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THERMODYNAMICS OF STRONGLY ANHARMONIC CRYSTALS

III. The Low Temperature Limit

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In paper /1/ the properties of the f.c.c. lattice with nearest neighbour central force interaction were considered in the case of the arbitrary external pressure. The instability temperature, the critical temperature, the phonon frequencies, the phonon widths and the thermodynamical properties of the f.c.c. lattice were calculated in the high temperature limit in /2/. In the present paper these quantities are calculated in the low temperature limit. Finally we discuss the results obtained in all three parts of our work.

The Low Temperature Limit $(\theta \ll \omega_D)$

In /3/ an expression for the self-energy operator (1.4)[x)] was obtained in the low temperature limit in the form

$$\Pi_k(\omega) = -\omega_k \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \{ \epsilon_0 \; S_{0k}\left(\frac{2\omega}{\omega_L}\right) + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} S_{1k}\left(\frac{2\omega}{\omega_L}\right) \} \tag{3.1}$$

where the dimensionless sums S_{0k} and S_{1k} are given in /3,4/, $\epsilon_0 \approx 1.02\,\omega_L$ is the zero-point energy per atom in pseudoharmonic approximation. The notations are the same as in /1,2/.

x) The formulae of our previous papers /1/ and /2/ are quoted as (1. . .) and (2. . .), respectively, e.g. (1.4) means formula (1.4) of /1/.

Equation /1.8/ can be written in the low temperature limit taking into account the explicit form (3.1) of the self-energy operator approximately as

$$\frac{Z}{2}\, f(\theta,\ell)\, \overline{u^2}(\ell) = \epsilon_0 \left[1 - \nu_0 \epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \right]^{-1} + \frac{3\pi^4}{5} \frac{\theta^4}{\omega_D^3} \left[1 + \nu_1 \epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)} \right] \tag{3.2}$$

with the numerical coefficients $\nu_0 \approx 7.3 \times 10^{-3}$, $\nu_1 \approx 0.10$ /3/.

Taking into account (1.17), (1.18) and (1.22) the S.C. equation (3.2) can be written approximately as follows

$$\lambda a\; y(a) = \left\{ 1 - \frac{0.4}{\lambda} \frac{\left[a^2 - \frac{P^*}{36}\left(\frac{\ell}{r_0}\right)^2 \right]^2}{a^5} \right\}^{-1} + 49.6 \left(\frac{r}{a} \right)^4 \left\{ 1 + \frac{5.4}{\lambda} \frac{\left[a^2 - \frac{P^*}{36}\left(\frac{\ell}{r}\right)^2 \right]^2}{a^5} \right\}, \tag{3.3}$$

where function $y(a)$ is given by (1.19) and (1.21).

In the low temperature limit it is interesting to investigate the crystals with weak coupling. The dependence of the real solutions of the S.C. equation (3.3) on the reduced temperature T^* and reduced pressure P^* is given in Fig. 3.1a for $\lambda = 3$ and in Fig. 3.1b for $\lambda = 2$. If $\lambda > \lambda_s = 2.24$ the solutions of the S.C. equation (3.3) (see Fig. 3.1a) have the similar behaviour as the solutions of the S.C. equation (2.3) (see Fig. 2.1) in the high temperature limit. Therefore we do not repeat here the discussions of /2/. The dependence of the instability temperature T_s^* on the reduced pressure P^* is similar to that which was found out in the high temperature limit (see Fig. 3.2 and Fig. 2.2). In the case $\lambda = 3$ we get the following value for the critical pressure $P_c^* \approx 1.5$ and critical temperature $T_c^* \approx 0.82$.

If the coupling constant is sufficiently small ($\lambda < \lambda_s$) the crystal becomes unstable even at $r. = 0$, because in this case the zero-point energy is sufficiently large. But when an external pressure is applied a stable crystal state appears which behaves in the analogous manner as in the case $\lambda \geq \lambda_s$ (see Fig. 3.1b).

