ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E4 - 5508

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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ON THE STABILITY OF AN ANHARMONIC CRYSTAL

1970

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Submitted to Acta Physica Hungarica

1. Introduction. Basic Equations

On the basis of the general method for investigating the properties of highly anharmonic crystals developed recently in /1,2/ in a previous work /3/ the conditions for stability of an anharmonic crystal were considered in the pseudoharmonic approximation with account of the third and fourth order anharmonic terms.

Such a restriction proved to be expedient since the relation between the mean square relative displacement $\sqrt{\overline{u}^2}$ of nearest neighbour atoms and the mean distance ℓ between them, $\sqrt{\overline{u}^2}/\ell$, is small enough up to the instability point, and improves the results of the pseudoharmonic theory as it permits us to diminish in a certain manner the undesirable effect of distortion due to the omission of all of the odd terms of anharmonicity. Calculations were considerably simplified, and the results approached to the ones of the case when the effect of damping of phonons is taken into account /4/.

In the present paper, which is the continuation of /3/, the properties of the face-cèntred cubic lattice with central nearest neighbour interaction are investigated in the same lowest order anharmonic terms approximation but with account of damping of phonons. The Lennard-Jones 12-6 interatomic potential is used. The properties of the crystal at fixed volume (section 2) and at fixed external pressure (section 3) are considered, and the results obtained in the case of anharmonicity are compared with the ones of the conventional perturbation theory.

The following investigation is carried out on the basis of the self-consistent system of equations for f.c.c. lattice consisting of identical atoms of mass M, the Hamiltonian of which in the central pair force approximation is of the form (see /4/)

$$H = \sum_{\ell} \frac{\vec{P}_{\ell}^{2}}{2M} + \frac{1}{2} \sum_{\ell \neq m} \phi (| \vec{R}_{\ell} - \vec{R}_{m} |) , \tag{1}$$

where

P_{ℓ}, R_{ℓ} -the momentum and position operators for the 1-th atom. Here and after the summation is performed only over the z nearest neighbours (in our case $z = 12$).

By using the double-time Green functions method /1,2/ the self-consistent system of equations for determination of the lattice constant can be obtained as well as the expression for the phonon frequency spectra $\epsilon_{\vec{k}j}$ and their damping $\Gamma_{\vec{k}j}$, the internal energy of the anharmonic crystal. Here we write down the expressions for the mentioned quantities (see /2,4/).

The equation of state from which the equilibrium lattice constant $d = \ell\sqrt{2}$ can be obtained is

$$P = -\frac{1}{3V} \sum_{\ell,a} \ell_a < \frac{\partial U}{\partial R_{\ell}^{a}} > = - \frac{z\ell}{6v} \tilde{\tilde{\phi}}^{(1)}(\ell) , \tag{2}$$

where P is the external pressure, $v = V/N = \ell^3/\sqrt{2}$, $\tilde{\tilde{\phi}}(\ell)$ is the self-consistent potential defined in the approximation used in this work as follows:

$$\tilde{\tilde{\phi}}(\ell) = <\phi(|\vec{R}_{\ell} - \vec{R}_{0}|)> \approx \exp\{\frac{1}{2} \sum <(u_{\ell}^{a} - u_{0}^{a})(u_{\ell}^{\beta} - u_{0}^{\beta})> \nabla_a \nabla_\beta\} \phi(\ell) \approx$$

$$\approx \phi(\ell) + \frac{1}{2} \sum_{a,\beta} <(u_{\ell}^{a} - u_{0}^{a})(u_{\ell}^{\beta} - u_{0}^{\beta})> \frac{\partial^2 \phi(\ell)}{\partial \ell_a \partial \ell_\beta} .$$

The renormalized phonon frequencies $\epsilon_{\vec{k}j}$ and phonon widths $\Gamma_{\vec{k}j}$ read

$$\varsigma_{\vec{k}j} = \omega_{\vec{k}j} + \mathrm{Re}\, M_{\vec{k}j}(\varsigma_{\vec{k}j}) \approx \tilde{\tilde{a}}\, \omega_{0\vec{k}j} \left[1 + \frac{\mathrm{Re}\, M_{\vec{k}j}(\varsigma_{\vec{k}j})}{\omega_{\vec{k}j}} \right], \qquad (4)$$

$$\Gamma_{\vec{k}j} = -\mathrm{Im}\, M_{\vec{k}j}(\varsigma_{kj} + i\epsilon) \approx -\mathrm{Im}\, M_{\vec{k}j}(\omega_{\vec{k}j} + i\epsilon), \qquad (5)$$

