CHANGES OF ELASTIC CONSTANTS IN STRUCTURAL PHASE TRANSITIONS. II. ELASTIC PHASE TRANSITIONS

By K. Parliński

Institute of Nuclear Physics, Cracow*

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In the framework of the Landau phenomenological theory the behaviour of the elastic constants associated with all elastic structural phase transitions induced by a one-dimensional irreducible representation of the high symmetry point group, are found. A dimensional analysis has established that the critical behaviour of the elastic constants is correctly described by the phenomenological theory.

1. Introduction

In the previous paper [1], further referred to as I, the general expansion of the free energy of the crystal (I-7) in the vicinity of the structural phase transition point was given. In this approach the state of a crystal is specified by the temperature T and the components of the normal strain S_α. The crystal is stable if all normal effective elastic constants are positive. If one normal elastic constant vanishes at a given temperature then the crystal becomes mechanically unstable and undergoes an elastic phase transition. This occurs either as a result of the vanishing of the normal elastic constant itself or as a result of soft behaviour of a normal mode that has the same symmetry as one of the components of the normal strain S_α.

All elastic phase transitions are equi-translational, which means that they are not accompanied by an enlargement of the unit cell; therefore the active normal mode which causes the symmetry reduction is always labelled by the wave vector $k = 0$. The elastic phase transitions have been listed by Aubry and Pick [2], who have also shown that the soft modes which induce the elastic phase transitions are always Raman active in the high and low symmetry phases. If the soft mode in the high symmetry phase is not Raman active then the phase transition is non-elastic. An example of the elastic phase transition is KH_2PO_4, which lowers its symmetry at 122 K from tetragonal ($I\bar{4}2d$) (point group $\bar{4}2m$) to orthorhombic ($Fdd2$) (point group $mm2$) by B_2 irreducible representation at $k = 0$ [3, 4].

* Address: Instytut Fizyki Jądrowej, Radzikowskiego 152, 31-342 Kraków, Poland.

In comparison with the non-elastic phase transitions [1], owing to the highly anisotropic nature of critical fluctuations, the elastic phase transitions exhibit completely different critical behaviour. It is well-known that a normal strain (except for a totally symmetric one) is related to a transverse elastic wave propagating in the crystal. Moreover, a softening of an effective normal elastic constant corresponds to a softening of specific elastic modes which propagate either along a definite direction (one-dimensional critical fluctuations) or in a definite plane (two-dimensional critical fluctuations). Such low dimensionality of critical fluctuations suppresses the critical behaviour to such a degree that the classical phenomenological theory gives a correct description for those elastic phase transitions which have a one-component order parameter.

Below, we shall confine the discussion to such elastic phase transitions which are induced by one-dimensional active irreducible representations of the high symmetry phase. Then, we consider the changes of the elastic constants in the vicinity of the phase transition and prove that the influence of different strain components on the critical behaviour of a given phase transition is inessential.

2. *The phenomenological theory*

The free energy (I-7) of a crystal in the vicinity of the elastic phase transition point written in terms of fluctuations at the absence of stress has a form

$$F = F(F, \{S_\alpha\}) + \tfrac{1}{2}\sum_{\alpha\beta} \tilde{c}_{\alpha\beta} s_\alpha s_\beta + \tfrac{1}{6}\sum_{\alpha\beta\gamma} \tilde{c}_{\alpha\beta\gamma} s_\alpha s_\beta s_\gamma + \ldots, \tag{1}$$

where

$$\tilde{c}_{\alpha\beta\gamma} = c_{\alpha\beta\gamma} - 3\sum_{j_c j_c'} K_{\alpha\beta}(j_c) M(j_c, j_c') N_\gamma(0, j_c')$$

$$-3 \sum_{\substack{j_c j_c' \\ j_c'' j_c'''}} N_\beta(0, j_c) M(j_c, j_c') L_\alpha(0, j_c', j_c'') M(j_c'', j_c''') N_\gamma(0, j_c'''),$$

and $M(j, j')$ stands for $M(^{00}_{jj'})$ in (I-11). This form arises if one introduces into (I-7) the effective elastic constants (I-14, 15) and substitutes the q_{kj} variable by a new variable t_{kj} according to (I-10). The mixed third order terms $s_\alpha s_\beta t_{0j}$ and $s_\alpha t_{0j} t_{0j'}$ have been omitted as not essential in the following discussion. Since, the considerations are confined to the case when the active normal mode transforms according to a one-dimensional irreducible representation, the third-order invariant vanishes i.e. $\tilde{c}_{\alpha\alpha\alpha} = 0$.