The frequencies of the renormalized phonons and their widths (1.3) according to (1.17), (1.18), (1.22) and (3.1) can be written in the following form

$$\frac{\epsilon_k}{\omega_{0k}} \approx a - \frac{6}{\lambda}\{ 2+1/\gamma\}^2\{\mathrm{Re}\, S_{0k} + \frac{3\pi^4}{5}(\frac{\tau}{a})^4 \mathrm{Re}\, S_{1k}\} \tag{3.4}$$

$$\frac{\Gamma_k}{\omega_{0k}} \approx \frac{6}{\lambda}\{ 2+1/\gamma\}^2\{\mathrm{Im}\, S_{0k} + \frac{3\pi^4}{5}(\frac{\tau}{a})^4 \mathrm{Im}\, S_{1k}\} \tag{3.5}$$

(In the calculations the following approximate values were taken /3/ $\mathrm{Re}\, S_{0k} \approx \mathrm{Im}\, S_{0k} \approx 1.85 \times 10^{-3}$, $\mathrm{Re}\, S_{1k} \approx \mathrm{Im}\, S_{1k} \approx 1.25 \times 10^{-3}$).

In Fig. 3.3 and in Fig. 3.4 the dependence of the renormalized phonon frequencies ϵ_k/ω_{0k} and phonon widths Γ_k/ω_{0k} on the reduced temperature is presented for $\lambda = 3$, respectively. It is seen from Fig. 3.3 and Fig. 3.4 that both of these properties depend slighly on the temperature in the region $T^* \leq T^*_s$. In the region $T^* > T^*_s$ the phonon widths grow rapidly but remain sufficiently small. This results for $P^* \ll 1$ coincide with those of work /3/.

In the low temperature limit according to /3,4/ we can write the expressions (1.12) and (1.13) for the free energy in the following form

$$F_0 = N\omega_L\{1 - \frac{\pi^4}{5}(\frac{\tau}{a})^4\}$$
$$\tilde{F}_3(\theta) = -N\epsilon_0 \frac{g^2(\theta,\ell)}{f^3(\theta,\ell)}\{\epsilon_0 B + \frac{3\pi^4}{5}\frac{\theta^4}{\omega_D^3} C\} \tag{3.6}$$

with the numerical coefficients $B \approx 1.85 \times 10^{-3}$, $C \approx 1.25 \times 10^{-2}$.

Taking into account (1.17), (1.18) and (3.6) the expression for the internal energy (1.10) and the free energy (1.11) takes the form

$$\frac{\Gamma_k}{\omega_{0k}} = \frac{1}{2} \cdot 10^{-2} T^* \frac{1}{a} (2 + \frac{1}{y})^2 . \tag{2.6}$$

(In the calculations the following approximate values were taken: $\mathrm{Re}\, S_k \approx 3 \times 10^{-2}$, $\mathrm{Im}\, S_k \approx 1 \times 10^{-2}$). In Fig. 2.3 the dependence of the renormalized phonon frequencies ϵ_k / ω_{0k} $(P^* = 0)$ on the reduced temperature T^* is presented for some values of P^*. In Fig. 2.4 Γ_k / ϵ_k is given as a function of T^*. The results obtained here for $P^* \ll 1$ coincide with those of work/2/.

In the high temperature limit according to /2,3/ we can write the expressions (2.12) and (2.13) in the following form

$$F_0 = 3N\theta \ln (0.65 \frac{\omega_L}{\theta}) , \tag{2.7}$$

$$\tilde{F}_3 (\theta) = - N\theta^2 A \frac{g^2(\theta, \ell)}{f^3(\theta, \ell)} ,$$

where the numerical coefficient $A \approx 5.6 \times 10^{-2}$. Taking into account (1.20), (2.2) and (2.7) the internal energy (1.10) and the free energy (1.11) can be written in the form

$$e = \frac{1}{3N\epsilon} E \approx 0.85\, T^* - 2a^2 (1 + 0.7\, y) + \frac{P^*}{4} (\frac{\ell}{r_0})^2 , \tag{2.8}$$

$$f = \frac{1}{3N\epsilon} F \approx T^* \ln (\frac{7.8}{\lambda} \frac{a}{T^*}) - \frac{T^*}{3} - 2a^2 (1 + \frac{y}{3}) + \frac{P^*}{4} (\frac{\ell}{r_0})^2 . \tag{2.9}$$

In the calculation of the free energy $\lambda = 20$ was taken. In Fig. 2.5 the reduced thermodynamical potential $g = f + P^* v^*$ is given as a function of the reduced temperature T^*. We note here, that the function $g(T^*)$ has a minimum at the temperature slighty lower than T_s^*. The dependence of the reduced internal energy e on the temperature T^* is presented in Fig. 2.6. We note here, that the decrease of the internal energy with the increase of the temperature does not appear in the pseudoharmonic approximation and in the low temperature limit. In the both cases the internal energy is an increasing function of the temperature and its curves have a van der Waals character.

