101 (1957); 8, 70 (1959)].

[2] K. Huang and C. N. Yang, Phys. Rev. 105, 767 (1957).

[3] T. D. Lee and C. N. Yang, Phys. Rev. 105, 1119 (1957).

[4] A. A. Abrikosov and I. M. Khalatnikov, Zh. Eksp. Teor. Fiz. 33, 1154 (1957) [Sov. Phys. JETP 6, 888 (1958)].

[5] V. M. Galitskiĭ, Zh. Eksp. Teor. Fiz. 34, 151 (1958) [Sov. Phys. JETP 7, 104 (1958)].

[6] J. Bardeen, G. Baym, and D. Pines, Phys. Rev. 156, 207 (1967).

[7] I. M. Khalatnikov, Teoriya sverkhtekuchesti (Theory of Superfluidity), Nauka, 1971.

[8] E. P. Bashkin and A. É. Meĭrovich, Pis'ma Zh. Eksp. Teor. Fiz. 26, 696 (1977) [JETP Lett. 26, 534 (1977)].

[9] E. P. Bashkin, Pis'ma Zh. Eksp. Teor. Fiz. 25, 3 (1977) [JETP Lett. 25, 1 (1977)]; Zh. Eksp. Teor. Fiz. 73, 1849 (1977) [Sov. Phys. JETP 46, (1977)].

[10] A. A. Abrikosov and I. E. Dzyaloshinskiĭ, Zh. Eksp. Teor. Fiz. 35, 771 (1958) [Sov. Phys. JETP 8, 535 (1959)].

[11] I. M. Khalatnikov, Zh. Eksp. Teor. Fiz. 55, 1919 (1968) [Sov. Phys. JETP 28, 1014 (1959)].

[12] N. R. Brubaker, D. O. Edwards, R. E. Sarwinski, P. Seligman, and R. A. Sherlock, Phys. Rev. Lett. 25, 715 (1970).

[13] B. N. Esel'son, V. A. Slyusarev, V. I. Sobolev, and M. A. Strzhemechnyĭ, Pis'ma Zh. Eksp. Teor. Fiz. 21, 253 (1975) [JETP Lett. 21, 115 (1975)].

[14] D. O. Edwards, E. M. Ifft, and R. E. Sarwinski, Phys. Rev. 177, 380 (1969).

[15] V. P. Silin, Zh. Eksp. Teor. Fiz. 33, 1227 (1957) [Sov. Phys. JETP 6, 945 (1958)].

[16] I. M. Khalatnikov, Pis'ma Zh. Eksp. Teor. Fiz. 5, 288 (1967) [JETP Lett. 5, 235 (1967)].

[17] A. A. Abrikosov and I. M. Khalatnikov, Zh. Eksp. Teor. Fiz. 32, 1083 (1957) [Sov. Phys. JETP 5, 887 (1957)].

[18] G. A. Brooker and J. Sykes, Phys. Rev. Lett. 21, 279 (1968).

[19] A. F. Andreev, V. I. Marchenko, and A. E. Meĭerovich, Pis'ma Zh. Eksp. Teor. Fiz. 26, 40 (1977) [JETP Lett. 26, 36 (1977)].

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Phonon spectrum and local vibrations in strongly anisotropic crystals

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The polarization of vibrations and behavior of the vibration plane in layer and chain crystals are investigated throughout the continuous spectral band. It is shown that there are at least four critical points. The density of flexural vibrations exhibits a standard square-root kink only is very narrow regions next to critical points located close to the lower limit of the spectrum. Outside these regions the behavior of the vibration density is quite different. The influence of anisotropy on the properties of local vibrations is considered. It is established that the threshold of appearance of local vibrations is considerably less than in an isotropic crystal and that the shape of the localization region is extremely anisotropic.

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1. INTRODUCTION

In 1952, I.M. Lifshitz[1] first drew attention to the existence—in strongly anisotropic crystals with layer or chain structures—of "flexural" vibrations resembling flexural waves in noninteracting atomic layers or chains. He pointed out a considerable qualitative difference between long-wavelength flexural vibrations and vibrations polarized in the plane of a layer or along a chain. This difference is manifested in a number of properties of a crystal and, in particular, it gives rise to an unusual temperature dependence of the specific heat at low temperatures.

