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ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

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**THERMODYNAMICS OF STRONGLY
ANHARMONIC CRYSTALS .**

II. The High Temperature Limit

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In paper^{/1/} the properties of the f.c.c. lattice with the nearest neighbour central force interaction were considered in the case of the arbitrary external pressure. In the present paper the instability temperature, the critical temperature, the phonon frequencies, the phonon widths and the thermodynamical properties of the f.c.c. lattice are calculated in the high temperature limit.

The High Temperature Limit ($\theta \gg \omega_D$)

In^{/2/} an expression for the self-energy operator (1.4)^{x/} was obtained in the high temperature limit in the form

$$\Pi_k(\omega) = -\theta \frac{g^2(\theta, \ell)}{f^3(\theta, \ell)} \omega_k S_k\left(\frac{2\omega}{\omega_L}\right), \quad (2.1)$$

where $S_k\left(\frac{2\omega}{\omega_L}\right)$ is a dimensionless sum which was calculated in^{/3/} for some values $\{\vec{k}, j\}$, $\omega_L = \sqrt{8f(\theta, \ell)/M}$ is the maximum frequency of the lattice in the pseudoharmonic approximation, $\omega_D \approx 1.05\omega_L$. The notations are the same as in^{/1/}.

^{x/}The formulae of our previous paper^{/1/} are quoted as (1...), e.g. (1.4) means formula (1.4) of^{/1/}.

Equation (1.8) can be written in the high temperature limit taking into account the explicit form (2.1) of the self-energy operator approximately as in [2]

$$\frac{Z}{2} f(\theta, \ell) \overline{u^2(\ell)} = 3\theta \left\{ \left[1 - 0.11 \cdot \theta \cdot \frac{g^2(\theta, \ell)}{f^3(\theta, \ell)} \right]^{-1} + \frac{1}{24} \frac{\omega_L^2}{\theta^2} \right\}, \quad (2.2)$$

Taking into account (1.17), (1.18) and (1.22) the S.C. equation (2.2) can be written approximately as follows

$$F(y) = \frac{4y}{T^*} \left\{ 1 - \left[\frac{P^* \left(\frac{\ell}{r_0} \right)^2}{6 T^*} - B \right] y \right\} - \left\{ 1 - \left[\frac{P^* \left(\frac{\ell}{r_0} \right)^2}{3 T^*} - B \right] y \right\}^2 e^y = 0, \quad (2.3)$$

where $T^* = \theta / \epsilon$ is the reduced temperature, $B = 0.22 \{ 2 + 1/\gamma \}^2$. It is also convenient to introduce the dimensionless temperature $r = \theta / \omega_{0L} = \lambda T^* / 11.76$, where $\lambda = Z \epsilon / \epsilon_0^{(0)}$ is the dimensionless coupling constant of atoms, $\epsilon_0^{(0)} \approx 1.02 \omega_{0L}$ is the zero-point energy per atom in the harmonic approximation, $\omega_{0L} = \sqrt{8f/M}$ is the maximum value of the harmonical vibrational frequency.

We point out here that the S.C. equation (2.3) has different number of real solutions depending on the P^* , T^* values. The physical solution is that one, which coincides with the harmonic solution if the anharmonic terms tend to zero. The harmonic solution is given by

$$y_h = \frac{T^*}{4 \alpha_h^2} = \frac{T^*}{2 \left\{ 1 + \frac{P^*}{6} \left(\frac{\ell}{r_0} \right)_h^2 + \sqrt{1 + \frac{P^*}{6} \left(\frac{\ell}{r_0} \right)_h^2} \right\}}. \quad (2.4)$$

The dependence of the real solutions of the S.C. equation (2.3) on the reduced temperature T^* and reduced pressure P^* is given in Fig. 2.1. If the pressure ($P^* < P_o^*$) and the temperature ($T^* < T_o^*(P^*)$) are sufficiently low the S.C. equation (2.3) has real

solutions, the smallest being the physical one. It corresponds to a stable crystal state S_1 . The instability temperature $T_g^*(P^*)$ is determined by the coincidence of the two real solutions: $y_1(T_g^*) = y_2(T_g^*)$. Consequently the instability temperature $T_g^*(P^*)$ determined by this condition can be obtained by solving the following system of equations: $F(y) = 0$ and $F'(y) = 0$. Solution y_2 corresponds to an unstable state. In all figures the dotted lines denote the unstable state. For $T^* > T_g^*(P^*)$ the solutions y_1 and y_2 become complex conjugate therefore the phonon frequencies become complex conjugate too which shows the vibrational instability of the lattice in the state S_1 corresponding to the solution y_1 . It is worth-while to note that if $P^* > 0$ in the region $T^* \geq T_g^*$, the self-consistent equation (2.3) has another real solution y_3 which corresponds to a stable state S_2 .