The dependence of the reduced volume $v^* = V\sqrt{2}/Nr_0^3 = (\ell/r_0)^3$ on the reduced pressure is given in Fig. 2.7. It is worth-while to note, that the curves have a van der Waals character. An analogous result was obtained in /4/.

The calculation of the f.c.c. lattice properties in the low temperature limit and a detailed discussion of the results will be given in the following paper.

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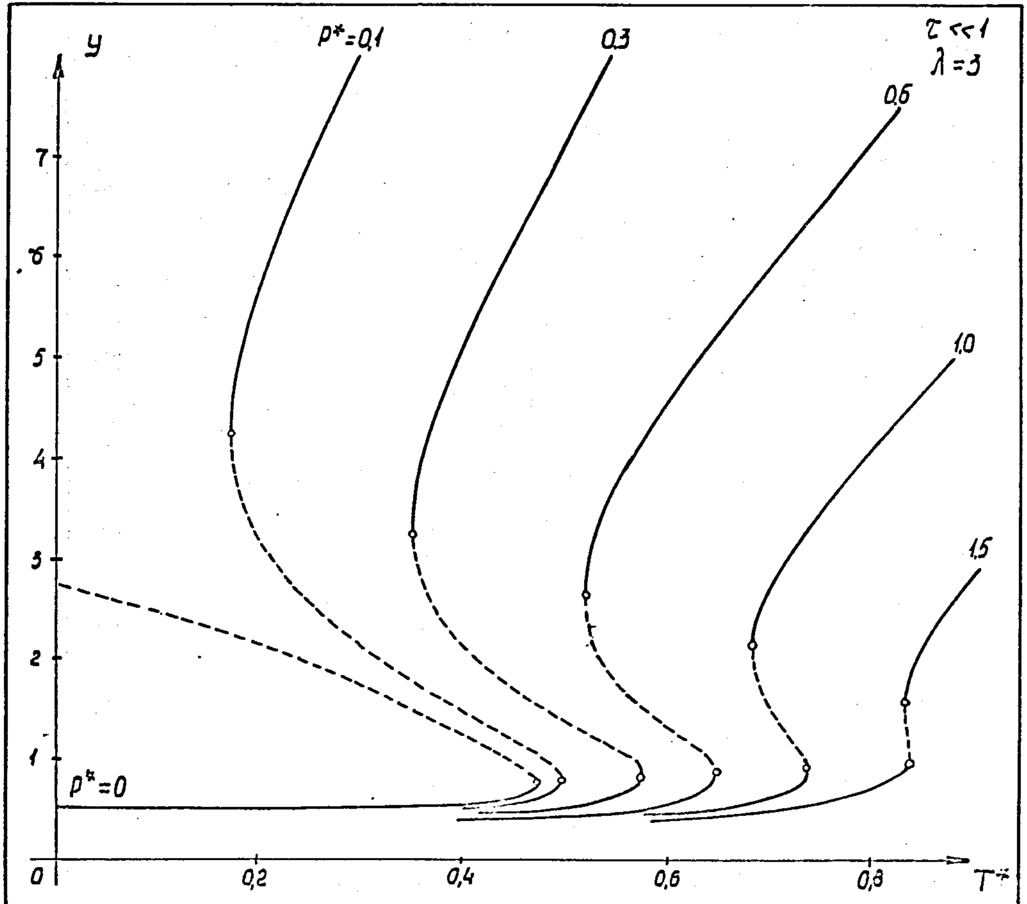

Fig. 3.1a. The real solutions of the S.C. equation for $\lambda = 3$.