The phase transition is elastic when at least one coefficient $U_\alpha(j_c)$ (see I-5) of the linear coupling between the normal strain and the active normal mode does not vanish. It happens when Γ_α — the associated irreducible representation of the normal strain is the same as Γ_{0j_c} — the irreducible representation of the active normal mode. In this case the equilibrium equation (I-12) can be approximately solved in the vicinity of the critical temperature. Neglecting the square terms, we find for non-zero components of $U_\alpha(j_c)$

$$c_\alpha S_\alpha + U_\alpha(j_c) Q_{0j_c} = 0, \tag{2}$$

and for the remaining components

$$c_\beta S_\beta = 0. \tag{3}$$

Thus, in the high symmetry phase $S_\alpha = Q_{0,j_c} = 0$ and the effective elastic constants are given by

$$\tilde{c}_{\alpha\alpha} = c_\alpha - \lambda_{0j_c}^{-1}(T)\,[U_\alpha(j_c)]^2. \tag{4}$$

The bare elastic constant c_α and the coefficient $[U_\alpha(j_c)]^2$ are positive and do not depend on temperature. On the other hand, the $\lambda_{0j_c}(T)$ is a linear function of temperature. Thus, the temperature of the elastic phase transition is defined by the condition $\tilde{c}_{\alpha\alpha}(T_{ce}) = 0$ for the active and effective elastic constant. Such transition can be initiated by the active soft mode for which the value $\lambda_{0j_c}(T)$ decreases when the transition temperature is approached from the high symmetry phase side. At T_{ce} the $\lambda_{0j_c}(T_{ce})$ remains still finite and positive. Above T_{ce}, the function $R(0, j_c, T)$ which stands for $R\binom{0\;0}{j_c j_c}$ in (I-19) can be simplified into the following form

$$R(0, j_c, T) = \lambda_{0j_c}(T) > 0. \tag{5}$$

In the low symmetry phase, according to (3), the static normal strains S_α which do not transform according to the active irreducible representation can be neglected. Hence,

$$\sum_{\alpha\beta} K_{\alpha\beta}(j_c) S_\alpha S_\beta = 0, \tag{6}$$

since $K_{\alpha\alpha}(j_c) = 0$ for active Γ_α. Furthermore, the expression $\sum_\alpha L_\alpha(0, j_c, j_c) S_\alpha$ vanishes since the non-zero components of $L_\alpha(0, j_c, j_c)$ are associated with the totally symmetric representation whereas the leading term in strain S_α belongs to active Γ_α. In the approximation, when $c_\alpha - \lambda_{0j_c}^{-1}[U_\alpha(j_c)]^2 > 0$, one finds

$$Q_{0j_c} = \pm\left\{-6B^{-1}\begin{pmatrix}0\\ j_c\end{pmatrix}[\lambda_{0j_c}(T) - c_\alpha^{-1}[U_\alpha(j_c)]^2]\right\}^{1/2} \sim |T - T_{ce}|^{1/2}, \tag{7}$$

and

$$S_\alpha = -c_\alpha^{-1} U_\alpha(j_c) Q_{0jc} \sim |T - T_{ce}|^{1/2}, \tag{8}$$

and from (I-13)

$$R(0, j_c, T) = -2[\lambda_{0jc}(T) - c_\alpha^{-1}[U_\alpha(j_c)]^2] + c_\alpha^{-1}[U_\alpha(j_c)]^2 > 0. \tag{9}$$