In the region of sufficiently high pressure or temperature: $P^* \geq P_0^*$ or $T^* \geq T_0^*$, the S.C. equation (2.3) has always two real solutions, the smallest of them is the physical one, which is a smooth function of the temperature and the pressure. In this case the phonon frequencies are always real. The critical temperature T_0^* and the critical pressure P_0^* are characterized by the disappearance of the vibrational instability of the lattice and they are determined by the coincidence of three real solutions of the S.C. equation (2.3): $y_1(T_0^*, P_0^*) = y_2(T_0^*, P_0^*) = y_3(T_0^*, P_0^*)$ consequently they can be obtained from the solution of the following system of equations $F(y) = 0$, $F'(y) = 0$, $F''(y) = 0$.

The dependence of the reduced instability temperature T_g^* on the reduced pressure P^* is presented in Fig. 2.2. In the high temperature limit we get the following value for the critical pressure $P_0^* \approx 1.35$ and the critical temperature $T_0^* \approx 0.98$.

The frequencies of the renormalized phonons and their widths (1.3) according to (1.17), (1.18), (1.22) and (2.1) can be written in the following form

$$\frac{\epsilon_k}{\omega_{0k}} \approx a - \frac{3}{2} \cdot 10^{-2} \frac{1}{a} \left(2 + \frac{1}{\gamma}\right)^2, \quad (2.5)$$

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

(In the calculations the following approximate values were taken: $\text{Re } S_k \approx 3 \times 10^{-2}$, $\text{Im } S_k \approx 1 \times 10^{-2}$). 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

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

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

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

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

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

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 slightly lower than T_g^* . 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.

References

1. T. Siklós and V.L. Aksienov. JINR, E4-5772, Dubna (1971).
2. N.M. Plakida and T. Siklós. phys.stat.sol., 39, 171 (1970).
3. A.A. Maradudin, A.E. Fein and G.H. Vineyard. phys.stat.sol., 2, 1479 (1962).
A.A. Maradudin. phys. stat. sol., 2, 1493 (1962).
4. L. von Heimendahl. Diplomarbeit, Physik-Department, T.H. München, 1970.