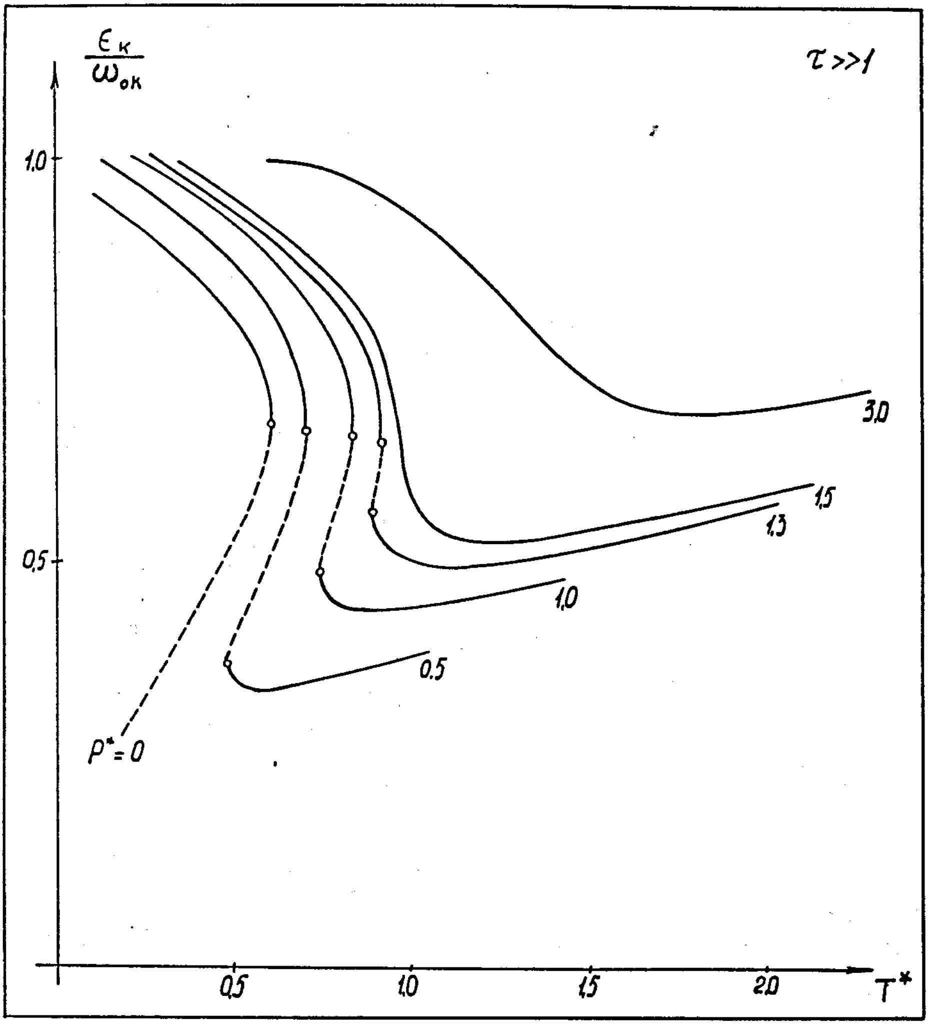

Fig. 2.3. The dependence of the renormalized phonon frequencies $\epsilon_k / \omega_{0k} (P^* = 0)$ on the reduced temperature T^*.