The recent years have seen concentration of attention on the conducting properties of strongly anisotropic crystals. Less work has been done on the phonon spectra of these crystals. This accounts for the absence, up until now, of a complete description of the properties of the density of vibrations in such crystals. Only some characteristic features of the behavior of this density are known for layer crystals at low frequencies[2] and these indicate that the influence of anisotropy on the phonon spectrum may be very considerable. For example, the formation of a sharp peak on the curve representing the density of flexural vibrations near the lower limit of the spectrum is reported by Kosevich.[2] However, the parameters of this peak have not yet been investigated. Moreover, the problem of the number, nature, and positions of the Van Hove critical points throughout the vibration spectrum of these crystals has not been tackled.

There is also considerable interest in the properties of local vibrations in strongly anisotropic crystals. The existence of local vibrations near point defects in crystals was first pointed out by I. M. Lifshitz in 1947.[3] These vibrations appear near various imperfections of the lattice and have been investigated quite thoroughly for isotropic crystals.[4,5] However, up to now the problem of the influence of a strong anisotropy on the properties of local vibrations has not been considered. We may expect local vibrations in strongly anisotropic crystals to have properties different from those in isotropic crystals. In fact, since planar layers and linear chains of atoms with a strong interaction are physically separate in layer and chain crystals, they should exhibit features characteristic of two- and one-dimensional systems (i.e., of systems existing in spaces with two or one dimension). However, it is clear from quantum mechanics [6] that the formation of a bound state, such a local vibration, occurs in such systems under conditions very different from those in the three-dimensional case. However, the problem does not reduce completely to a standard situation. A strongly anisotropic crystal is a three-dimensional body and although the three-dimensional effects can, in a sense, be regarded as "weak," they cannot be excluded completely. Therefore, the nature of vibrations in layer and chain crystals is governed by the competition between two factors: the three-dimensional nature of the crystal and its "low-dimensional" aspect, i.e., the tendency for the appearance of properties typical of two- and one-dimensional systems. A strongly anisotropic crystal behaves as two- or one-dimensional throughout most of its frequency spectrum and only in the immediate vicinity of singularities on the frequency axis and near the limits of the spectrum do the three-dimensional properties become of primary importance.

We shall investigate the phonon spectrum and properties of local vibrations near a point defect in layer and chain crystals. In our study of the vibration density $g(\epsilon)$ ($\epsilon = \omega^2$ is the square of the vibration frequency) attention will be concentrated on the behavior of this density near the Van Hove critical points. This is greatly facilitated by the circumstance that the properties of $g(\epsilon)$ near singularities are governed primarily by the topology of the constant-frequency surfaces of a crystal and depend relatively weakly on the detailed form of the dispersion law. Therefore, it is sufficient to know only the first few terms of the expansion of the dispersion law in the vicinity of singularities in the k space (corresponding to the critical points) at which there are changes in the topology of the constant-frequency surfaces.[7]

In Sec. 2 we shall discuss the polarization of vibrations in strongly anisotropic crystals. In Secs. 3 and 4 we shall analyze the properties of chain crystals and in Secs. 5 and 6 those of layer crystals.

2. POLARIZATION OF VIBRATIONS IN STRONGLY ANISOTROPIC CRYSTALS

The branches of vibrations in planar and linear structures may be classified in accordance with their polarization.[8] We may distinguish "longitudinal" vibrations with the polarization vector lying in the plane of a layer or along the line of a chain and "flexural" vibrations for which the polarization vector is normal to the plane of a layer or to the direction of a chain. Deviations from this classification in the case of strongly anisotropic crystals, in which planar layers or linear chains of strongly interacting atoms are physically separate, are small because of the weakness of the coupling between the layers or chains. At all frequencies ω at which the weak coupling between the layers or chains can be ignored (i.e., if $|\omega - \omega_i| \gg \omega_1$, where ω_i are the boundaries of the Brillouin zone or singular points inside it and ω_1 is a low frequency representing the coupling between layers or chains) the branches of vibrations in strongly anisotropic crystals can also be classified in accordance with their polarization into longitudinal and flexural. The density of vibrations in each branch for such values of ω, i.e., practically throughout the zone, is identical with the density of vibrations of the corresponding branch of a planar or linear structure to within small corrections of the order of ω_1^2.