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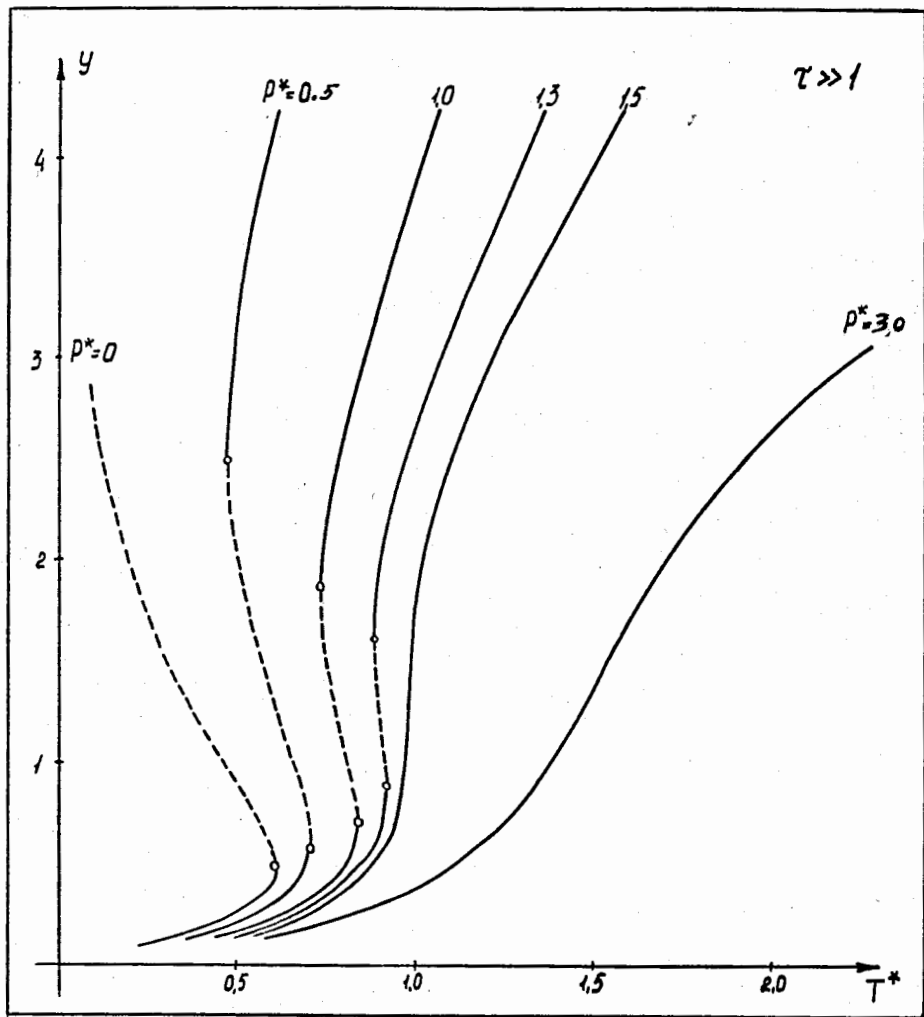


Fig. 2.1. The real solutions of the S.C. equation.