where $\omega_{0\vec{k}j}$ are the phonon frequencies in the harmonic approximation and $\omega_{\vec{k}j}$ -the ones in pseudoharmonic approximation, $\tilde{\tilde{a}}^2 = \{\tilde{\tilde{\phi}}^{(2)}(\ell) + \frac{c}{\ell}\tilde{\tilde{\phi}}^{(1)}(\ell)\} / f_0$ – the renormalization coefficient ($f_0 = \phi^{(2)}(r_0)$, $c = 3\delta - 1$, $\delta = \omega_k^2 / \omega_{\vec{k}j}^2 = \sum_j \omega_{\vec{k}j}^2 / 3\omega_{\vec{k}j}^2 \approx 1{,}40$ /3/), $M_{\vec{k}j}$ is the self-energy operator (see /4/). The internal energy of the system can be written in the form:

$$E = \langle H \rangle = \frac{N}{2} \{ z \tilde{\tilde{\phi}}(\ell) + \epsilon(\theta) \} + 5 \tilde{\tilde{F}}_3(\theta), \qquad (6)$$

where

$$\epsilon(\theta) = \frac{z}{2} \tilde{\tilde{a}}^2 f_0 \bar{u}_\ell^2 = \frac{1}{N} \sum_k \frac{1}{2\pi\omega_k} \int_0^\infty \frac{d\omega^2}{2\omega} \omega_k^2 \coth\frac{\omega}{2\theta} \{-\mathrm{Im}\, G_k(\omega + i\epsilon)\}, \qquad (7)$$

$\tilde{\tilde{F}}_3(\theta)$ is the anharmonic contribution of odd-derivative terms to the free energy and reads

$$\tilde{\tilde{F}}_3(\theta) = \frac{1}{12\pi} \int_0^\infty d\omega \coth\frac{\omega}{2\theta} \sum_k \frac{\omega^2 - \omega_k^2}{\omega_k} \{ -\mathrm{Im}\, G_k(\omega + i\epsilon) \}. \qquad (8)$$

In the formula (7) $\bar{u}_\ell^2$ is the mean square relative longitudinal displacement of neighbouring atoms.

In the high and low temperature the quantities $M_k (k \equiv \{\vec{k}j\})$, $\tilde{\tilde{F}}_3(\theta)$ and $\epsilon(\theta)$ can be written explicitly. For high temperatures ($\theta \gg \omega_D$ where $\omega_D \approx 1{,}05\, \omega_L$ is the Debaye energy in the pseudoharmonic approximation) we have (see /4/):

$$M_k(\omega) = -\theta \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \omega_k S_k(\nu),$$

where

$$g(\theta,\ell) = \tilde{\tilde{\phi}}^{(3)}(\ell), \qquad f(\theta) = \tilde{\tilde{\phi}}^{(2)}(\ell),$$

$$S_k(\nu) = \frac{1}{32N}\sum \frac{\Delta(\vec{p}+\vec{p}'-\vec{k})}{\Lambda_k^2\Lambda_p^2\Lambda_{p'}^2} F^2(-k,p,p')\left\{\frac{(\Lambda_p+\Lambda_{p'})^2}{(\Lambda_p+\Lambda_{p'})^2-\nu^2}+\frac{(\Lambda_p-\Lambda_{p'})^2}{(\Lambda_p-\Lambda_{p'})^2-\nu^2}\right\}$$

$\left(\nu=\frac{\omega}{\omega_L/2}, \omega_L=\omega_{0L}\sqrt{\frac{f(\theta,\ell)}{f_0}}, \omega_{0L}=\sqrt{\frac{8f_0}{M}}\right.$ is the maximum frequency in the harmonic approximation); the dimensionless sum $S_k(\nu)$ was calculated for some values $\{\vec{k}j\}$ in /5/;

$$\tilde{\tilde{F}}_3(\theta) \approx -N\theta\, A\,\frac{g^2(\theta,\ell)}{f^3(\theta,\ell)}, \quad A \approx 5{,}6 \cdot 10^{-2}, \tag{10}$$

$$\epsilon(\theta) \approx 3\theta\left\{\frac{1}{1-\mu\theta\,\frac{g^2(\theta,\ell)}{f^3(\theta,\ell)}}+\frac{\omega_L^2}{24\theta^2}\right\}, \tag{11}$$

$$\mu = 2A \approx 0{,}11 .$$

In the low temperature limit ($\theta \ll \omega_D$) the corresponding quantities are:

$$M_k(\omega) = -\omega_k\,\frac{g^2(\theta,\ell)}{f^3(\theta,\ell)}\left\{\epsilon_0\, S_{0k}(\nu)+\frac{3\pi^4\theta^4}{5\omega_0^3}S_{1k}(\nu)\right\}, \tag{12}$$

where

$$S_{0k}(\nu) = \frac{1}{(1.02)8^2N}\sum_{p,p'}\frac{\Delta(\vec{p}+\vec{p}'-\vec{k})}{\Lambda_k^2\Lambda_p\Lambda_{p'}}F^2(-k,p,p')\frac{(\Lambda_p+\Lambda_{p'})}{(\Lambda_p+\Lambda_{p'})^2-\nu^2},$$

$$S_{1k}(\nu) = \frac{1}{(120.8)8^2}\sum_{j_1,j_2}\int_{-1}^{1} d\cos\theta\int_0^{2\pi}d\phi\,\frac{G^2(\vec{k}j;\phi\theta,j_1;\vec{k}j_2)}{\Lambda_{\vec{k}j}^2\Lambda_{\vec{k}j_2}^2 d_{j_1}^5(\theta\phi)}\,\frac{2\Lambda_{\vec{k}j_2}}{\Lambda_{\vec{k}j_2}^2-\nu^2},$$

(the notations in S_{0k} and S_{1k} are the same as in /4/,

$\epsilon_0 = \epsilon_0^0 \sqrt{\frac{f(\theta,\ell)}{f_0}} \approx 1{,}02\,\omega_L$ where ϵ_0^0 is the zero point energy per atom in the harmonic approximation);

$$\tilde{\tilde{F}}_3(\theta) \approx -N\epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \{ \epsilon_0 B + \frac{3\pi^4\theta^4}{5\,\omega_D^3} C \} ,$$

$$B \approx 1{,}85 \,.\, 10^{-3} , \qquad C \approx 1.25 \,.\, 10^{-2} , \tag{13}$$

$$\epsilon(\theta) = \frac{\epsilon_0}{1 - \nu_0 \epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)}} + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} \{ 1 + \nu_1 \epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \} ,$$

$$\nu_0 = 4B \approx 7{,}3 \,.\, 10^{-3} , \qquad \nu_1 = 8C \approx 0{,}10 . \tag{14}$$

2. The Lattice at Fixed Volume

As mentioned above, in investigating the self-consistent system of equations for the crystal lattice we shall use the Lennard-Jones (12-6) model potential

$$\phi_{L-J}(\ell) = D \{ (\frac{r_0}{\ell})^{12} - 2(\frac{r_0}{\ell})^6 \} . \tag{15}$$

Substituting (15) into (3) and performing the summation with account of all of the terms in the derivatives of the pair potential we easily get

$$\tilde{\tilde{\phi}}(\ell) = D \{ \xi^{12} - 2\xi^6 + \frac{1}{6} y [(13-c)\xi^{14} - (7-c)\xi^8] \} , \tag{16}$$

where we introduced the notation $\xi \equiv \frac{r_0}{\ell}$ and the dimensionless variable $y = (6/r_0)^2 u_\ell^{-2}$.

In this section we consider the properties of the f.c.c. lattice at fixed volume with $\ell = r_0 =$ const. Determining the force constants and the renormalization coefficient $\tilde{\tilde{\alpha}}$ with the help of (16) and substituting them into eq. (7) we obtain the equation for y as a function of temperature and external pressure. Below this equation is analized in the high and low temperature limits.

<u>2a. High temperatures ($\theta \gg \omega_D$)</u>. In the case of high temperatures (7) and (11) give us the following equation for y :

$$\{\Lambda_1 y\,[1+\frac{D(H_1-H_2)}{f_0^2}y]-\beta\}(1+\frac{DH_2}{f_0^2}y)\{1-\frac{zA}{6}\theta\frac{g_0^2}{f_0^3}[1+\frac{D}{f_0}(\frac{2H_3}{g_0}-\frac{3H_2}{f_0})y]\}=1,$$

where

$$\Lambda_1=\frac{zD}{3\theta}=\frac{4D}{\theta}=\frac{M\omega_{0L}^2 r_0^2}{144\,\theta},\quad \beta=\frac{\omega_{0L}^2}{24\theta^2}\ll 1,$$

$$H_1=h_0+\frac{c}{r_0}(2g_0+\frac{(c-2)f_0}{r_0}),\quad H_2=h_0+\frac{c}{r_0}(g_0-\frac{2f_0}{r_0}),$$

$$H_3=\phi^{(5)}(r_0)+\frac{c}{r_0}(h_0-\frac{3g_0}{r_0}+\frac{6f_0}{r_0^2}),$$

$$h_0=\phi^{(4)}(r_0),\qquad g_0=\phi^{(3)}(r_0).$$

The equation (17) shows that in the constant volume case the lattice is stable in the whole region of temperatures (the solution of (17) is real for $y>0$ in the whole region of the parameters Λ_1). However, it is necessary to note that in the present case the problem of the dynamics stability of a lattice can be solved consistently only if the short range correlations due to the hard core part of the interatomic potential are carefully taken into account.

