VARIATION OF THE NATURE OF THE ENERGY SPECTRUM THRESHOLD CHARACTERISTICS UNDER PRESSURE

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Possible changes in the nature of the decay threshold of quasiparticles in liquid He^4 due to increasing pressure are investigated. It is shown that when $k_c > 2k_0$ the energy spectrum begins to bend above 2Δ. Pressure-induced decay in the optical phonon spectrum of the crystal is also considered.

1. INTRODUCTION

PITAEVSKIĬ[1] has shown that the energy spectrum of elementary excitations of the Bose type has singularities at the points of the threshold of the decay of the excitations. It has turned out that there exist different types of thresholds, depending on the properties of the quasiparticles produced in the decay. At a given pressure, of course, one of the threshold types is realized. However, if the pressure is varied, then one type of threshold may go over, at a certain critical pressure, into another type. The threshold may also disappear completely. The present paper is devoted to an investigation of the properties of the spectrum at pressures close to critical.

In the second section we investigate the possible change of the character of the decay threshold in liquid He^4, and in the third we study the case of the appearance of a decay threshold under pressure in the optical phonon spectrum of a crystal.

2. THRESHOLD PHENOMENA IN LIQUID He^4

The experimental data[2] on the scattering of neutrons indicate that, actually, in liquid He^4 at normal pressure, there is probably realized a threshold for the decay of the quasiparticle into two rotons which are emitted at a certain angle to each other. The momentum and energy of the quasiparticle at the threshold point are $k_c < 2k_0$ and $\epsilon_c = 2\Delta$, while the momenta of the rotons are equal to k_0 and the dispersion law near this point is given by

$$\varepsilon(k) = 2\Delta - \alpha \exp\left\{-\frac{\beta}{k_c - k}\right\}, \tag{1}$$

where $\alpha > 0$ and $\beta > 0$ are certain constants, while the constants k_0 and Δ are determined by the form of the roton spectrum:

$$\varepsilon(k) = \Delta + \frac{1}{2\mu}(k - k_0)^2, \quad k = |\mathbf{k}|.$$

The spectrum curve terminates at the threshold point. Further experiments[3] have shown, however, that at increased pressure the spectrum curve possibly rises above the value $\epsilon = 2\Delta$. This can occur only if the threshold momentum k_c becomes larger than k_0 with increasing pressure. The pressure P_0 at which $k_c = 2k_0$ is the critical pressure. When $P > P_0$ the quasiparticle will decay into two rotons with parallel momenta.

In this section we investigate the properties of the spectrum at $k_c \approx 2k_0$ and $P \approx P_0$. The elementary-excitation spectrum is determined by the poles of the Green's function. The Dyson equation for the Green's function G and the equation for the total vertex Γ are[1]

$$G^{-1}(k) - G_0^{-1}(k) = i\int \Gamma_0(k; q, k-q) G(q) G(k-q)\ \Gamma(k; q, k-q)\frac{d^4q}{(2\pi)^4}$$

$$\Gamma(k; q, k-q) - \Gamma_0(k; q, k-q) = i\int \Gamma(k; q_1, k-q_1) G(q_1) G(k-q_1) \times \gamma(q_1, k-q_1; q, k-q)\frac{d^4q_1}{(2\pi)^4}, \tag{2}$$

where G_0 is the free Green's function, Γ_0 is the bare vertex part, γ is the irreducible four-particle vertex part[1)], and $k = \{\mathbf{k}, \epsilon\}$ and $q = \{\mathbf{q}, \omega\}$ are the four-momenta. In the calculation of the Green's function near the threshold, greatest interest attaches to the nonregular terms, which occur in the case of the singular integration in (2). In the case of the threshold connected with the decay into two rotons, such a singular integral is[1]

$$I(k) = \int \frac{d^3\mathbf{q}}{\varepsilon(\mathbf{q}) + \varepsilon(|\mathbf{k} - \mathbf{q}|) - \varepsilon}. \tag{3}$$