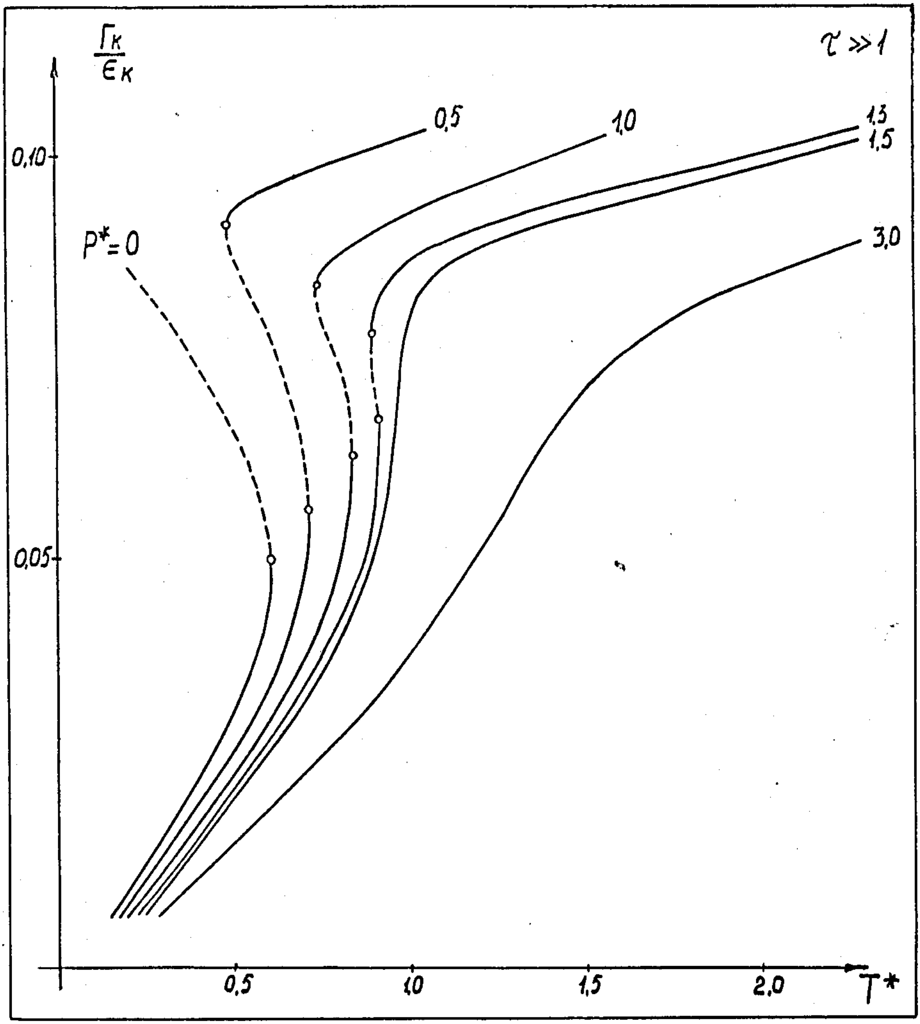

Fig. 2.4. The dependence of the phonon widths Γ_k / ϵ_k on the temperature T^* .

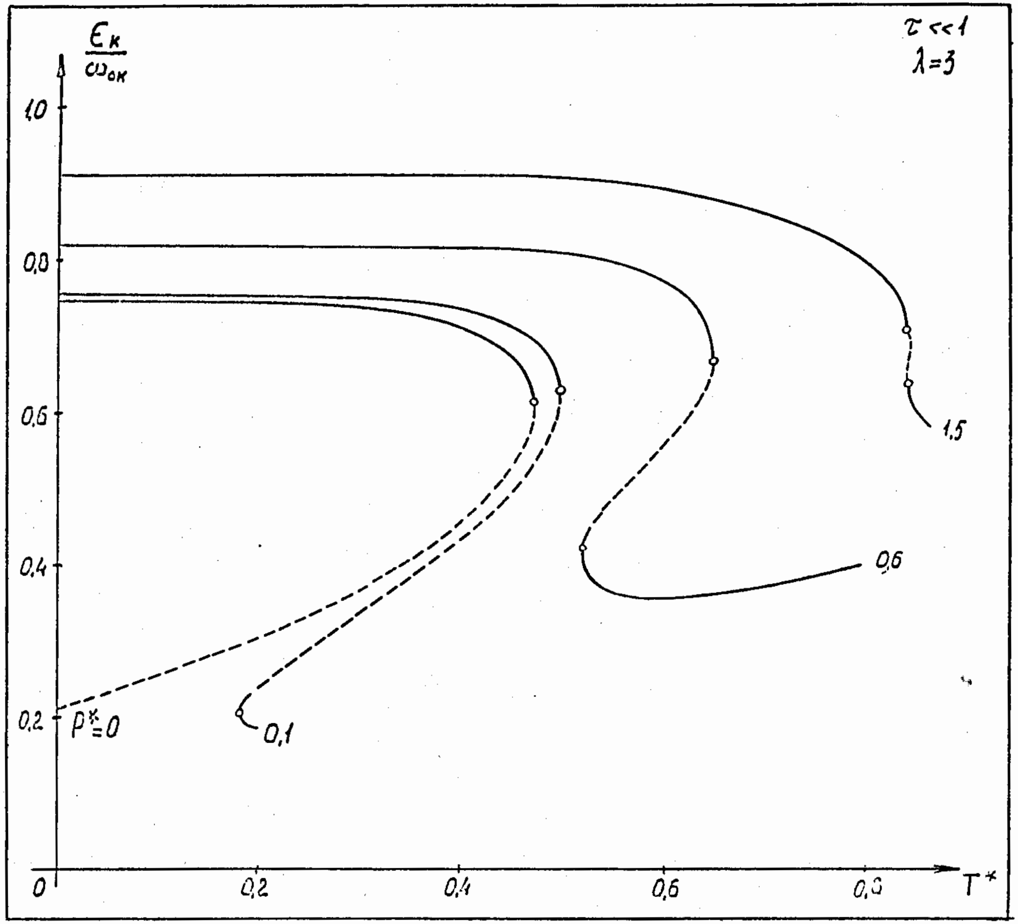

Fig. 3.3. The dependence of the renormalized phonon frequencies ϵ_k / ω_{0k} on the reduced temperature T^* ($\lambda = 3$).