In the case of small anharmonicity ($\theta \ll D$, $y \ll 1$) the solution of equation (17) can be written in the form

$$y=\frac{\theta}{4D}\{1+\theta\,[2A\frac{g_0^2}{f_0^3}-\frac{1}{4}\frac{H_1}{f_0^2}]+\beta\,[1-\frac{\theta}{4}\frac{(2H_1-H_2)}{f_0^2}]\}$$

and leads to the expression for the physical quantities coinciding with the results of the conventional perturbation theory if $c = 0$, i.e. in the approximation in which only the leading highest order derivatives of the interatomic potential are taken into account (see, for example, /6,7/).

From (18) we obtain the following expressions for the physical characteristics of the crystal:

the renormalized frequencies:

$$\varsigma_{\vec{k}j} \approx \omega_{0\vec{k}j} \{ 1 + \frac{\theta}{8} \frac{H_1}{f_0^2} (1+\beta) - \theta \frac{g_0^2}{f_0^3} \operatorname{Re} S_{\vec{k}j} \} , \quad (19)$$

the phonon widths:

$$\Gamma_{\vec{k}j} \approx \theta \frac{g_0^2}{f_0^3} \omega_{0\vec{k}j} \operatorname{Im} S_{\vec{k}j} , \quad (20)$$

where $\operatorname{Re} S_{\vec{k}j} \equiv \operatorname{Re} S_{\vec{k}j}(\Lambda_{\vec{k}j})$, $\operatorname{Im} S_{\vec{k}j} \equiv \operatorname{Im} S_{\vec{k}j}(\Lambda_{\vec{k}j} + i\epsilon)$;

the internal energy:

$$\frac{1}{N} E \approx -\frac{zD}{2} + 3\theta \{ 1+\beta - \theta [\frac{1}{8} \frac{H_1}{f_0^2} - \frac{1}{16} \frac{H_4}{f_0^2}) - \frac{A}{3} \frac{g_0}{f_0^3}] \} ,$$

$$H_4 = h_0 + \frac{c}{r_0} (2g_0 + \frac{cf_0}{r_0}) ; \quad (21)$$

the external pressure:

$$P = \frac{21\ell}{2vr_0} (1+a_1)\theta \{ 1+\beta - \theta [0{,}25 \frac{H_1}{f_0^2} - 0{,}10 \frac{(1+a_2)}{(1+a_1)} \frac{h_0}{f_0^2} - 2A \frac{g_0^2}{f_0^3}] \} , \quad (22)$$

where

$$a_1 = \frac{cf_0}{r_0 g_0} , \quad a_2 = \frac{c}{r_0 \phi^{(5)}(r_0)} \frac{1}{} \{ 2h_0 + \frac{(c-2)g_0}{r_0} - \frac{2cf_0}{r_0^2} \} .$$

We note here that for determining the internal energy and pressure with an accuracy to the terms of θ^2 inclusively it was necessary to take into account the terms of the order of y^2 in the self-consistent potential $\tilde{\phi}(\ell)$.

<u>2b. Low temperatures ($\theta \ll \omega_D$).</u> Equation (7) with the account of (14) gives us the following equation for determining y:

$$\Lambda y \left(1 + \frac{DH_2}{f_0^2} y\right)^{-1/2} \left(1 + \frac{DH_1}{f_0^2} y\right) = 1 + \eta \left(1 + \frac{DH_2}{f_0^2} y\right)^{-2} +$$

$$+ \epsilon_0^0 \frac{g_0^2}{f_0^3} \left(1 + \frac{DH_2}{f_0^2} y\right)^{1/2} \left[1 + \frac{D}{f_0}\left(\frac{2H_3}{g_0} - \frac{3H_2}{f_0}\right) y\right] \left[\nu_0 + \nu_1 \eta \left(1 + \frac{DH_2}{f_0^2} y\right)^{-2}\right], \tag{23}$$

where $\Lambda = zD/\epsilon_0^0$ – the dimensionless coupling parameter for atoms; $\eta = \frac{3\pi^4}{5}\left(\frac{\theta}{\omega_{0D}}\right)^4 \ll 1$. Equation (23) has the real solutions in the whole region of the parameter Λ, however, it is necessary to make the same remarks as in the case of high temperatures relatively to the problem of the stability of the lattice.