Quantity $R(0, j_c, T)$ as a function of temperature is twice as steep in the low as in the high symmetry phase. At T_{ce}, it has a finite positive value. The $R(0, j_c, T)$ may represent the square of the energy of the soft optic phonon at $\boldsymbol{k} = 0$. From (I-8) and (I-11), we find also that

$$N_\alpha(0, j_c) = U_\alpha(j_c), \quad M(0, j_c) = R^{-1}(0, j_c). \tag{10}$$

The effective elastic constants can be calculated on the basis of the formula (I-15). The symmetries of the tensors $U_i(j_c)$, $K_{ij}(j_c)$ and $L_i(0, j_c, j_c)$ have been found by the method described in I. The non-zero components of the third order elastic constants are listed in [5]. In Table I the tensor of the effective elastic constants, the high G and low F symmetry

TABLE I

Tensors of elastic constants in a vicinity of equi-translational elastic phase transitions induced by one-dimensional irreducible representations

	c_{il}						G	Γ_{0j_c}	F
Monoclinic	A	F	D	a	I	d	$2/m$ $(m \perp Y)$	B_g	1
		E	G	b	J	e	m $(m \perp Y)$	A''	1
			C	c	M	f	2 $(2 \parallel Y)$	B	1
				u	g	v			
					H	h			
						w	$V_4 = V_6 = 0$		
Orthorhombic	A	F	D	0	0	d	mmm	B_{1g}	$2/m$ $(m \perp Z)$
		E	G	0	0	e	$mm2$	A_2	2 $(2 \parallel Z)$
			C	0	0	f	222	B_1	2 $(2 \parallel Z)$
				b_{44}	p	0			
					b_{55}	0			
						w	$V_4 = V_5 = V_6 = 0$		
Tetragonal I	N	T	V	0	0	r	$4/m$	B_g	$2/m$ $(2 \parallel Z)$
		P	W	0	0	s	$\bar{4}$	B	2 $(2 \parallel Z)$
			S	0	0	t	4	B	2 $(2 \parallel Z)$
				m	p	0			
					n	0			
						w	$V_1 = V_2$, $V_4 = V_5 = V_6 = 0$		
Tetragonal II	A	B	D	0	0	d	$4/mmm$	B_{2g}	mmm
		A	D	0	0	d	$\bar{4}2m$	B_2	$mm2$
			C	0	0	f	422	B_2	222
				b_{44}	p	0	$4mm$	B_2	$mm2$
					b_{44}	0			
						w	$V_1 = V_2$, $V_4 = V_5 = V_6 = 0$		
Tetragonal III	N	T	V	0	0	0	$4/mmm$	B_{1g}	mmm
		P	W	0	0	0	$\bar{4}2m$	B_1	222
			S	0	0	0	422	B_1	222
				m	0	0	$4mm$	B_1	$mm2$
					n	0			
						b_{66}	$V_1 = V_2$, $V_4 = V_5 = V_6 = 0$		

point groups, the symmetry of the active normal mode and the restrictions imposed on the strain components V_n (I-17), are listed. The abbreviations are summarized in Table II. The tensors in the high and low symmetry phases are written in the conventional coordinate