We shall now analyze in greater detail the polarization of the vibrations in various branches. We shall consider only the acoustic vibration mode. To be specific, we shall discuss a simple tetragonal lattice and assume that the interaction of atoms along the fourfold axis z differs greatly from the interaction in the basal plane (x, y). We shall consider a chain crystal bearing in mind that the conclusions drawn apply essentially also to layer crystals.

A chain crystal can be represented as a set of chains of strongly interacting atoms along the z axis with a weak coupling between the chains.[2] We shall use $\alpha_{ik}(\mathrm{n})$ for the dynamic matrix of a crystal; n is the vector number of a lattice site. To determine the frequencies $\omega_s(\mathbf{k})$ and the polarization vectors $\mathrm{e}_s(\mathrm{k})$ $(s = 1, 2, 3)$ of the vibrations, we have to solve the problem of reducing to the diagonal form the matrix

$$A_{ik}(\mathbf{k}) = \sum_{\mathbf{n}} \alpha_{ik}(\mathbf{n}) \exp[i\mathbf{k}\mathbf{r}(\mathbf{n})], \tag{2.1}$$

which depends on the quasiwave vector k; the quantity r(n) in Eq. (2.1) is the radius vector of a lattice site whose number is n. In our case, the matrix $A_{ik}(\mathrm{k})$ is real and symmetric.

For a chain crystal the elements of the matrix $\alpha_{ik}(\mathrm{n})$ with the vector n lying along the z axis are much greater than the elements $\alpha_{ik}(\mathrm{n})$ with other values of n representing the weak interaction between the chains. Consequently, we shall divide the summation over n in Eq. (2.1) into two parts:

$$\begin{gathered} A_{ik}(\mathbf{k}) = A_{ik}^{(0)}(k_z) + A_{ik}^{(1)}(\mathbf{k}), \\ A_{ik}^{(0)}(k_z) = \sum_{n_x=0,\, n_y=0} \alpha_{ik}(n_z) \exp[ik_z z(n_z)], \\ A_{ik}^{(1)}(\mathbf{k}) = \sum_{(n_x,\, n_y)\neq 0} \alpha_{ik}(\mathbf{n}) \exp[i\mathbf{k}\mathbf{r}(\mathbf{n})], \end{gathered} \tag{2.2}$$

where $A_{ik}^{(0)}(k_z)$ describes the strong interaction of atoms in a chain and $A_{ik}^{(1)}(\mathrm{k})$ is a small, compared with $A_{ik}^{(0)}(k_z)$ correction due to the weak coupling between the chains. In other words, for almost all the values of k, we have

$$A_{ik}^{(1)}(\mathbf{k}) \sim \eta^2 A_{ik}^{(0)}(k_z), \quad \eta = \omega_1/\omega_0 \ll 1, \tag{2.3}$$

where ω_0 is a high frequency representing the coupling of atoms in a chain.

For some values of k, Eq. (2.3) is not obeyed and the values of $A^{(0)}$ and $A^{(1)}$ become of the same order of magnitude. In fact, it follows from the familiar relationship for the elements of the force matrix

$$\sum_{\mathbf{n}} \alpha_{ik}(\mathbf{n}) = 0 \tag{2.4}$$

that

$$A^{(0)}_{ik}(0) = -A^{(1)}_{ik}(0) \sim \eta^2\omega_0^2.$$

The quantities $A^{(0)}_{ik}(k_z)$ retain the same order of magnitude in a narrow region of width $\Delta k_z \sim \eta k_{z\,\max}$ near the point $k_z = 0$. Outside this region we have $A^{(0)}_{ik}(k_z) \sim \omega_0^2$.