In the case of small anharmonicity ($\epsilon_0^0 \ll zD$, $y \ll 1$) the solution of (23) takes the form

$$y = \frac{\epsilon_0^0}{zD} \left\{1 + \epsilon_0^0 \left[\nu_0 \frac{g_0^2}{f_0^3} - \frac{(2H_1 - H_2)}{24 f_0^2}\right] + \eta \left[1 + \epsilon_0^0 \left(\nu_1 \frac{g_0^2}{f_0^3} - \frac{(2H_1 + H_2)}{12 f_0^2}\right)\right]\right\} \tag{24}$$

and gives the results for the physical quantities coinciding with the ones of the conventional perturbation theory when $c = 0$, i.e. $H_1 = H_2 = h_0$.

With the help of (24) the characteristics of the system are obtained in the following form:

$$\varsigma_{\vec{k}j} \approx \omega_{0\vec{k}j} \left\{1 + \epsilon_0^0 \left[\frac{1}{24} \frac{H_1}{f_0^2}(1+\eta) - \frac{g_0^2}{f_0^3}\left(\mathrm{Re}\, S_{0\vec{k}j} + \eta\, \mathrm{Re}\, S_{1\vec{k}j}\right)\right]\right\}; \tag{25}$$

$$\Gamma_{\vec{k}j} \approx \omega_{0\vec{k}j}\, \epsilon_0^0 \frac{g_0^2}{f_0^3} \left(\mathrm{Im}\, S_{0\vec{k}j} + \eta\, \mathrm{Im}\, S_{1\vec{k}j}\right); \tag{26}$$

$$\frac{1}{N} E \approx -\frac{zD}{2} + \epsilon_0^0 \left\{1 + \epsilon_0^0 \left[\frac{(H_4 + 2H_2 - 2H_1)}{48 f_0^2} - \frac{g_0^2}{f_0^3}(5B - \nu_0)\right] + \right.$$

$$\left. + \eta \left[1 - \epsilon_0^0 \left(\frac{(2H_1 + 2H_2 - H_4)}{24 f_0^2} - \frac{g}{f_0^3}(\nu_1 - 5C)\right)\right]\right\}; \tag{27}$$

$$P \approx \frac{21\ell}{6vr_0}(1+a_1)\epsilon_0^0\{1+\epsilon_0^0[\nu_0\frac{g_0^2}{f_0^3}-\frac{(2H_1-H_2)}{24f_0^2}+0,034\frac{(1+a_2)}{(1+a_1)}\frac{h_0}{f_0^2}]+$$

$$+\eta[1-\epsilon_0^0(-\nu_1\frac{g_0^2}{f_0^3}+\frac{(2H_1+H_2)}{12f_0^2}-0,069\frac{(1+a_2)}{(1+a_1)}\frac{h_0}{f_0^2})]\} . \tag{28}$$

It is clear that due to the account of the zero-point vibrations of atoms the pressure is different from zero even when $\theta = 0$. In obtaining the expressions for E and P, as in the high temperature case, the terms of the order of y^2 in $\tilde{\phi}(\ell)$ were taken into account.

3. The Lattice at Constant External Pressure

In the case of isotopic external pressure P = const. the mean distance ℓ between atoms dependent on temperature can be determined from equation (2) after substituting into it the expression for $\tilde{\phi}^{(1)}(\ell)$ obtained with the help of (16). In the approximation of small pressure, considered in this work, ℓ is given by

$$\ell = \ell_0 - \frac{1}{18} r_0 p , \tag{29}$$

where $\ell_0 = \ell|_{p=0} = r_0(1+\frac{\sigma_1}{4}y)$, $p = P(\frac{3v_0 r_0}{2zD\ell_0}) \ll 1$ is a dimensionless small pressure ($v_0 = \ell_0^3/\sqrt{2}$).

The renormalization coefficient $\tilde{\tilde{a}}$ and force constants in this case read

$$\tilde{\tilde{a}}^2 = 1 - \sigma y + \sigma_1 p ,$$

$$f = f_0 (1 - \sigma y + \frac{7}{6} p) , \quad (30)$$

$$g = g_0 (1 - y + p) .$$

The following notations were introduced in (29)-(30):

$$\sigma \equiv \frac{35 + c}{36} , \qquad \sigma_1 \equiv \frac{21 - c}{18} .$$

Below the cases of high and low temperatures are considered separately.