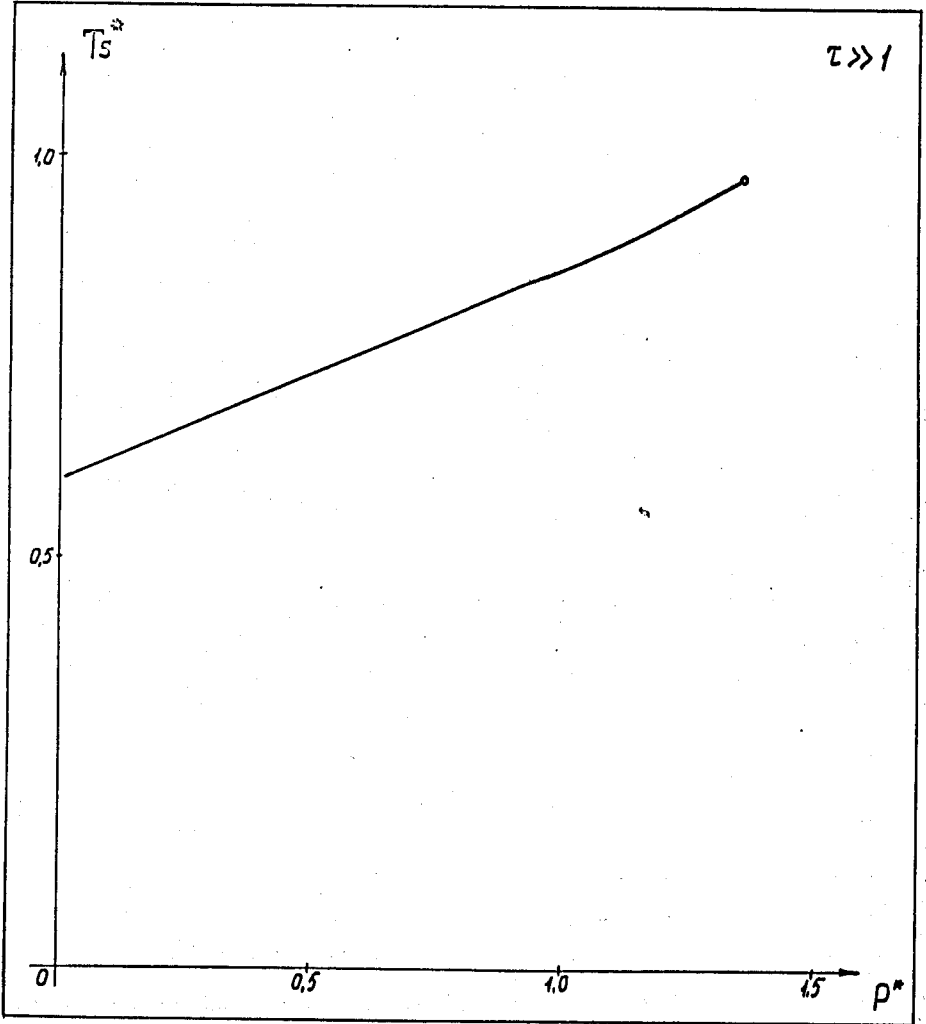


Fig. 2.2. The dependence of the instability temperature T_s^* on the reduced pressure P^* .

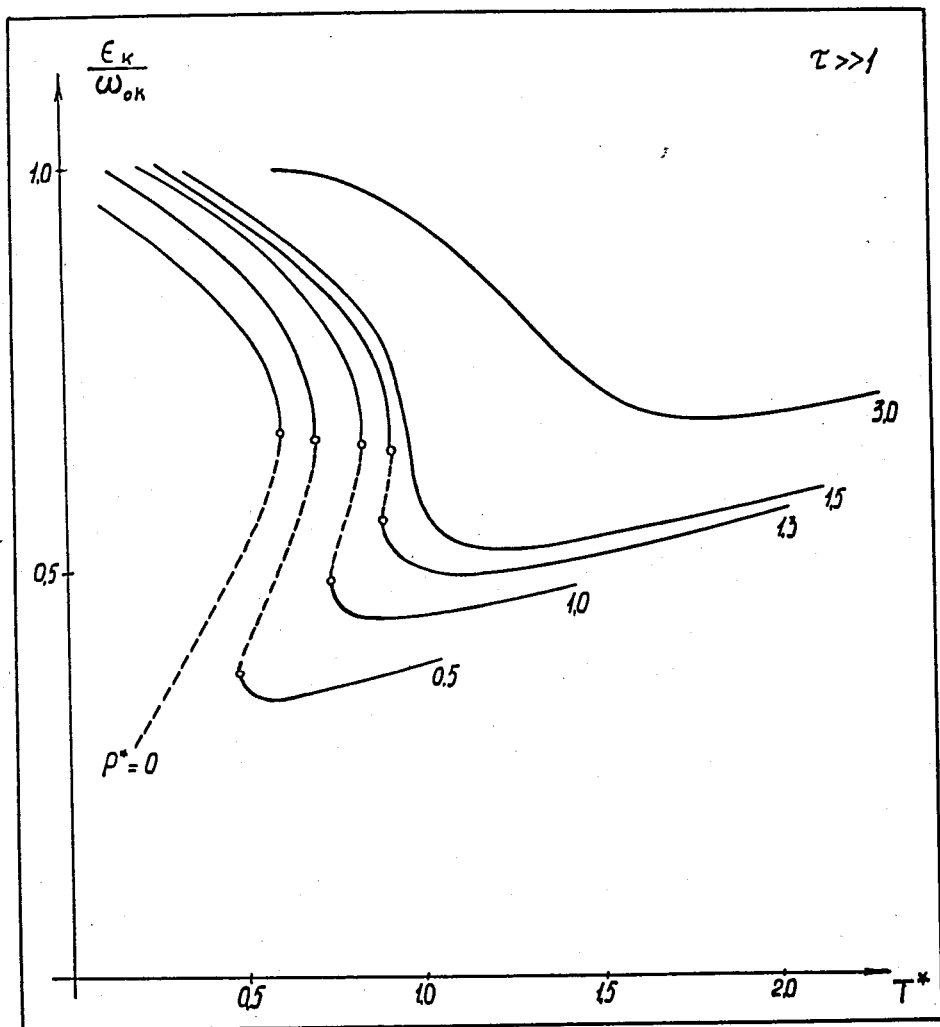


Fig. 2.3. The dependence of the renormalized phonon frequencies ϵ_k / ω_{0k} ($P^* = 0$) on the reduced temperature T^* .