In the arguments of the functions, k will denote $\{\mathbf{k}, \epsilon\}$, and in all other cases it will denote $|\mathbf{k}|$. The integration (3) is carried out in the region $|\mathbf{q} - \mathbf{q}_c| \ll k_0$, where $\mathbf{q}_c$ is the threshold momentum of one of the rotons. The singularity in the integral (3) is connected with the fact that the denominator of the integrand vanishes at the threshold point we have $\mathbf{k} = \mathbf{k}_c$, $\mathbf{q} = \mathbf{q}_c$, and $\epsilon = \epsilon_c$:

$$\varepsilon_c = \varepsilon(\mathbf{q}_c) + \varepsilon(|\mathbf{k}_c - \mathbf{q}_c|),$$

where $\mathbf{q}_c$, $\mathbf{k}_c - \mathbf{q}_c$, and $\epsilon(\mathbf{q}_c)$, $\epsilon(|\mathbf{k}_c - \mathbf{q}_c|)$ are the momenta and the energies of the rotons produced in the decay.

We shall calculate (3) assuming $|k - 2k_0| \ll k_0$. For convenience in the calculation, we shall use the following device[4]. We determine the roton spectrum accurate to terms of fourth order in $k - k_0$, so that accurate to these terms we can write

$$\frac{(k - k_0)^2}{2\mu} \approx \frac{(k^2 - k_0^2)^2}{8k_0^2\mu}.$$

1) $\gamma(\mathbf{q}_1, \mathbf{k} - \mathbf{q}_1; \mathbf{q}, \mathbf{k} - \mathbf{q})$ is the set of all those three-particle diagrams which cannot be divided between the points $\mathbf{q}_1$, $\mathbf{k} - \mathbf{q}_1$, and $\mathbf{q}$, $\mathbf{k} - \mathbf{q}$ into two parts joined only by one or two lines.

We then have in place of (3)

$$I(k)=\int\left\{2\Delta-\varepsilon+\frac{(q^2-k_0^2)^2}{8k_0^2\mu}+\frac{(|\mathbf{k}-\mathbf{q}|^2-k_0^2)^2}{8k_0^2\mu}\right\}^{-1}d^3\mathbf{q}. \quad (4)$$

Now the integration in (4) can be extended to infinity, since the integral converges and the main contribution is made by the region of interest to us. Let us make the change of variable

$$\mathbf{u}=(2k_0\sqrt{\mu})^{-1/2}(\mathbf{q}-{}^1/_2\mathbf{k}),$$

and then

$$I(k)\infty\int\left\{2\Delta-\varepsilon+\left[u^2+\frac{1}{8k_0\sqrt{\mu}}(k^2-4k_0^2)\right]^2+\frac{(\mathbf{ku})^2}{2k_0\sqrt{\mu}}\right\}^{-1}d^3\mathbf{u}$$

(the symbol ∞ denotes equality apart from a regular coefficient and a regular addition).

As the result of the integrations we obtain the singular term

$$I(k)\infty\ln\frac{\sqrt{2\Delta-\varepsilon+s^2}+s}{a}, \quad (5)$$

where

$$s=\frac{1}{8k_0\sqrt{\mu}}(k^2-4k_0^2)\approx\frac{1}{2\sqrt{\mu}}(k-2k_0).$$

The corresponding singular term in the Green's function is

$$G^{-1}(k)\infty\left[\ln\frac{\sqrt{2\Delta-\varepsilon+s^2}+s}{\alpha_1}\right]^{-1}, \qquad \alpha_1>0. \quad (6)$$

The threshold is characterized by the presence of a branch point in the Green's function at $k = k_c$ and $\epsilon = \epsilon_c$. It is seen from (6) that two types of branch point are possible, and consequently two cases of threshold.

1. $s < 0$, $k_c < 2k_0$, $\epsilon_c = 2\Delta$. In this case there is a logarithmic branch point, and the threshold is connected with the decay of the excitation into two rotons with momenta k_0, emitted at an angle $\theta = 2\sqrt{(2k_0 - k_c)/k_0}$ relative to each other.

2. $s > 0$, $k_c > 2k_0$, $\epsilon_c = 2\Delta + (k_c - 2k_0)^2/4\mu$. In this case there is a root branch point, and the threshold is connected with the decay of the excitation into two rotons emitted parallel to each other, with momenta $q_c = k_c/2$.