3a. High temperatures ($\theta \gg \omega_D$). Substituting (30) into equation (7) and taking into account (11) we get the equation for determining the parameter y in the form:

$$\{ \Lambda_1 y \frac{(1-\sigma y+\sigma_1 p)}{(1-\sigma y+\frac{7}{6} p)} - \beta \} (1-\sigma y+\frac{7}{6}p) \{1 - 2A\theta \frac{g_0^2}{f_0^3} \frac{(1-y+p)^2}{(1-\sigma y+\frac{7}{6}p)^3}\} = 1. \quad (31)$$

In the region of temperatures $\theta \lesssim \theta_c$, where

$$\frac{\theta_c}{D} \approx 0,5 (1 + 2,1 p - 0,18 \beta_c) , \quad (32)$$

the solution of (31) is real and in the vicinity of the critical point ($r \lessapprox 1$) takes the following form):

$$y \approx 0,4 \{ 1 + 1,2 p + 0,34 \beta_c - 1,9 \sqrt{1 - r} \} , \quad (33)$$

where $r \equiv \theta / \theta_c$.

The physical quantities in this case read:

$$\varsigma_{\vec{k}j} \approx 0,8 \omega_{0\vec{k}j} \{1 + 0,32 p + 0,48\sqrt{1-r} - 2,86 r \operatorname{Re} S_{\vec{k}j} \} , \quad (34)$$

$$\Gamma_{\vec{k}j} \approx 2,3 r \omega_{0\vec{k}j} \operatorname{Im} S_{\vec{k}j} , \quad (35)$$

$$\frac{1}{N}E \approx -\frac{zD}{2} + 3\theta_c \{2 - 2{,}2\,p + 1{,}1\beta_c - 2{,}3\sqrt{1-r}\} , \quad (36)$$

$$C_p = \frac{k}{N}\left[\frac{\partial}{\partial\theta}(E + 3PV)\right]_p \approx 3k\,\frac{1{,}15}{\sqrt{1-r}} , \quad (37)$$

$$\alpha_p = \frac{k}{\ell}\left[\frac{\partial\ell}{\partial\theta}\right]_p \approx \frac{k r_0}{\ell\theta_c}\,\frac{0{,}10}{\sqrt{1-r}} . \quad (38)$$

It is clear from expressions obtained here that the dynamic instability of the system occurs if $\theta > \theta_c$ (the renormalized phonon frequency $\varsigma_{\vec{k}j}$ becomes complex) as in the pseudoharmonic approximation /3/. The internal energy remains finite at $\theta \lessapprox \theta_c$, but the specific heat at constant pressure C_p and the coefficient of the linear thermal expansion α_p tend to infinity as $\theta \to \theta_c$.

Far from critical point, i.e. in the small anharmonicity limit, when $\theta \ll D$, $y \ll 1$, the solution of e.q. (31) is given by

$$y \approx \frac{1}{\Lambda_1}\{1 + \beta - \sigma_1 p + \theta\left[\frac{\sigma}{20{,}6}\,\frac{h_0}{f_0^2} + 2A\,\frac{g_0^2}{f_0^3}\right]\} , \quad (33')$$

and the corresponding physical quantities are:

$$\varsigma_{\vec{k}j} \approx \omega_{0\vec{k}j}\{1 + \frac{\sigma_1}{2}p - \theta\left[\frac{\sigma}{41{,}2}\,\frac{h_0}{f_0^2}(1+\beta) + \frac{g_0^2}{f_0^3}\,\mathrm{Re}\,S_{\vec{k}j}\right]\} , \quad (34')$$

$$\Gamma_{\vec{k}j} \approx \omega_{0\vec{k}j}\,\theta\,\frac{g_0^2}{f_0^3}\,\mathrm{Im}\,S_{\vec{k}j} , \quad (35')$$

$$\frac{1}{N}E \approx -\frac{zD}{2} + 3\theta\{1 + \beta - \frac{\sigma_1}{2}p + \theta\left[\frac{\sigma}{41{,}2}\,\frac{h_0}{f_0^2} + \frac{1}{16}\,\frac{H_4}{f_0^2} + \frac{A}{3}\,\frac{g_0^2}{f_0^3}\right]\} \quad (36')$$

$$C_p = 3k \{ 1 + \beta + \theta [\frac{\sigma}{20,6} \frac{h_0}{f_0^2} + \frac{1}{8} \frac{H_4}{f_0^2} + \frac{2A}{3} \frac{g_0^2}{f_0^3}] \} , \qquad (37')$$

$$\alpha_p \approx \frac{\sigma_1 k r_0}{16 \ell D} \{ 1 + \beta + \theta [\frac{\sigma}{10,3} \frac{h_0}{f_0^2} + 4A \frac{g_0^2}{f_0^3}] \} . \qquad (38')$$