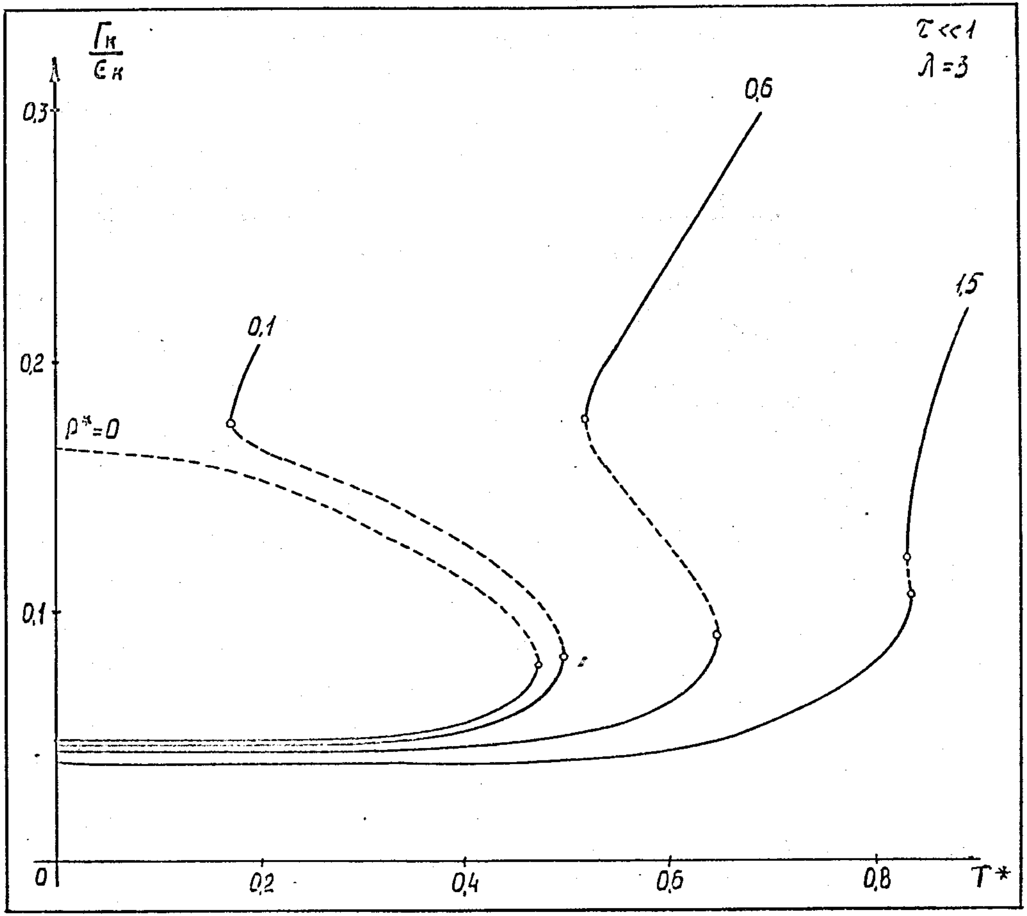

Fig. 3.4. The dependence of the phonon widths Γ_k / ϵ_k on the temperature T^* ($\lambda = 3$) .