Let us see how k_c varies when the pressure changes in this region. Assume that at a certain pressure P_0 we have $k_c(P_0) = 2k_0(P_0)$. We obtain the total Green's function at $k_c = 2k_0$ and $\epsilon_c = 2\Delta$ by adding to the irregular term the regular ones; recognizing also that $G^{-1}(2k_0, 2\Delta) = 0$, we have

$$G^{-1}(k)=A^{-1}\left[\beta\left(\ln\frac{\sqrt{2\Delta-\varepsilon+s^2}+s}{\alpha_1}\right)^{-1}-(k-2k_0)\right], \quad (7)$$

where $\alpha_1 > 0$ and $\beta > 0$ are certain constants.

To determine the dependence of k_c and ϵ_c on the pressure, we assume that the pressure decreases by ΔP, and then k_c and ϵ_c also change. We expand in (7) accurate to terms of first order in $\Delta P = P - P_0$, $\Delta k_c = k_c - 2k_0$, $\Delta\epsilon_c = \epsilon_c = 2\Delta$. It is assumed here that all the coefficients are regular functions of the pressure.

At the new threshold point we have

$$G^{-1}(k_c)= \quad (8)$$

$$=A^{-1}\left[\beta\left(\ln\frac{\sqrt{-\Delta\varepsilon_c+(\Delta k_c)^2/4\mu}+\Delta k_c/2\sqrt{\mu}}{\alpha_1}\right)^{-1}-\Delta k_c+\lambda\Delta P\right]=0.$$

An investigation of this equation shows that the following solutions are possible.

1. $\lambda\Delta P < 0$; in this case

$$\varepsilon_c=2\Delta,\ \Delta k_c=\lambda\Delta P<0. \quad (9)$$

2. $\lambda\Delta P > 0$; in this case

$$\varepsilon_c=2\Delta+(\Delta k_c)^2/4\mu,\ \ \Delta k_c>0$$

and is determined from the equation

$$\beta\left[\ln\frac{\Delta k_c}{2\alpha_1\sqrt{\mu}}\right]^{-1}-\Delta k_c+\lambda\Delta P=0. \quad (10)$$

This equation has a solution at any arbitrarily small $\lambda\Delta P > 0$.

Let us determine the form of the spectrum near the threshold in both cases.

1. $k_c < 2k_0$. In this case the Green's function and $\epsilon(k)$ near the threshold are given by

$$G^{-1}(k)=A^{-1}\left[\beta\left(\ln\frac{\sqrt{2\Delta-\varepsilon+s^2}+s}{\alpha_1}\right)^{-1}-(k-k_c)\right], \quad (11)$$

$$\varepsilon(k)=2\Delta-\alpha_1\exp\left\{-\frac{\beta}{k_c-k}\right\}\left(\frac{2k_0-k_c}{\sqrt{\mu}}+\alpha_1\exp\left\{-\frac{\beta}{k_c-k}\right\}\right) \quad (12)$$

or, accurate to exponentially small terms,

$$\varepsilon(k)=2\Delta-\bar{\alpha}(2k_0-k)\exp\left\{-\frac{\beta}{k_c-k}\right\} \qquad k<k_c<2k_0. \quad (13)$$

We note that in (13), unlike in (1), the pre-exponential coefficient depends essentially on k.

2. Analogously, when $k_c > 2k_0$, we have

$$G^{-1}(k)=A^{-1}\left[\beta\left(\ln\frac{\sqrt{2\Delta-\varepsilon+s^2}+s}{\alpha_1}\right)^{-1}-\beta\left(\ln\frac{s}{\alpha_1}\right)^{-1}-(k-k_c)\right] \quad (14)$$

and the spectrum is given by

$$\varepsilon(k)=2\Delta-\alpha_1e^{-r}\left(\frac{2k_0-k}{\sqrt{\mu}}+\alpha_1e^{-r}\right), \qquad k<k_c, \quad (15)$$

where

$$r=\beta\Big/\left[(k_c-k)-\beta\left(\ln\frac{k-2k_0}{2\alpha_1\sqrt{\mu}}\right)^{-1}\right]. \quad (16)$$

$$k_c-k\gg-\beta\left(\ln\frac{k-2k_0}{\alpha_2}\right)^{-1},$$

i.e., when $k \approx 2k_0$, the spectrum, as expected, goes over into (12) and has an exponential character. When

$$k_c-k\ll-\beta\left(\ln\frac{k-2k_0}{\alpha_2}\right)^{-1},$$

i.e., when $k \approx k_c$, it assumes a power-law form

$$\varepsilon(k)=2\Delta+\frac{1}{4\mu}(k-2k_0)^2. \quad (17)$$

In this region, the spectrum bends above 2Δ.