3b. Low temperatures ($\theta \ll \omega_D$). The equation for determining y is obtained from (30), (7) and (14) and has the following form:

$$\Lambda y \{ 1 - \frac{49}{8} \frac{z}{\Lambda} \nu_0 \frac{(1-y)^2}{(1-\sigma y)^{5/2}} \} =$$

$$= \frac{1}{(1-\sigma y)^{1/2}} \{ 1 - \Lambda p y \frac{(\sigma_1 - 7/12)}{(1-\sigma y)^{1/2}} + \frac{\eta}{(1-\sigma y)^2} [1 + \frac{49}{8} \frac{z}{\Lambda} (\nu_1 - \nu_0) \frac{(1-y)^2}{(1-\sigma y)^{5/2}}] \} . \qquad (39)$$

The critical parameters Λ_0 and θ_c restricting the region of existence of real solutions of equation (39) for $y > 0$, $\Lambda \tilde{\geq} \Lambda_0$, $\theta \leq \theta_c$ are given by the formulae

$$\frac{\theta_c}{\omega_{0D}} \approx \frac{1}{2,5\pi} (\Lambda - \Lambda_0)^{1/4} , \quad \Lambda_0 \approx 3,5 (1-p) . \qquad (40)$$

The solution near the critical point ($\theta \lessapprox \theta_c$) can be written in the form

$$y \approx 0,6 \{ 1 + 0,8p - 0,47(\Lambda - \Lambda_0) - 0,52\sqrt{(\Lambda - \Lambda_0)(1-r^4)} [1 - 0,47(\Lambda - \Lambda_0)] + 0,6(\Lambda - \Lambda_0)(1-r^4) \} \qquad (41)$$

and leads to the following expressions for the physical characteristics of the lattice:

$$\varsigma_{\vec{k}j} \approx 0,63 \omega_{0\vec{k}j} \{ 1 + 0,65p + 0,35(\Lambda - \Lambda_0) + 0,4\sqrt{(\Lambda - \Lambda_0)(1-r^4)} - 33,2 \, \mathrm{Re}\, S_{0\vec{k}j} - 2,07 . 10^2 \eta_o \mathrm{Re}\, S_{1\vec{k}j} \{ \} ,$$

$$\Gamma_{\vec{k}j} \approx 21 \, \omega_{0\vec{k}j} \{ \mathrm{Im}\, S_{0\vec{k}j} + 6,25 \eta_o \mathrm{Im}\, S_{1\vec{k}j} \} , \qquad (43)$$

$$\frac{1}{N} E \approx -\frac{zD}{2} + \epsilon_0^0 \{ 0,96 - 0,13p + 0,17(\Lambda - \Lambda_0) - 0,11\sqrt{(\Lambda - \Lambda_0)(1-r^4)} [1 + 2,2(\Lambda - \Lambda_0)] \} , \qquad (44)$$

$$C_p = 3{,}7\,k\,\frac{12\pi^4}{5}\,\frac{\theta^3}{\omega^3_{0D}}\,\frac{[1+2{,}2(\Lambda-\Lambda_0)]}{\sqrt{(\Lambda-\Lambda\ )(1-r^4)}}, \tag{45}$$

$$a_p \approx 10{,}4\,\frac{k r_0}{\ell}\,\frac{3\pi^4}{5}\,\frac{\theta^3}{\omega^4_{0D}}\,\{\frac{1-0{,}5(\Lambda-\Lambda_0)}{\sqrt{(\Lambda-\Lambda_0)(1-r^4)}} - 2{,}3\}. \tag{46}$$

We see, as in the pseudoharmonic approximation, that the system becomes unstable when $\Lambda < \Lambda_0$ or $\theta > \theta_0$ (see (42)). The internal energy is finite at $\theta \leq \theta_c$, but the specific heat and the coefficient of the linear thermal expansion tend to infinity as $\theta \to \theta_0$.

