ОБЪЕДИНЕННЫЙ
ИНСТИТУТ
ЯДЕРНЫХ
ИССЛЕДОВАНИЙ

Дубна

E4 - 5521

T. Siklós

THEORY OF ANHARMONIC CRYSTALS IN PSEUDOHARMONIC APPROXIMATION

III. Crystal with Weak Coupling

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

1970

E4 - 5521

T. Siklós

THEORY OF ANHARMONIC CRYSTALS IN PSEUDOHARMONIC APPROXIMATION

III. Crystal with Weak Coupling

Submitted to "Acta Physica Hungarica"

In the paper [1] the properties of the anharmonic linear chain were considered in pseudoharmonic approximation in the case of the arbitrary external tension. In this paper we present an additional investigation of the properties of the anharmonic linear chain with weak coupling of atoms $[\lambda = (\pi D/\omega_{0L}) \lesssim 2]$. As follows from the results of paper [1] it is necessary to investigate in this case the properties of the chain in the low temperature limit.

It was shown in [1] that the self-consistent equation, which determines the properties of the chain, can be written as follows:

$$\lambda \alpha\, y(\alpha) = \int_0^{\pi/2} d\varphi \sin\varphi \coth \frac{\alpha \sin\varphi}{2\tau}, \qquad (1)$$

where the notations are the same as in [1] and

$$y(\alpha) = \ln \frac{\alpha^2 - \frac{P^*}{6}}{\left(\alpha^2 - \frac{P^*}{3}\right)^2}\,. \qquad (2)$$

In the low temperature limit the self-consistent equation (1) can be rewritten in the following form:

$$\lambda \alpha\, y(\alpha) = 1 + \frac{\pi^2}{3}\left(\frac{\tau}{\alpha}\right)^2. \qquad (3)$$

According to [1], the instability temperature can be obtained as a simultaneous solution of the equation (3) and its derivative:

$$\lambda \left\{ y(\alpha) + \alpha\, y'(\alpha) \right\} = -\frac{2\pi^2}{3} \frac{\tau^2}{\alpha^3} . \qquad (4)$$

The critical temperature can be obtained as a simultaneous solution of the equations (3), (4) and the second derivative of (3):

$$\lambda \left\{ 2\, y'(\alpha) + \alpha\, y''(\alpha) \right\} = 2\pi^2 \frac{\tau^2}{\alpha^3} . \qquad (5)$$

It is convenient to rewrite the equations (3) – (5) in the following form:

$$\lambda = \frac{1 + \frac{\pi^2}{3}\left(\frac{\tau}{\alpha}\right)^2}{\alpha\, y(\alpha)} \qquad (6)$$

$$\lambda = -\frac{1 + \pi^2\left(\frac{\tau}{\alpha}\right)^2}{\alpha^2\, y'(\alpha)} \qquad (7)$$

$$\lambda = 2\,\frac{1 + 2\pi^2\left(\frac{\tau}{\alpha}\right)^2}{\alpha^3\, y''(\alpha)} . \qquad (8)$$

It is easy to see, that in the case of $P^* = 0$ the equations (7) and (8) are incompatible, consequently the critical temperature does not exist if $P^* = 0$. The analytical solution of the system of equations (6) - (8) in the case of $\tau = 0$ gives the following value for the critical tension $P_c^* = 0.055$, than $\alpha_c \approx 0.266$, $\lambda_0^{(c)} \approx 1,21$.

The results of numerical solutions of these systems of equations are given in Fig.1, 2. In Fig.1 the dependence of the instability temperature $\tau_s = (\theta_s / \omega_{oL})$ on the dimensionless coupling constant $\lambda = (\pi D / \omega_{oL})$ is given for some values of P^*. In Fig.2 the instability temperature is presented as a function of reduced tension P^* for some values of λ. In all Figures the critical curves are denoted by the dotted line.

We note here, that the results at the temperature τ= 0.1-0.2 agree quite well with the results of the paper [1] for the same temperature. The results obtained here agree quite well with the asymptotic expressions of work [2] for $P^* \ll 1$.

It is interesting to point out, that the critical temperature is equal to zero at finite pressure $P_c^* = 0.055$. As was shown in [3], the behaviour of the three-dimensional lattice does not differ qualitatively from the one-dimensional lattice discussed in [1] and consequently an analogous situation should take place in the three-dimensional case.