The difference between the orders of magnitude of the quantities $A^{(0)}$ and $A^{(1)}$ over a large part of the Brillouin zone allows us to apply the perturbation theory[6] in reducing the matrix $A_{ik}(\mathbf{k})$ to the diagonal form. This is done by expressing $A_{ik}(\mathbf{k})$ in a coordinate system linked to the crystallographic axes of the crystal. In terms of these coordinates the quantity $A^{(0)}_{ik}(k_z)$ becomes diagonal; one of its eigenvectors $\mathbf{e}_3^{(0)}$ is directed along the z axis and the other two, $\mathbf{e}_1^{(0)}$ and $\mathbf{e}_2^{(0)}$, are orthogonal to one another and can be oriented in an arbitrary manner in the basal plane. We shall assume that they are directed along the x and y axes, respectively. The eigenvalues $A_1^{(0)}(k_z)$ and $A_2^{(0)}(k_z)$, corresponding to the x and y axes are equal and different from the eigenvalue $A_3^{(0)}(k_z)$ for the z axis. The difference $A_3^{(0)}(k_z) - A_1^{(0)}(k_z)$ is generally of the same order of magnitude as each of these quantities. Considerations of symmetry do not impose any other requirements on the magnitude of this difference nor do they require that the difference vanishes or is anomalously small at some values $k_z \neq 0$; this may happen only for accidental reasons. We shall not consider such accidental situations.

The eigenvector $\mathbf{e}_3(\mathbf{k})$ of the matrix $A_{ik}(\mathbf{k})$ is, in the first approximation,

$$e_3^j(\mathbf{k}) = e_3^{(0)j} + \sum_{s=1,2} \frac{A^{(1)}_{3s}(\mathbf{k})}{A_3^{(0)}(k_z) - A_1^{(0)}(k_z)} e_s^{(0)j}, \tag{2.5}$$

where the index j labels the components of the vector $\mathbf{e}_s(\mathbf{k})$. The corresponding eigenvalue is

$$A_3(\mathbf{k}) = A_3^{(0)}(k_z) + A^{(1)}_{33}(\mathbf{k}) + \sum_{s=1,2} \frac{A^{(1)}_{3s}(\mathbf{k}) A^{(1)}_{s3}(\mathbf{k})}{A_3^{(0)}(k_z) - A_1^{(0)}(k_z)}. \tag{2.6}$$

The formulas (2.5) and (2.6) determine the polarization and dispersion law of that branch of vibrations of a chain crystal which is closest to the properties of a longitudinal branch of a linear chain; we shall call it quasilongitudinal. It follows from Eq. (2.5) that for all values of k satisfying $|k_z| \gg \eta k_{z\,\max}$ and, consequently, $\omega \gg \omega_1$, the polarization of vibrations in a quasilongitudinal branch of a chain crystal differs from the case of a purely longitudinal polarization in a linear chain only by small quantities of the order of $\eta^2 \ll 1$. If the vector k is almost orthogonal to the chain direction, $|k_z| \lesssim \eta k_{z\,\max}$ ($\omega \lesssim \omega_1$), and also differs significantly from the values of $\mathbf{k}_0$, $\mathbf{k}_1$, and $\mathbf{k}_2$ corresponding to points of the type 0, 1, and 2 in Fig. 1, the polarization of the quasilongitudinal branch deviates considerably from the direction parallel to the chains. In this small part of the Brillouin zone the perturbation theory formulas cease to be valid. However, in the direct vicinity of the points of the 0, 1, and 2 type correction to the vector $\mathbf{e}_3^{(0)}$ of the purely longitudinal polarization is again small and of the $(a\varkappa)^2$ type, and the second correction to the square of the frequency is a small quantity of the $\eta^2(a\varkappa)^4$ type ($|\varkappa|$ is the distance to the corresponding point in the **k** space). At all points on the boundary of the Brillouin zone of high symmetry (points of the 1-5 type in Fig. 1) the polarization of a quasilongitudinal branch becomes rigorously longitudinal.

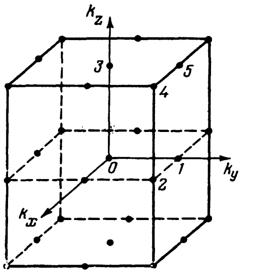

FIG. 1. Brillouin zone of a crystal with a simple tetragonal lattice.