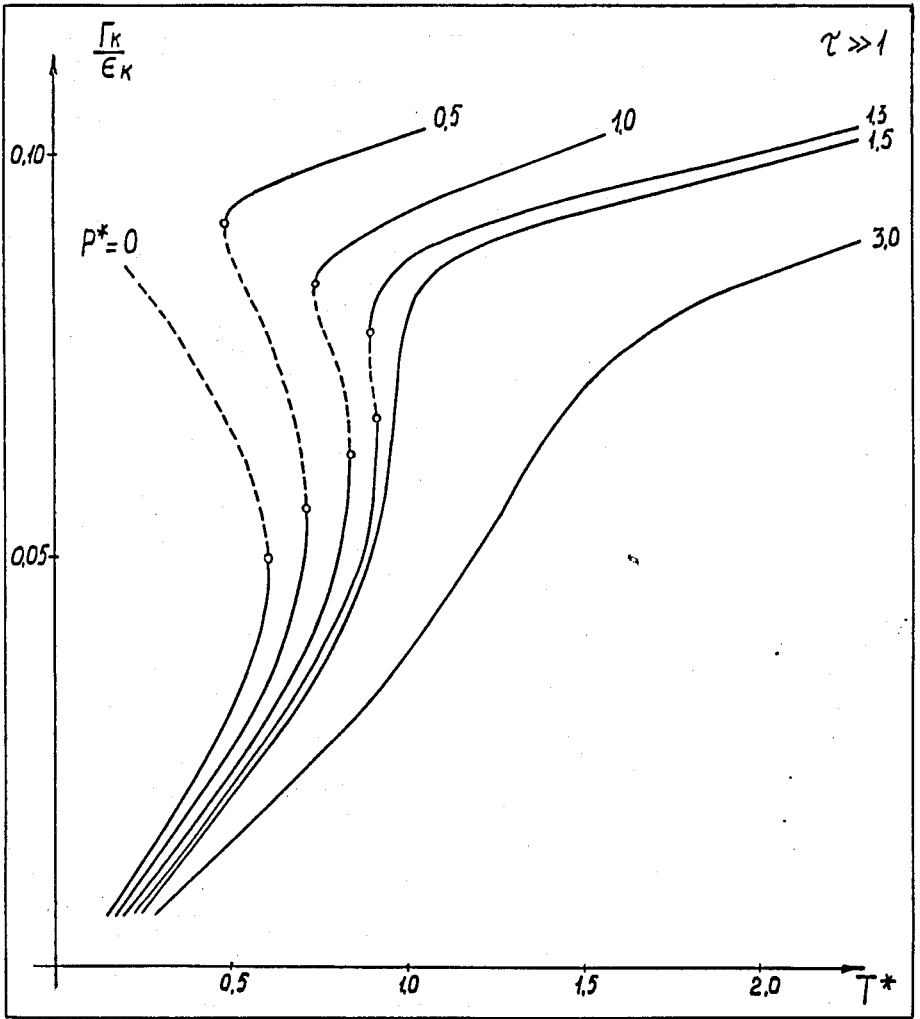


Fig. 2.4. The dependence of the phonon widths Γ_k / ϵ_k on the temperature T^* .