TABLE II

Summary of abbreviations

$R = R(0, j_c, T)$	$L_i = L_i(0, j_c, j_c)$
$Q = Q_{0j_c}$	$K_{il} = K_{il(j_c)}$
$U_i = U_i(j_c)$	$b_{il} = c_{il} + \sum_{j=1}^{6} c_{ilj}V_j$
$A = b_{11} - L_1^2Q^2R^{-1}$	$a = K_{14}Q - L_1U_4QR^{-1}$
$B = b_{12} - L_1^2Q^2R^{-1}$	$b = K_{24}Q - L_2U_4QR^{-1}$
$C = b_{33} - L_3^2Q^2R^{-1}$	$c = K_{34}Q - L_3U_4QR^{-1}$
$D = b_{13} - L_1L_3Q^2R^{-1}$	$d = K_{16}Q - L_1U_6QR^{-1}$
$E = b_{22} - L_2^2Q^2R^{-1}$	$e = K_{26}Q - L_2U_6QR^{-1}$
$F = b_{12} - L_1L_2Q^2R^{-1}$	$f = K_{36}Q - L_3U_6QR^{-1}$
$G = b_{23} - L_2L_3Q^2R^{-1}$	$g = K_{45}Q - L_5U_4QR^{-1}$
$H = b_{55} - L_5^2Q^2R^{-1}$	$h = K_{56}Q - L_5U_6QR^{-1}$
$I = b_{15} - L_1L_5Q^2R^{-1}$	$m = b_{44} + K_{44}Q$
$J = b_{25} - L_2L_5Q^2R^{-1}$	$n = b_{44} - K_{44}Q$
$M = b_{35} - L_3L_5Q^2R^{-1}$	$p = K_{45}Q$
$N = b_{11} + K_{11}Q - (L_1Q + U_1)^2R^{-1}$	$r = b_{16} + K_{16}Q - (L_1Q + U_1)U_6R^{-1}$
$P = b_{11} - K_{11}Q - (L_1Q - U_1)^2R^{-1}$	$s = -b_{16} + K_{16}Q - (L_1Q - U_1)U_6R^{-1}$
$S = b_{33} - L_3^2Q^2R^{-1}$	$t = K_{36}Q - L_3U_6QR^{-1}$
$T = b_{12} - (L_1^2Q^2 - U_1^2)R^{-1}$	$u = b_{44} - U_4^2R^{-1}$
$V = b_{13} + K_{13}Q - (L_1Q + U_1)L_3QR^{-1}$	$v = b_{46} - U_4U_6R^{-1}$
$W = b_{13} - K_{13}Q - (L_1Q - U_1)L_3QR^{-1}$	$w = b_{66} - U_6^2R^{-1}$

systems with one exception, namely, the tensors for *mmm*, *mm*2, 222 and *mm*2 point groups appearing as a result of symmetry lowering of 4/*mmm*, $\bar{4}2m$, 422, 4*mm* point groups by B_{2g}, B_2, B_2 and B_2 irreducible representations, respectively, are turned around z axis by 45° with respect to the orthorhombic conventional coordinate system. For the elastic phase transitions listed in Table I the difference $c_{11}-c_{12}$ remains constant. Also, all effective elastic constants are continuous functions of temperature. Their temperature dependence can be easily deduced from the relations (5)–(9).

3. *Critical fluctuations*

The critical behaviour of the order parameter of the elastic phase transition was studied by Folk, Iro and Schwabl [6]. Below, we discuss the influence of other strain components on the critical fluctuations of the soft normal strain. We write down the local free energy density in terms of the long-wavelength strains. Making use of (1), and writting down the coefficients in Cartesian axes notation one finds in the hydrodynamic limit

$$F = F_0 + \tfrac{1}{2}\int d^dx \sum_{ijkl} \tilde{c}_{ijkl} v_{ij}(\boldsymbol{x}) v_{kl}(\boldsymbol{x}) + \tfrac{1}{6}\int d^dx \sum_{ijklpq} \tilde{c}_{ijklpq} v_{ij}(\boldsymbol{x}) v_{kl}(\boldsymbol{x}) v_{pq}(\boldsymbol{x}) + \dots \tag{11}$$

where $i = x, y, z$ and d denotes the dimensionality of the space. We denote

$$v_{ij}(x) = \sum_{k\alpha} \sigma_{ij}(\alpha) \exp(i\boldsymbol{k}\cdot\boldsymbol{x}) s_\alpha(\boldsymbol{k}), \tag{12}$$

where $s_\alpha(\boldsymbol{k})$ is the Fourier component of the normal strain characterized by the wave vector $\boldsymbol{k}$. The local strain is related to the local displacement vector

$$u_i(\boldsymbol{x}) = \sum_{\boldsymbol{k}\varrho} e_i(\boldsymbol{k}, \varrho) \exp(i\boldsymbol{k} \cdot \boldsymbol{x}) u_{\boldsymbol{k}\varrho} \tag{13}$$

via

$$v_{ij}(\boldsymbol{x}) = \tfrac{1}{2}\left(\frac{\partial u_i(\boldsymbol{x})}{\partial x_j} + \frac{\partial u_j(\boldsymbol{x})}{\partial x_i}\right). \tag{14}$$