In both cases the spectrum terminates at the threshold point. It is not clear at present, however, whether k_c actually increases with increasing pressure and whether the pressure P_0 is reached before the helium solidifies.

3. THRESHOLD PHENOMENA IN CRYSTALS

In this part of the paper we consider the dependence of the spectrum of the vibrational excitations of the crystal on the pressure near threshold. Just as in the first part, we shall consider only the threshold of decay into two excitations. However, unlike in liquid He^4, in a crystal the decay-causing interaction between the quasiparticles is weak, and therefore the corresponding investigation can be carried out more completely. The three-particle interaction of interest to us is connected with anharmonicity and is described in the Hamiltonian by the following term:

$$H_{int}=\frac{\gamma}{\sqrt{V}}\sum_{\mathbf{k},\mathbf{q}}\sqrt{\varepsilon_0(\mathbf{k})\,\varepsilon_1(\mathbf{q})\,\varepsilon_2(\mathbf{k}-\mathbf{q})}\,a_{\mathbf{q}}^{+}a_{\mathbf{k}-\mathbf{q}}^{+}a_{\mathbf{k}}+\text{c.c.},\qquad(18)$$

where $\gamma\sim(\rho c^2)^{1/2}$ is the interaction constant, ρ the density, and c the velocity of sound.[2)] The summation over the polarizations has been omitted. The dimensionless interaction constant is here $\alpha\sim(\rho c a^4)^{-1/2}\ll 1$, and a is the interatomic distance. We shall assume that $\epsilon_0(\mathbf{k})$, which is the spectrum of the decaying excitations without allowance for the interaction), and $\epsilon_1(\mathbf{q})$ and $\epsilon_2(\mathbf{q})$, which are the spectra of the produced quasiparticles, are all specified, and that the pressure dependence of the parameters that enter in the spectra is also known. To determine the threshold, however, it is necessary to know the exact spectrum $\epsilon(\mathbf{k})$, i.e., the spectrum of the excitations with allowance for the interaction. Nonetheless, by virtue of the weakness of the interaction, $\epsilon(\mathbf{k})$ does not differ strongly from $\epsilon_0(\mathbf{k})$, and consequently that region of the values of k, q, and P, in which the solution of the equation $\epsilon_0(\mathbf{k})=\epsilon_1(\mathbf{q})+\epsilon_2(\mathbf{k}-\mathbf{q})$ appears, will be close to the true threshold region. On the other hand, an exact determination of the threshold and of its pressure dependence will be carried out only after $\epsilon(\mathbf{k})$ is determined. Let us assume that in the threshold region the decaying excitation has a spectrum with minimum at k = 0, and the spectrum of the produced excitations is symmetrical with respect to q with a maximum at $\mathbf{q}=\pm\mathbf{q}_0$, it being assumed also that the crystal has a symmetry center[3)]. Without allowance for the interaction, all the coefficients in the spectrum are assumed to be regular functions of the pressure. Just as in the first part of the paper, a diagram of the type shown in Fig. 1 is significant. We have

$$G^{-1}(k)=G_0^{-1}(k)-\Sigma(k),\qquad(19)$$

$$\Sigma(k)=\frac{i\gamma^2}{(2\pi)^4}\int G_0(q)\,G_0(k-q)\,d^4q,\qquad(20)$$

$$G_0(k)=\frac{\varepsilon_0^2(\mathbf{k})}{\varepsilon^2-\varepsilon_0^2(\mathbf{k})+i\delta},\qquad(21)$$

$$\begin{aligned}\Sigma(k)&=\frac{i\gamma^2}{(2\pi)^4}\int\frac{\varepsilon_1^2(\mathbf{q})}{\omega^2-\varepsilon_1^2(\mathbf{q})+i\delta}\,\frac{\varepsilon_2^2(\mathbf{k}-\mathbf{q})}{(\varepsilon-\omega)^2-\varepsilon_2^2(\mathbf{k}-\mathbf{q})+i\delta}\,d^3\mathbf{q}\,d\omega\\&=\frac{\gamma^2}{16\pi^3}\int\varepsilon_1(\mathbf{q})\,\varepsilon_2(\mathbf{k}-\mathbf{q})\,\frac{\varepsilon_1(\mathbf{q})+\varepsilon_2(\mathbf{k}-\mathbf{q})}{\varepsilon^2-[\varepsilon_1(\mathbf{q})+\varepsilon_2(\mathbf{k}-\mathbf{q})]^2+i\delta}\,d^3\mathbf{q}.\end{aligned}\qquad(22)$$