Two other branches of vibrations in a chain crystal have properties close to those of flexural branches of a linear chain; we shall call them quasiflexural. The deviation of the polarization of quasiflexural branches from one which is rigorously transverse may be considerable in the same small part of the Brillouin zone where there is a corresponding deviation for the quasilongitudinal branch. Outside this region the polarization of the quasiflexural branches differs from the rigorously transverse only by a small amount of the order $\eta^2 \ll 1$. However, the interaction between chains lifts the degeneracy along the directions of polarization in the plane which is transverse relative to the chains; the vectors $\mathbf{e}_1(\mathbf{k})$ and $\mathbf{e}_2(\mathbf{k})$ rotate with **k** varying along the direction of chains but remain orthogonal to one another and almost orthogonal to the direction of chains in the $\omega \gg \omega_1$ case. At points of the 1-5 type (Fig. 1) the quasiflexural branches are polarized rigorously along the crystallographic axes and in the vicinity of these points the polarization is almost transverse, to within corrections of the order of $(a\varkappa)^2$.

Layer crystals have one quasiflexural branch and two quasilongitudinal. The deviation of the polarizations of these branches from that rigorously transverse relative to the plane of a layer or from the rigorously longitudinal orientation becomes considerable only when the wave vector **k** is almost normal to the plane of a layer, $|k_\perp| \lesssim \eta k_{\perp\,\max}$ ($\omega \lesssim \omega_1$), and differs significantly from the value $\mathbf{k}_3$ corresponding to a type 3 point. Since longitudinal branches of a planar lattice are generally nondegenerate, the interaction between layers does not result in their coupling of the kind observed between two flexural vibrations in a chain crystal.

3. CHAIN CRYSTAL. QUASILONGITUDINAL BRANCH

In the case of strongly anisotropic crystals we shall be interested mainly in the influence of the anisotropy of a crystal on the position and nature of the Van Hove critical points and on the properties of local vibrations near point defects. In investigating the behavior of the vibration density $g(\epsilon)$ near these critical points we have to know only, as pointed out in the Introduction, the first few terms of the expansion of the dispersion law of vibrations in the vicinity of singularities in the **k** space at which there is a change in the topology of the constant-frequency surfaces.[7] Such expansions were obtained by I. M. Lifshitz[1] for strongly anisotropic crystals in the

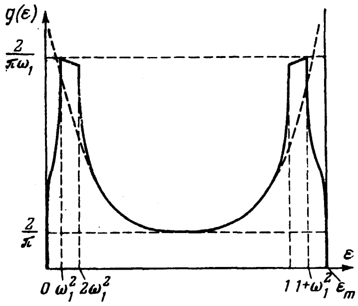

FIG. 2. Density of quasilongitudinal vibrations in a chain crystal ($\omega_1^2 \ll 1$). The dashed curve is the density of longitudinal vibrations in a corresponding linear chain.

long-wavelength range; they can be constructed in the vicinity of each of the singularities on the basis of the crystal lattice symmetry and the known anisotropy of the forces of interaction between atoms. As before, we shall assume that a chain crystal has a simple tetragonal lattice. We shall use a system of units in which the frequency of the strong coupling between atoms in chains (or layers) is taken as unity.

Omitting simple calculations, we shall give the resultant density of vibrations in a quasilongitudinal branch. The graph of the function $g(\epsilon)$ then has the form shown schematically in Fig. 2. There are four Van Hove critical points. Two of them lie near the lower limit of the spectrum at a distance ω_1^2 from it and the other two at the same distance from the upper limit ϵ_m. Throughout the frequency band between these limits, with the exception of narrow ($\sim \omega_1^2$) regions near the limits of the spectrum, the density $g(\epsilon)$ has no singularities and, to within small corrections of the order of ω_1^2, it is equal to the vibration density $g_0(\epsilon)$ of a corresponding linear chain. Near the limits of the spectrum the density $g(\epsilon)$ has large values of the order of $1/\omega_1$. At all critical points the density $g(\epsilon)$ exhibits a standard square-root kink.