The orthonormalized eigenvectors $e_i(\boldsymbol{k}, \varrho)$ and corresponding eigenvalues $\tilde{c}_\varrho(\boldsymbol{k})$ of elastic modes are determined by the Christoffel equation

$$\sum_k A_{ik}(\boldsymbol{k}) e_k(\boldsymbol{k}, \varrho) = \tilde{c}_\varrho(\boldsymbol{k}) e_i(\boldsymbol{k}, \varrho), \tag{15}$$

where

$$A_{ik}(\boldsymbol{k}) = \sum_{jl} \tilde{c}_{ijkl} k_j k_l, \tag{16}$$

and k_j, k_l are the Cartesian components of the wave vector $\boldsymbol{k}$. The knowledge of the polarization vector of an elastic mode ϱ propagating along $\boldsymbol{k}$ permits us to describe the square of the wave speed

$$\tilde{c}_\varrho(\boldsymbol{k}) = \sum_{ik} e_i(\boldsymbol{k}, \varrho) A_{ik}(\boldsymbol{k}) e_k(\boldsymbol{k}, \varrho). \tag{17}$$

Now, the local free energy density can be expressed in terms of normal coordinates of the elastic waves, namely

$$F = F_0 + \tfrac{1}{2} \sum_{\boldsymbol{k}\varrho} \tilde{c}_\varrho(\boldsymbol{k}) u_{\boldsymbol{k}\varrho} u_{-\boldsymbol{k}\varrho}$$
$$+ \frac{i^3}{6} \sum_{\substack{\boldsymbol{k}_1\boldsymbol{k}_2\boldsymbol{k}_3 \\ \varrho_1\varrho_2\varrho_3}} d\begin{pmatrix} \boldsymbol{k}_1 & \boldsymbol{k}_2 & \boldsymbol{k}_3 \\ \varrho_1 & \varrho_3 & \varrho_3 \end{pmatrix} u_{\boldsymbol{k}_1\varrho_1} u_{\boldsymbol{k}_2\varrho_2} u_{\boldsymbol{k}_3\varrho_3} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3) + \ldots, \tag{18}$$

where

$$d\begin{pmatrix} \boldsymbol{k}_1 & \boldsymbol{k}_2 & \boldsymbol{k}_3 \\ \varrho_1 & \varrho_2 & \varrho_3 \end{pmatrix} = \sum_{ikp} \left(\sum_{jlq} \tilde{c}_{ijklpq} k_{1j} k_{2l} k_{3q} \right) e_i(\boldsymbol{k}_1, \varrho_1) e_k(\boldsymbol{k}_2, \varrho_2) e_p(\boldsymbol{k}_3, \varrho_3).$$

Near to elastic phase transition associated with one-component order parameter the softening of the transverse elastic mode occurs in one special direction $\boldsymbol{k}^{(c)}$ (and equivalent directions allowed by the symmetry) for which $\tilde{c}_{\varrho_c}(\boldsymbol{k}^{(c)}) \to 0$ as $T \to T_{ce}$. The critical fluctuations are expected to occur just around this special direction. Apart from the soft elastic mode, there are two other elastic modes $\tilde{c}_{\varrho_1}(\boldsymbol{k}^{(c)})$ and $\tilde{c}_{\varrho_2}(\boldsymbol{k}^{(c)})$ propagating along the same direction $\boldsymbol{k}^{(c)}$ with generally different speeds. The special direction $\boldsymbol{k}^{(c)}$ and the elastic wave velocities and their polarization vectors together with those normal expressions of elastic constants which vanish at T_{ce}, are listed in Table III.