I should like to thank Dr. N.Plakida for helpful discussions and Dr. J.Esszenszki for his help in the numerical calculations.

References

1. T. Siklós. Acta Phys.Hung. (to be published);
JINR Report, E4-5389, Dubna, 1970.
2. N.M.Plakida, T.Siklós. Acta Phys.Hung., 26, 387 (1969).
3. T.Siklós. Acta Phys.Hung. (to be published);
JINR Report, E4-5390, Dubna, 1970.

Received by Publishing Department
on December 16, 1970

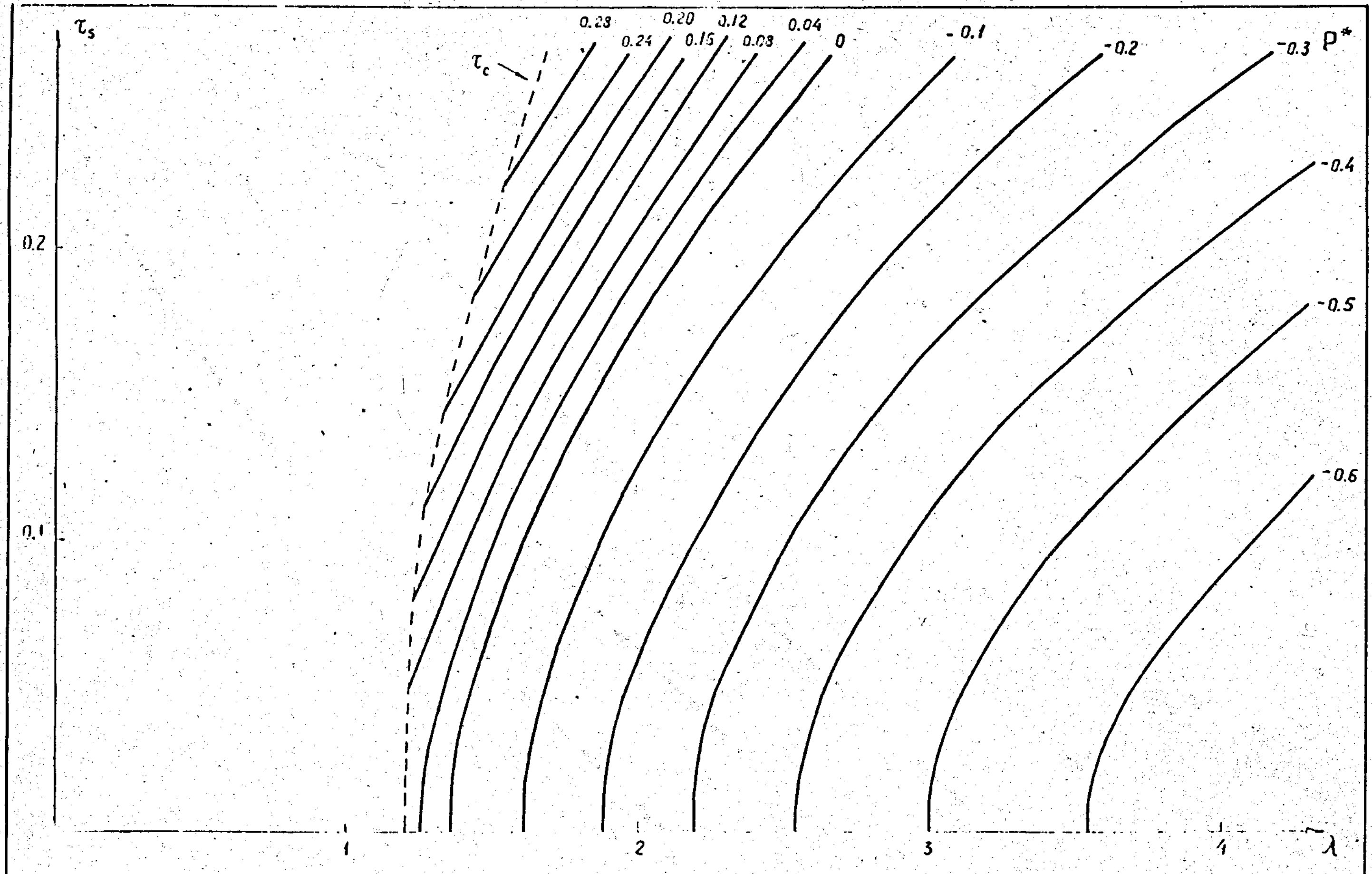

Fig.1 The dependence of the instability temperature $\tau_s = \Theta_s / \omega_{oc}$ on the dimensionless coupling constant λ of the atoms.