An irregular term appears in (22) upon integration in the vicinity of the threshold value of q in the threshold region of the variables ϵ and k. To simplify the subsequent derivations, we use the simplest form of the expansion of $\epsilon_0(\mathbf{k})$, $\epsilon_1(\mathbf{q})$, and $\epsilon_2(\mathbf{q})$ in the threshold region:

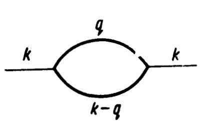

FIG. 1

[2)]We use a system of units in which h = 1.

[3)]It is possible to take the spectrum of the decaying excitations with a maximum at k = 0, and the spectrum of the decay excitations with a minimum at $q=\pm q_0$.

$$\begin{aligned}&\varepsilon_0(k)=\Delta+\frac{1}{2\mu}k^2,\qquad \varepsilon_1(\mathbf{q})=\Delta_1-\frac{1}{\mu_1}(\mathbf{q}-\mathbf{q}_0)^2,\\&\varepsilon_2(\mathbf{q})=\Delta_1-\frac{1}{\mu_1}(\mathbf{q}+\mathbf{q}_0)^2,\qquad \Delta(P_0)=2\Delta_1(P_0).\end{aligned}\qquad(23)$$

It is easy to generalize the results obtained below to include the case of the more general expansion (23).

Using the expansion (23), we obtain for the irregular term the following expression:

$$\begin{aligned}\Sigma(k)&\propto\int\frac{d^3\mathbf{q}}{\varepsilon-2\Delta_1+\mu_1^{-1}[(\mathbf{q}-\mathbf{q}_0)^2+(\mathbf{k}-\mathbf{q}+\mathbf{q}_0)^2]+i\delta}\propto\\&\propto\int\frac{d^3\mathbf{q}}{\varepsilon-\varepsilon_{\text{thr}}(\mathbf{k})+2\mu_1^{-1}[(\mathbf{q}-\mathbf{q}_0)+{}^1/_2\mathbf{k}]^2+i\delta},\end{aligned}\qquad(24)$$

where $\epsilon_{\text{thr}}=2\Delta_1-k^2/2\mu_1$. In (24), the integration is carried out in the region $|\mathbf{q}-\mathbf{q}_0-\frac{1}{2}\mathbf{k}|\ll q_0$. The exact value of the coefficient in front of the irregular term will be given later. To calculate (24), we use the following device. We introduce $\xi=\epsilon-\epsilon_{\text{thr}}(\mathbf{k})$ and differentiate Σ with respect to ξ; then

$$\frac{\partial\Sigma}{\partial\xi}\propto-\int\frac{d^3\mathbf{q}}{[\xi+2(\mathbf{q}-\mathbf{q}_0-{}^1/_2\mathbf{k})^2/\mu_1+i\delta]^2}.\qquad(25)$$

It is possible to extend the integration in the resultant integral to infinity, since the integral converges and the main contribution is made by the region of interest to us. Therefore the integral in (25) can be readily calculated by making the change of variable $\mathbf{u}=\mathbf{q}-\mathbf{q}_0-\frac{1}{2}\mathbf{k}$:

$$\frac{\partial\Sigma}{\partial\xi}\propto-\int_{-\infty}^{+\infty}\frac{u^2du}{[\xi+2u^2/\mu_1+i\delta]^2}\propto-\frac{1}{\sqrt{\xi}},$$

$\xi>0$, whence

$$\Sigma\propto-\sqrt{\xi},\quad \xi>0.\qquad(26)$$

When $\xi<0$, it is easy to show that

$$\Sigma\propto-i\sqrt{|\xi|},\qquad(27)$$

and the coefficients in (26) and (27) are identical. As the result we find that the Green's function near the pole in the threshold region is given by

$$\begin{aligned}&G^{-1}(k)=A^{-1}[\varepsilon-\varepsilon_0(k)+2b\sqrt{\varepsilon-\varepsilon_{\text{thr}}(k)+i\delta}],\\&b=\frac{\gamma^2}{128\pi}\Delta^3\left(\frac{\mu_1}{2}\right)^{3/2}\sim\alpha^2\sqrt{\Delta}.\end{aligned}\qquad(28)$$

The regular term that arises in (22) following integration over the remote regions is included in Δ, leading to an inessential ($\sim\alpha^2$) renormalization of Δ.