TABLE III

Eigenvalues $c_\varrho(k^{(c)})$ and polarization vectors $e(k^{(c)}, \varrho)$ of the elastic modes which propagate along the soft special directions $k^{(c)}$

	$k^{(c)}$	Transverse soft mode	Longitudinal mode	Transverse mode	The c which vanishes at T_{ce}
Monoclinic	[0, 1, 0]	$\alpha(1-\gamma)k_y^2$ $(\delta_+, 0, \varepsilon\delta_+)$	$c_{22}k_y^2$ $(0, 1, 0)$	$\alpha(1+\gamma)k_y^2$ $(\delta_-, 0, \varepsilon\delta_-)$	$c_{44}c_{66}-c_{46}^2$
Orthorhombic	[1, 0, 0]	$c_{66}k_x^2$ $(0, 1, 0)$	$c_{11}k_x^2$ $(1, 0, 0)$	$c_{55}k_x^2$ $(0, 0, 1)$	c_{66}
Tetragonal I	$[k_1, k_2, 0]$ $k_1 = k^{(c)}\cos\tau$ $k_2 = k^{(c)}\sin\tau$	$(\chi-\varkappa)\varphi^2(k^c)^2$ $(-\vartheta\varphi, \varphi, 0)$	$(\zeta-\varkappa)\varphi^2(k^c)^2$ $(\varphi, \vartheta\varphi, 0)$	$c_{44}(k^{(c)})^2$ $(0, 0, 1)$	$(c_{11}-c_{12})c_{66}-2c_{16}^2$
Tetragonal II	[1, 0, 0]	$c_{66}k_x^2$ $(0, 1, 0)$	$c_{11}k_x^2$ $(1, 0, 0)$	$c_{44}k_x^2$ $(0, 0, 1)$	c_{66}
Tetragonal III	[1, 1, 0]	$\frac{1}{2}(c_{11}-c_{12})(k^{(c)})^2$ $\frac{1}{\sqrt{2}}(-1, 1, 0)$	$\frac{1}{2}(c_{11}+c_{12}+2c_{66})(k^c)^2$ $\frac{1}{\sqrt{2}}(1, 1, 0)$	$c_{44}(k^{(c)})^2$ $(0, 0, 1)$	$\frac{1}{2}(c_{11}-c_{12})$

$\alpha = \frac{1}{2}(c_{44}+c_{66})$

$\beta = (c_{66}-c_{44})(c_{46})^{-1}$

$\gamma = [1-(c_{44}c_{66}-c_{46}^2)\alpha^{-2}]^{-\frac{1}{2}}$

$\delta_{+,-} = [1+(\beta\pm\sqrt{1+\beta^2})^2]^{-\frac{1}{2}}$

$\varepsilon = \beta+\sqrt{1+\beta^2}$

$\eta = (c_{11}-c_{12}-2c_{66})(4c_{16})^{-1}$

$\vartheta = -\eta-\sqrt{1+\eta^2}+\sqrt{2}[1+\eta^2+\eta\sqrt{1+\eta^2}]^{\frac{1}{2}}$

$\varphi = (1+\vartheta^2)^{-\frac{1}{2}}$

$\varkappa = \vartheta(3-\vartheta)c_{16}$

$\zeta = c_{11}+\vartheta^2(2c_{66}+c_{12})$

$\chi = (c_{11}-c_{12})\vartheta^2+(1-\vartheta^2)c_{66}$

$\tau = -\frac{1}{4}\operatorname{arct}\left(\frac{1}{\eta}\right)$

Consider elastic modes which propagate along a direction $\boldsymbol{k}$ slightly deviated from a special direction $\boldsymbol{k}^{(c)}$ and decompose the three-dimensional wave vector $\boldsymbol{k} = (p, r, t)$ into a special component $p = k^{(c)}$ of dimensionality $m = 1$ and remaining $d-m = 2$ components r and t (d — dimensionality of $\boldsymbol{k}$ space). The approximate speed of three elastic waves in the slightly deviated direction $\boldsymbol{k}$ can be found from (17) by substituting there the relevant polarization vectors $e(\boldsymbol{k}^{(c)}, \varrho)$ of a mode propagating along $\boldsymbol{k}^{(c)}$, instead of an exact polarization vector $e(\boldsymbol{k}, \varrho)$. After such modifications the free energy density takes the form