Far from the critical point ($\Lambda \gg 1$, $y \ll 1$) the solution of (39) is given by

$$y \approx \frac{\epsilon^0_0}{zD}\{1-(\sigma_1-\frac{7}{12})p+\epsilon^0_0[\frac{\sigma}{6.\,20{,}6}\frac{h_0}{f^2_0}+\nu_0\frac{g^2_0}{f^3_0}]+\eta[1+\epsilon^0_0(\frac{\sigma}{20{,}6}\frac{h}{f^2_0}+\nu_1\frac{g^2_0}{f^3_0})]\} \tag{41'}$$

and leads to the following expressions for the physical quantities:

$$\varsigma_{\vec{k}j} \approx \omega_{0\vec{k}j}\{1+\frac{\sigma_1}{2}p-\epsilon^0_0[\frac{\sigma}{6.20{,}6}\frac{h_0}{f^2_0}(1+\eta)+\frac{g^2_0}{f^3_0}(\mathrm{Re}\,S_{0\vec{k}j}+\eta\,\mathrm{Re}\,S_{1\vec{k}j})]\}, \tag{42'}$$

$$\Gamma_{\vec{k}j} \approx \omega_{0\vec{k}j}\,\epsilon^0_0\,\frac{g^2_0}{f^3_0}\,\{\mathrm{Im}\,S_{0\vec{k}j}+\eta\,\mathrm{Im}\,S_{1\vec{k}j}\}, \tag{43'}$$

$$\frac{1}{N}E \approx -\frac{zD}{2}+\epsilon^0_0\{1-\epsilon^0_0[\frac{(\sigma_2-\sigma)}{6.20{,}6}\frac{h_0}{f^2_0}+\frac{g^2_0}{f^3_0}(5B-\nu_0)]+$$
$$+\eta[1+\epsilon^0_0(\frac{(3\sigma-\sigma_2)}{3.20{,}6}\frac{h_0}{f^2_0}+\frac{g^2_0}{f^3_0}(\nu_1-5C))]\}, \tag{44'}$$

where $\sigma_2 \equiv \sigma + \frac{12-c}{4} - \frac{DH_4}{2f_0^2} \approx 1{,}5$;

$$C_p \approx k \frac{12\pi^4}{5} \frac{\theta^3}{\omega^3_{0D}} \{1+\epsilon_0^0 [\frac{(3\sigma-\sigma_2)}{3.\,20{,}6} \frac{h_0}{f_0^2} + \frac{g_0^2}{f_0^3}(\nu_1 - 5C)]\} , \qquad (45')$$

$$a_p \approx \frac{\sigma_1 k r_0}{12\,\ell D} \frac{3\pi^4}{5} \frac{\theta^3}{\omega^3_{0D}} \{1+\epsilon_0^0 [\frac{\sigma}{20{,}6} \frac{h_0}{f_0^2} + \nu_1 \frac{g_0^2}{f_0^3}]\} . \qquad (46')$$

4. Discussion

Using the general method developed in /1,2/ we have considered the properties of the three-dimensional lattice in the lowest order anharmonic approximation.

Comparing the results of the present work with those of /3/ in which the similar consideration of the crystal has been performed in the pseudoharmonic approximation we see that the account of phonon damping leads to the decrease of the critical temperature θ_c and increase of the critical value of the dimensionless coupling parameter λ . The same result was obtained in the case when the higher order anharmonic terms were taken into account /4,8/.

The value of the critical parameters and physical quantities obtained in this paper, especially in the high temperature limit, approach well to those obtained earlier in /4/ with account of the higher order anharmonicities and using the Morse interatomic model potential.

Thus, due to the sufficient smallness of the values of the mean square relative displacements of atoms in the lattice up to the critical point (the evaluation of the longitudinal ones from the calculations of Section 3 gives

$$\frac{\sqrt{\overline{u^2_{\ell_c}}}}{\ell_c} = \frac{r_0\sqrt{\overline{Y_c}}}{6\ell_c} \approx \begin{cases} 0{,}10, & \theta \gg \omega_D \\ 0{,}11, & \theta \ll \omega_D \end{cases}) .$$

it appears to be expedient in many cases to use the lowest order anharmonic approximation when using the developed self-consistent theory for investigating the properties of anharmonic crystals in wide intervals of temperatures and external pressure. Such a procedure simplifies considerably the calculations and makes it possible to use the more realistic Lennard-Jones pair potential in comparison with other model potentials. We note also that the account of all of the lower order terms in calculating the derivatives of the pair potential in this work (see (16)), as in /3/, leads to more accurate results.

The results obtained in the case of small anharmonicity agree well with the ones of the ordinary perturbation theory. The critical temperature obtained in this work, as in /4/, corresponds to the transition of the system from the crystal state to the uniform density state and is close to the melting temperature (see discussion in /4/).

Acknowledgement

The author should like to thank Dr. N.M. Plakida for many valuable discussions.

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Received by Publishing Department
on December 10, 1970.