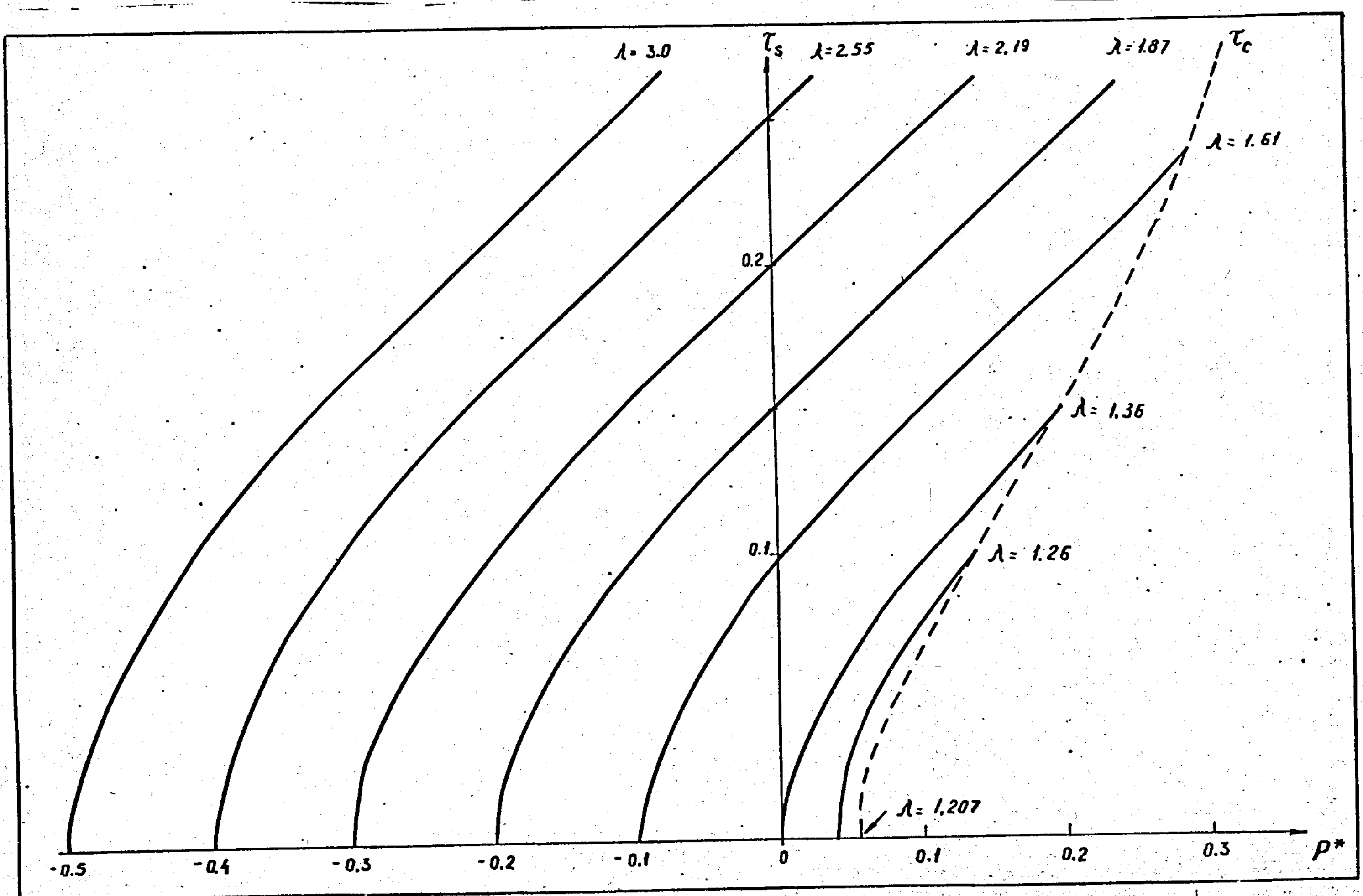

Fig.2 The dependence of the instability temperature τ_s

the reduced tension P^*