$$F = F_0 + \tfrac{1}{2} \sum_{\boldsymbol{k}}^{(1)} \{(\tilde{c}_{\varrho_c} p^2 + p^4 + A_{\varrho_c} r^2 + B_{\varrho_c} t^2) u_{\boldsymbol{k}\varrho_c} u_{-\boldsymbol{k}\varrho_c}$$
$$+ (\tilde{c}_{\varrho_1} p^2 + A_{\varrho_1} r^2 + B_{\varrho_1} t^2) u_{\boldsymbol{k}\varrho_1} u_{-\boldsymbol{k}\varrho_1} + (\tilde{c}_{\varrho_2} p^2 + A_{\varrho_2} r^2 + B_{\varrho_2} t^2) u_{\boldsymbol{k}\varrho_2} u_{-\boldsymbol{k}\varrho_2}\}$$
$$+ \left(\frac{-i}{6}\right) \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}^{(1)} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3) \{(d' p_1 p_2 r_3 + d'' p_1 p_2 t_3) u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_c}$$
$$+ d_1 p_1 p_2 p_3 u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_1} + d_2 p_1 p_2 p_3 u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_2}\}. \tag{19}$$

One notices here an additional term p^4 which represents the gradient term [6] along the special direction $k^{(c)}$ of the active strain component. The summations over the wave vector can be restricted into a cylinder around the special direction. This soft sector is indicated on top of the summation symbols. The A_ϱ, B_ϱ coefficient are expressed by the remaining effective elastic constants. The third order terms follow immediately from the symmetry of d_{ijklpq} coefficients [5]. In the above free energy density only those third order terms are left which might be relevant in the critical behaviour. The first two terms represent a coupling of different components of the same critical mode and the remaining two describe the coupling between two displacement modes. One notices an analogy between these third order terms and the coupling terms $L_\alpha s_\alpha(\boldsymbol{k}_1) q_{\boldsymbol{k}_2} q_{-\boldsymbol{k}_1-\boldsymbol{k}_2}$(I-26) which prove to be relevant in the non-elastic phase transitions. The coefficient standing by the term $p_1 p_2 p_3 u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_c}$ vanishes by symmetry.

The orthorhombic point group 222 will be used for illustration. The elastic phase transition is associated with the B_1 irreducible representation. The transverse elastic mode that propagates along the x axis with the speed specified by the c_{66} elastic constant and with the polarization vector parallel to the y axis is expected to be soft (Table I). The relevant free energy density (19) then takes the form

$$F = F_0 + \tfrac{1}{2} \sum_{\boldsymbol{k}}^{(1)} \{(\tilde{c}_{66} k_x^2 + \tilde{c}_{22} k_y^2 + \tilde{c}_{44} k_z^2) u_{\boldsymbol{k}\varrho_c} u_{-\boldsymbol{k}\varrho_c}$$
$$+ (\tilde{c}_{11} k_x^2 + \tilde{c}_{66} k_y^2 + \tilde{c}_{55} k_z^2) u_{\boldsymbol{k}\varrho_1} u_{-\boldsymbol{k}\varrho_1} + (\tilde{c}_{55} k_x^2 + \tilde{c}_{44} k_y^2 + \tilde{c}_{33} k_z^2) u_{\boldsymbol{k}\varrho_2} u_{-\boldsymbol{k}\varrho_2}\}$$
$$+ \left(\frac{-i}{6}\right) \sum_{\boldsymbol{k}_1 \boldsymbol{k}_2 \boldsymbol{k}_3}^{(1)} \delta(\boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{k}_3) \{3 d_{266} k_{1x} k_{2x} k_{3y} u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_c}$$
$$+ d_{166} k_{1x} k_{2x} k_{3x} u_{\boldsymbol{k}_1\varrho_c} u_{\boldsymbol{k}_2\varrho_c} u_{\boldsymbol{k}_3\varrho_1}\}.$$