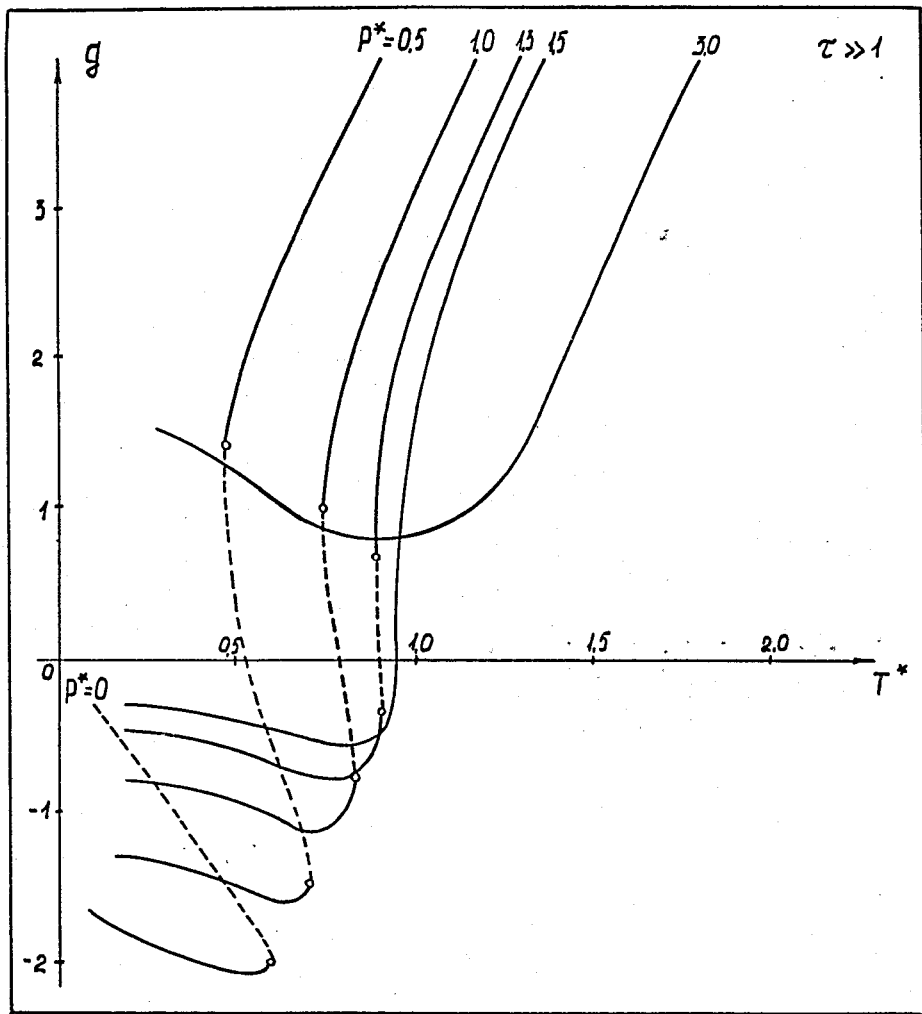


Fig. 2.5. The thermodynamical potential $g = f + p^* v^*$ as a function of the temperature T^* .