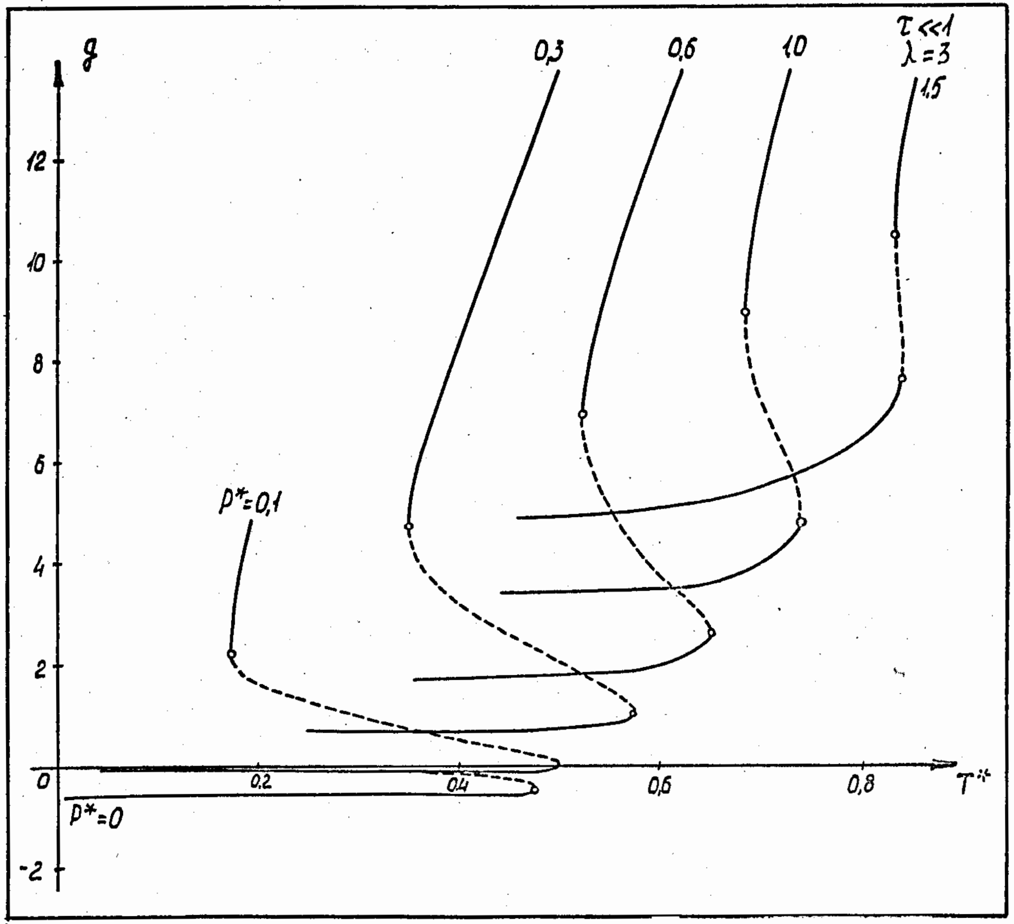

Fig. 3.5. The thermodynamical potential $g = f + 3P^* v^*$ as a function of the temperature T^* ($\lambda = 3$).