To apply the renormalization group procedure to the local free energy density (19) the summations over the wave vector $\boldsymbol{k}$ should be changed into the integrals over the shell of the cylinder $b^{-1} < p < 1$ and $b_0^{-1} < r, t < 1$. Then new variables $p' = bp$, $r' = b_0 r$, $t' = b_0 t$ should be introduced and the normal coordinates $u_{k\varrho_c} \to \zeta_c u'_{k'\varrho_c}$ and $u_{k\varrho_{1,2}} \to \zeta_{1,2} u'_{k'\varrho_{1,2}}$ should be rescaled. The coefficients standing by p^4, A_{ϱ_c}, $\tilde{c}_{\varrho_1}$ terms yield the conditions: $b^{-4-m} b_0^{-d+m} \zeta_c^2 = 1, b^{-m} b^{-d+m-2} \zeta_c^2 = 1, b^{-2-m} b_0^{-d+m} \zeta_{1,2}^2 = 1$, respectively. Hence, $b_0 = b^2$, $\zeta_c^2 = b^{2d-m+4}$ and $\zeta_{1,2}^2 = b^{2d-m+2}$. After such specification the factors for the corresponding coupling constants in the renormalized free energy density are

$$\tilde{c}_{\varrho_c} \qquad -b^2$$

$$p^4, A_{\varrho_c}, B_{\varrho_c}, \tilde{c}_{\varrho_1}, \tilde{c}_{\varrho_2} \qquad -1$$

$$A_{\varrho_{1,2}}, B_{\varrho_{1,2}} \qquad -b^{-2}$$

$$d', d'', d_1, d_2 \qquad -b^{-d+2+m/2}.$$

We see from this dimensional analysis [7] that at the fixed point $\tilde{c}^*_{\varrho_c} = 0$, as it should be. (In [5] it has been shown that the fourth order term does not introduce any corrections.) The coupling constants $A_{\varrho_{1,2}}$, $B_{\varrho_{1,2}}$ become irrelevant for critical fluctuations in the vicinity of the fixed point. The third order coupling coefficients d', d'', d_1, d_2 also become irrelevant provided the dimensionality of the k-space and soft sector are $d = 3$ and $m = 1$, respectively. For the phase transitions listed in Table I we have $m = 1$.

The coupling coefficients A_{ϱ_c}, B_{ϱ_c}, $\tilde{c}_{\varrho_1}$, $\tilde{c}_{\varrho_2}$ are not themselves renormalized. However, in the second order of perturbation expansion, they can depend on the third order coupling coefficients, d', d'', d_1, d_2 similarly to the elastic constants (I-30) for the non-elastic phase transitions. Nevertheless, since the d', d'', d_1, d_2 become irrelevant when the fixed point is approached all effective elastic constants will behave as predicted by the phenomenological theory, the results of which are quoted in Table I and II. This conclusion applies also to the normal elastic constant associated with the totally symmetric strain and, therefore, dilatation does not accompany the elastic phase transition. So, the elastic phase transition exhibits the classical critical behaviour for which the phenomenological Landau theory becomes exact and for which the critical exponents assume the Landau values.

REFERENCES

[1] K. Parliński, *Acta Phys. Pol.* **A58**, 183 (1980).
[2] S. Aubry, R. Pick, *J. Phys.* (France) **32**, 657 (1971).
[3] C. W. Garland, D. B. Nowotny, *Phys. Rev.* **177**, 971 (1969).
[4] E. M. Brody, H. Z. Cummins, *Phys. Rev. Lett.* **21**, 1263 (1968).
[5] K. Brugger, *J. Appl. Phys.* **36**, 759 (1965).
[6] R. Folk, H. Iro, F. Schwabl, *Z. Phys.* **B25**, 69 (1976).
[7] K. G. Wilson, J. Kogut, *Phys. Rep.* **12C**, 77 (1974).