The spectrum $\epsilon(\mathbf{k})$ is of the form

$$\varepsilon(k)=\varepsilon_0(k)+2b^2-2b\sqrt{b^2+\varepsilon_0(k)-\varepsilon_{\text{thr}}(k)}\qquad(29)$$

and is determined by the choice of the branch of the root in (28) in accordance with (26) and (27). We note also that

$$\varepsilon_{\text{thr}}(k)=\max[\varepsilon_1(\mathbf{q})+\varepsilon_2(\mathbf{k}-\mathbf{q})],$$

and the threshold is determined from the condition

$$\varepsilon_c=\varepsilon(k_c)=\varepsilon_{\text{thr}}(k_c).\qquad(30)$$

Let us determine now the dependence of the spectrum and of the threshold on the pressure. To this end we substitute $\epsilon_0(\mathbf{k})$ and $\epsilon_{\text{thr}}(\mathbf{k})$ in (28) and (29) and expand with respect to the pressure accurate to terms of first order in $P-P_0$. It is important here that the quantities ϵ_0, ϵ_1, and ϵ_2 are independent of the interaction and are therefore regular functions of the pressure:

$$G^{-1}(k) = A^{-1}\left[\Delta\varepsilon - \frac{k^2}{2\mu} + 2b\sqrt{\Delta\varepsilon + \frac{k^2}{2\mu_1} + \eta}\right], \tag{31}$$

$$\varepsilon(k) = \Delta + \frac{k^2}{2\mu} + 2b^2 - 2b\left[b^2 + \frac{1}{2}k^2\left(\frac{1}{\mu} + \frac{1}{\mu_1}\right) + \eta\right]^{1/2}, \tag{32}$$

where

$$\Delta\varepsilon = \varepsilon - \Delta, \quad \eta = \left(\frac{\partial\Delta}{\partial P} - 2\frac{\partial\Delta_1}{\partial P}\right)_{P=P_0}(P - P_0).$$

An investigation of the expressions (30)—(32) shows that there are the following regions of the behavior of the spectrum as a function of the pressure.

1. $\eta > 0$. There are no threshold points for any value of k.

2. $\eta = 0$. A threshold point arises at $k_c = 0$ and $\epsilon_c = \Delta$.

3. $\eta < 0$. Then

$$k_c = \left[2|\eta|\frac{\mu_1\mu}{\mu_1 + \mu}\right]^{1/2}, \quad \varepsilon_c = \varepsilon_{\text{thr}}(k_c) = \Delta + \frac{k_c^2}{2\mu}.$$

The spectrum exists when $k > k_c$, and k_c is the termination point of the spectrum. The spectrum vanishes when $k < k_c$. The behavior of the spectrum is shown schematically in Fig. 2. Here $\eta_1 = b^2\mu(\mu + 2\mu_1)/\mu_1^2$ and is determined from the condition

$$\left.\frac{\partial^2\varepsilon}{\partial k^2}\right|_{k=0,\ \eta=\eta_1} = 0.$$

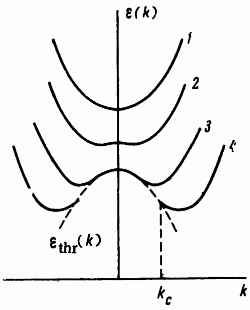

FIG. 2. Schematic diagram of the behavior of the spectrum: $1 - \eta > \eta_1 > 0$, $2 - \eta_1 > \eta > 0$, $3 - \eta = 0$, $4 - \eta < 0$.

Attention should be called to the fact that in the pre-threshold region, when $\eta < \eta_1$, the minimum on the curve of the spectrum must be replaced by a maximum. This can facilitate an experimental observation of the phenomenon. One might assume that such a behavior of the spectrum at $P = P_0$ would lead to singularities in the thermodynamic functions of the crystal. It can be shown, however, that this is not the case. The thermodynamic potential of the crystal is a regular function of the pressure at $P = P_0$.

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