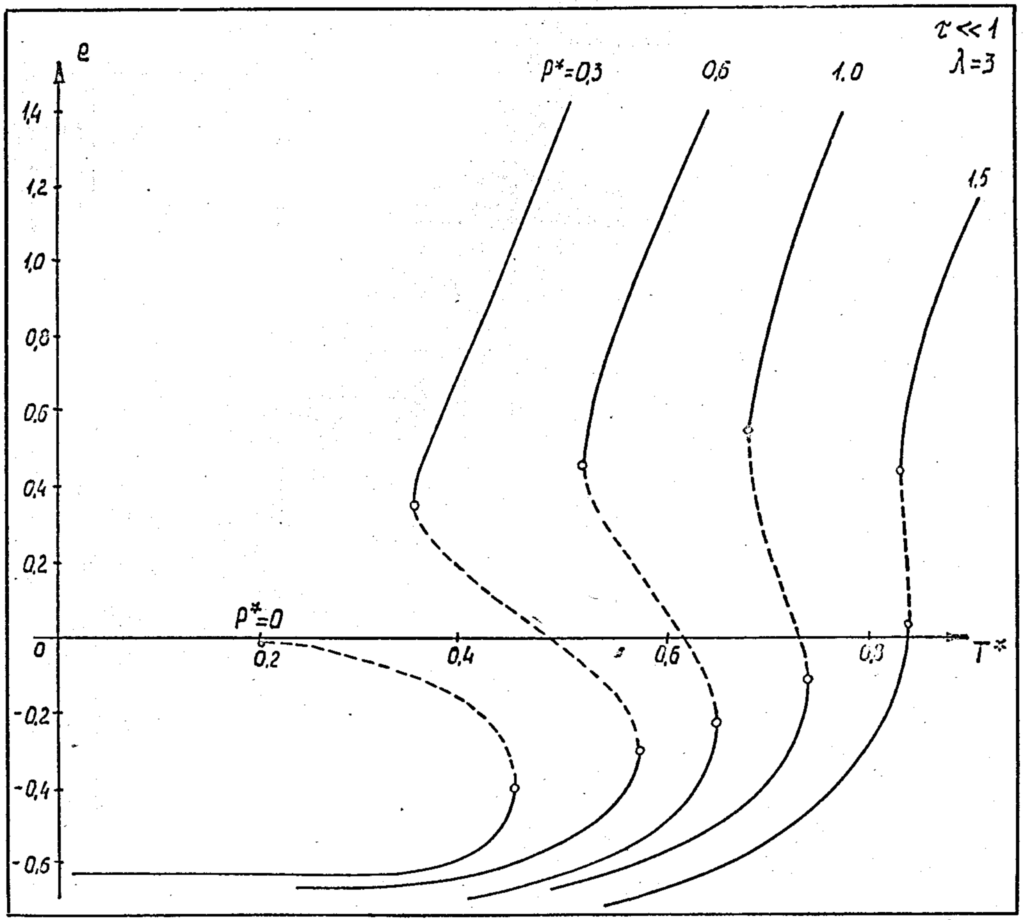

Fig. 3.6. The internal energy $e = \frac{1}{N\omega_{0L}} E$ as a function of the temperature T^* ($\lambda = 3$).

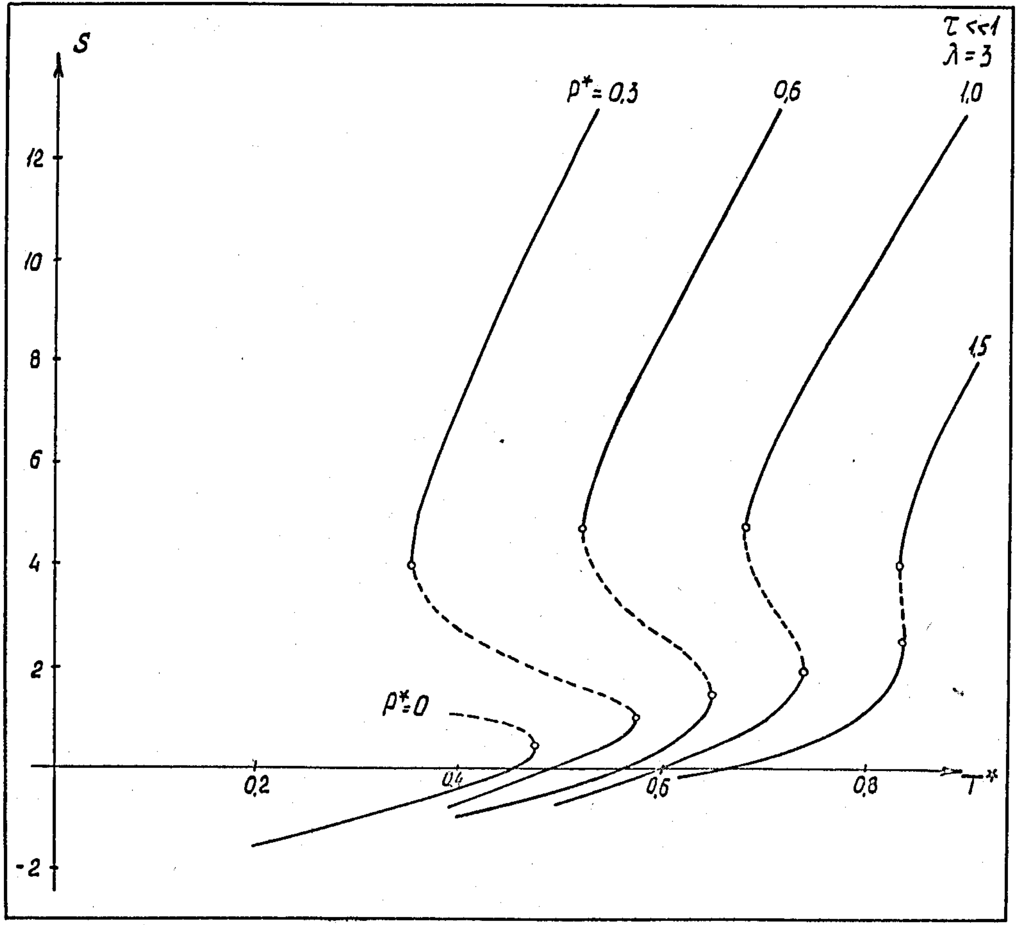

Fig. 3.7. The entropy $s = (1/Nk)S$ as a function of the temperature T^* ($-$ λ = 3).