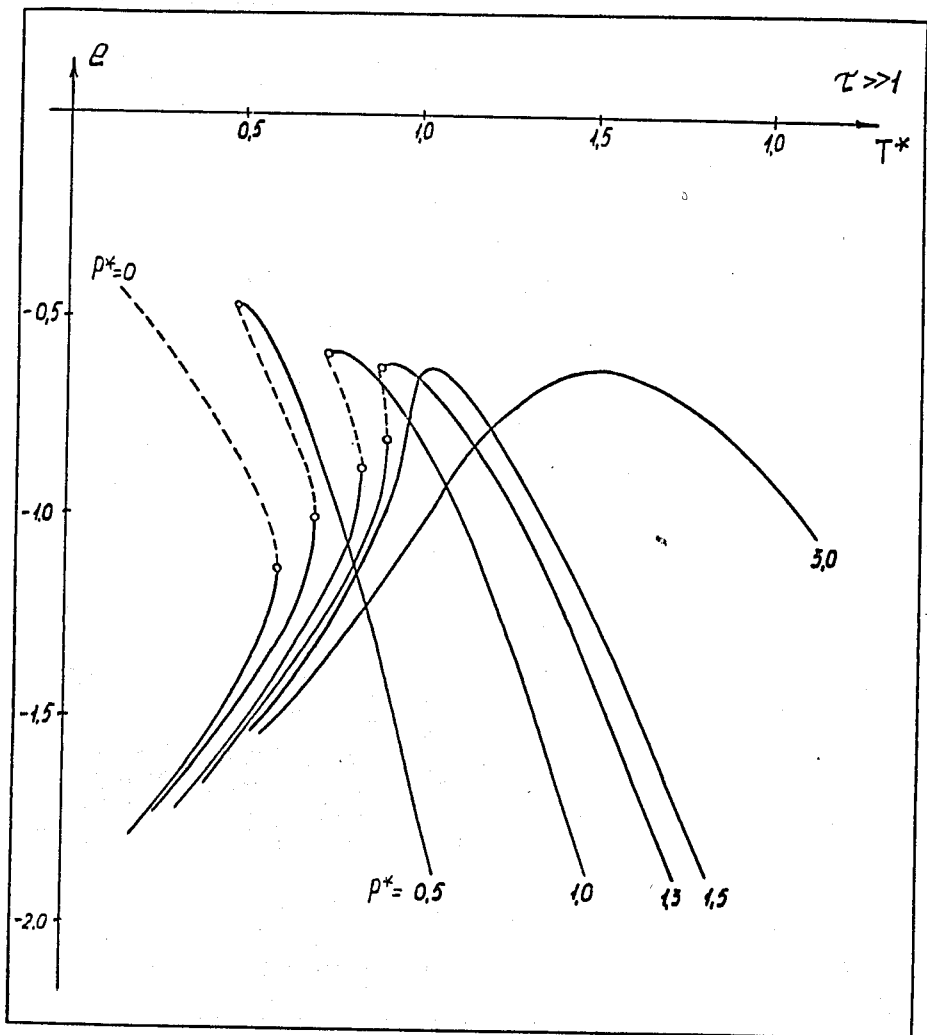


Fig. 2.6. The internal energy $e = (1/3 N \epsilon) E$ as a function of the temperature T^* .

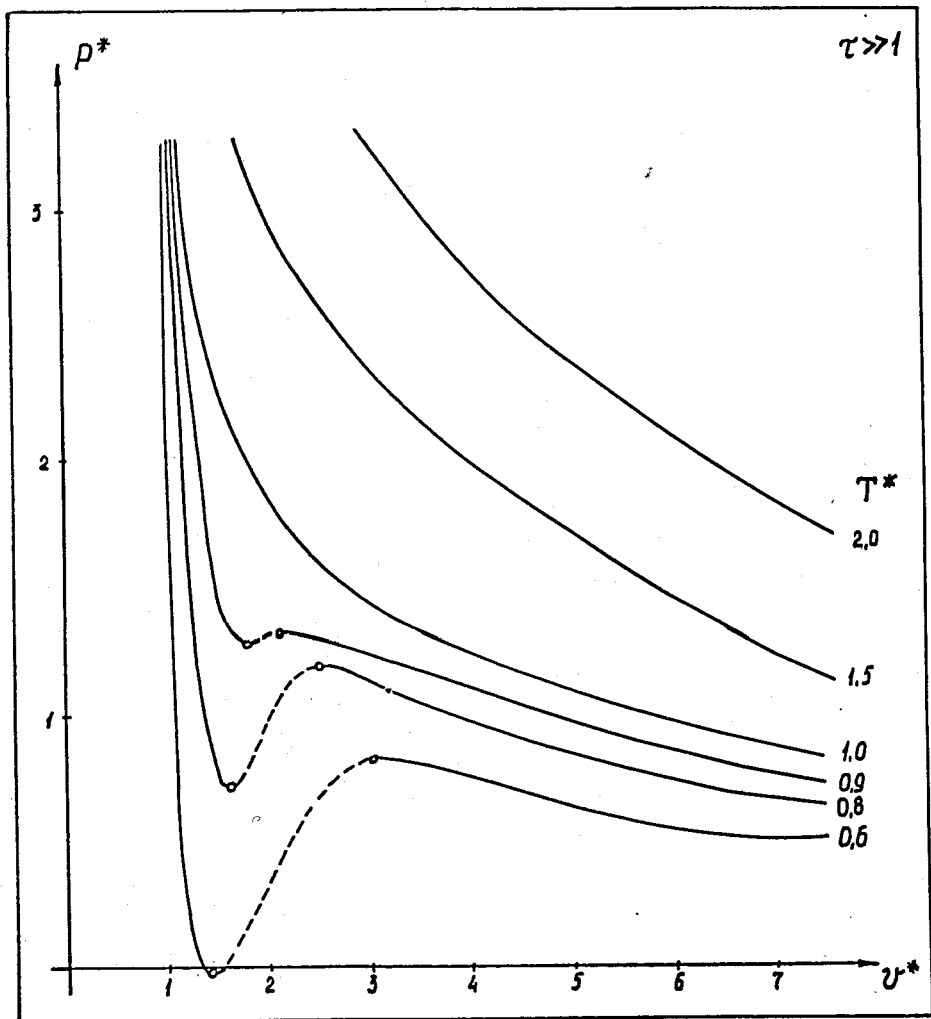


Fig. 2.7. The dependence of the reduced volume $v^* = (\ell/r_0)^3$ on the reduced pressure P^* .