physically attained only for *pinned boundary conditions*. In the case of constant external pressure ( $v_0 > 0$ ) or when anisotropy is present a 1st order transition is always expected.

However a criterion for the *observability* of the 1st order discontinuity shows that the transition looks like a continuous one even for strong electrostrictive

coupling in ferroelectrics; in this case the apparent behaviour must be very similar to that of the incompressible system (without Fisher renormalization).

The «pseudo»-tricritical behaviour experimentally encountered may be identified with the limit of observability of the 1st order transition.

**Appendix I.** — In the particular case of cylindrical symmetry one has

$$\Delta' = \frac{1}{2} \left( \frac{f_1^2 c_{33} - 2 f_1 f_3 c_{13} + f_3^2 c_1}{c_1 c_{33} - c_{13}^2} \right)$$

and

$$\Delta(\theta) = \frac{1}{2} \left[ \frac{f_1^2 \sin^2 \theta (c_{33} \cos^2 \theta + c_{44} \sin^2 \theta) - 2 f_1 f_3 (c_{13} + c_{44}) \sin^2 \theta \cos^2 \theta + f_3^2 \cos^2 \theta (c_1 \sin^2 \theta + c_{44} \cos^2 \theta)}{(c_1 \sin^2 \theta + c_{44} \cos^2 \theta) (c_{33} \cos^2 \theta + c_{44} \sin^2 \theta) - (c_{13} + c_{44})^2 \sin^2 \theta \cos^2 \theta} \right]$$

where

$$c_1 = \frac{c_{11} + c_{12}}{2}.$$

Elastic stability conditions require the denominator of  $\Delta'$  and of  $\Delta(\theta)$  to be positive; one may easily check that this implies that both these quantities must be non-negative. One may also note that  $\Delta(\theta)$  reduces to  $\Delta'$  when  $c_{44} = 0$ , as in the isotropic case, and one obtains :

$$v(\theta) = \Delta' - \Delta(\theta) = \frac{c_{44} [f_1 (c_{33} \cos^2 \theta - c_{13} \sin^2 \theta) + f_3 (c_1 \sin^2 \theta - c_{13} \cos^2 \theta)]^2}{2 D' D(\theta)}$$

where  $D'$  and  $D(\theta)$  are the denominators of  $\Delta'$  and  $\Delta(\theta)$  respectively.

One can thus conclude that  $v(\theta) \geq 0$  as in the isotropic case.

One may conjecture that  $v(\hat{q})$  is positive in the general anisotropic problem, although a direct proof of this does not seem to be an easy task !

## References

- [1] RICE, O. K., *J. Chem. Phys.* **22** (1954) 1535.
- [2] DOMB, C., *J. Chem. Phys.* **24** (1956) 783.
- [3] MATTIS, D. C. and SCHULTZ, T. D., *Phys. Rev.* **129** (1963) 175.
- [4] LARKIN, A. J. and PIKIN, S. A., *Sov. Phys. JETP* **29** (1969) 891.
- [5] SAK, J., *Phys. Rev. B* **10** (1974) 3957.
- [6] DE MOURA, M. A., LUBENSKY, T. L., IMRY, Y. and AHARONY, A., *Phys. Rev. B* **13** (1976) 2176.
- [7] KHMEL'NITSKII, D. E. and SHNEERSON, V. L., *Sov. Phys. JETP* **42** (1976) 560.
- [8] BERGMAN, D. J. and HALPERIN, B. I., *Phys. Rev. B* **13** (1976) 2145.
- [9] BAKER, G. A. Jr., and ESSAM, J. W., *Phys. Rev. Lett.* **24** (1970) 447.
- [10] FISHER, M. E., *Phys. Rev.* **176** (1968) 257.
- [11] AHARONY, A., *J. Mag. Materials* **7** (1978) 215.
- [12] IMRY, Y., *Phys. Rev. Lett.* **33** (1974) 1304.
- [13] RUDNICK, J., BERGMAN, D. J. and IMRY, Y., *Phys. Lett. A* **46** (1974) 449.
- [14] AHARONY, A., *Phys. Rev. B* **13** (1976) 2092.
- [15] WEGNER, F. J. and RIEDEL, E. K., *Phys. Rev. B* **7** (1973) 248.
- [16] See also :  
LYUKSTYUKOV, I. F., *Sov. Phys. JETP* **46** (1978) 383.
- [17] AHARONY, A. and HALPERIN, B. I., *Phys. Rev. Lett.* **35** (1975) 1308.
- [18] AHARONY, A., *Phys. Rev. B* **8** (1973) 3363 and **9** (1974) 3946 (E).
- [19] NAKAMURA, E., NAGAI, T., ISHIDA, K., ITOH, K. and MITSUI, T., *J. Phys. Soc. Japan* **28** (1970) suppl. 271.
- CAMNASIO, A. J. and GONZALO, J. A., *J. Phys. Soc. Japan* **39** (1975) 451.
- [20] BASTIE, P., LAJZEROWICZ, J., SCHNEIDER, J. R., *J. Phys. C. Solid State Phys.* **11** (1978) 1203.
- [21] ALS-NIELSEN, J., HOLMES, L. M. and GUGGENHEIM, H. J., *Phys. Rev. Lett.* **32** (1974) 610.
- ALHERS, G., KORNBLOT, A. and GUGGENHEIM, H. J., *Phys. Rev. Lett.* **34** (1975) 1227.
- [22] SCHMIDT, V. H., WESTERN, A. B., BAKER, A. G., *Phys. Rev. Lett.* **37** (1976) 839.
- BASTIE, P., VALLADE, M., VETTER, C. and ZEYEN, C., *Phys. Rev. Lett.* **40** (1978) 337.
- [23] PEERCY, P. S., *Phys. Rev. Lett.* **35** (1975) 1581.
- [24] LANDOLT-BORNSTEIN, groupe III, vol. 3, *Ferro and antiferroelectric substances* (Springer Verlag, Berlin, Heidelberg, New York) 1969.
- [25] The elastic constants of TGS are found in a paper by KONSTANTINOVA, V. P., SIL'VESTROVA, I. M. and ALEKSANDROV, K. S., *Sov. Phys. Crystallogr.* **4** (1959) 63.
- [26] FUJII, Y. and YAMADA, Y., *J. Phys. Soc. Japan* **30** (1971) 1676.
- [27] PAUL, G. L., COCHRAN, W., BUYERS, W. J. L. and COWLEY, R. A., *Phys. Rev. B* **2** (1970) 4603.
- [28] EHSES, K. H. and MUSER, H. E., *Ferroelectrics* **12** (1976) 247.
- [29] NATTERMANN, T., *Phys. Status Solidi* (b) **85** (1978) 291.
- [30] In the case of KDP, one must also remember that it is a ferroelectric-ferroelastic crystal since a linear coupling exists between a shear strain and the polarization. For such a ferroelastic transition the marginal dimensionality is less than 3 and the critical behaviour is expected to be purely classical for  $d = 3$ . (See for example FOLK, R., IRO, H. and SCHWABL, F., *Phys. Lett.* **57a** (1976) 112 and COWLEY, R. A., *Phys. Rev. B* **13** (1976) 4877.)
- [31] BASTIE, P., VALLADE, M., VETTER, C., ZEYEN, C. and MEISTER, H., To be published.