We shall consider the question of local vibrations which appear near a point defect in a chain crystal. In considering the influence of the anisotropy of a crystal on the properties of such vibrations it is natural to restrict the analysis to the simplest of point defects, which is an isotropic atom at one of the lattice sites. Kagan and Iosilevskiĭ[9] showed that an isotopic point defect is an isotropic perturbation and it does not give rise to a coupling between vibrations of different polarizations. Consequently, in lattices of symmetry not lower than orthorhombic the local vibrations near an isotopic atom are polarized strictly along the crystallographic axes.[9] In other words, the local vibrations in a chain crystal with a simple tetragonal lattice can be divided, in accordance with their polarization, into strictly flexural and longitudinal. Local vibrations with each of these polarizations are generally formed from all the independent vibration branches simultaneously. Consequently, there is a characteristic coupling between the various vibration branches within the same polarization and this, as is known, may convert a local frequency into a quasilocal one on condition that the maximum vibration frequencies in the different branches are different. However, in strongly anisotropic crystals this coupling between quasilongitudinal and quasiflexural vibrations is negligible. In fact, the formation of local vibrations above the acoustic zone is dominated by vibrations above the acoustic zone is dominated by vibrations of an ideal crystal with near-maximal frequencies. It is shown in Sec. 2 that in this frequency range the deviation of the polarization of a quasiflexural branch from rigorously transverse is very small, of the order of $\omega_1^2 \ll 1$. An admixture of vibrations of a quasiflexural branch to longitudinal local vibrations is proportional to the square of the projection of the polarization vector of the quasiflexural branch onto the direction of the chain $[e_1{}^{s}(\mathbf{k})]^2$, which is a small quantity of the order of ω_1^4 over a considerable range of $\mathbf{k}$. In other words, local vibrations polarized along the chains form mainly from vibrations of the quasilongitudinal branch. Broadening of local frequencies of the order of $\omega_1{}^4 \ll \omega_1{}^2$ will be ignored; moreover, we shall not discuss here a possible coupling between two quasiflexural branches in a chain crystal and two quasilongitudinal branches in a layer crystal but we shall assume that, for example, the maximum frequencies in these branches are identical.

Consequently, the frequency of local vibrations polarized along chains can be found from the Lifshitz equation[3]

$$1+U_0\varepsilon\int_0^{\varepsilon_m}\frac{g(z)\,dz}{\varepsilon-z}=0,\quad U_0=\frac{M-m}{m},\tag{3.1}$$

where $g(z)$ is the density of vibrations in a quasilongitudinal branch, M is the mass of the isotope, and m is the mass of the host lattice atom.

We shall investigate Eq. (3.1) in the case when the frequency of local vibrations ϵ_l lies fairly close to the upper limit of ϵ_m of the continuous spectrum: $\epsilon_l - \epsilon_m \ll \epsilon_m$. For such values of ϵ the main contribution to the integral defining the Green function

$$G_\varepsilon(0)=\int_0^{\varepsilon_m}\frac{g(z)\,dz}{\varepsilon-z}\tag{3.2}$$

is due to the values of z near the upper limit of the spectrum. The integral (3.2) converges for all values $\epsilon \geqslant \epsilon_m$, as in the isotropic case, because $g(\epsilon)$ vanishes at the point $\epsilon = \epsilon_m$. However, its value is much greater than in the isotropic case because of the square-root singularity of $g(\epsilon)$ near the upper limit of the spectrum, which is characteristic of one-dimensional crystals and which is cut off at a distance of the order of ω_1^2 from the upper limit in the case of a chain crystal.

To investigate the integral (3.2) as a function of ϵ, it is convenient to express it in terms of a function $\varphi(x)$ defined by

$$g(z)=\frac{1}{\pi\varepsilon_m[t(1-t)]^{1/2}}\varphi([t(1-t)]^{1/2}),\quad z=\varepsilon_m t\ .\tag{3.3}$$

A comparison of Eq. (3.3) with the expansion $g(\epsilon)$ in the limit $\epsilon \to 0$ shows that

$$\varphi(x)=2\varepsilon_m^{3/2}x^2/\pi\omega_1{}^2,\quad x\ll\omega_1.\tag{3.4}$$

For $x \gtrsim \omega_1$, the function $\varphi(x)$ is of the order of unity.

Simple transformations give

$$G_\varepsilon(0)=\frac{2}{\pi\varepsilon_m}\int_0^{1/2}\frac{\varphi(x)\,dx}{\gamma+x^2},\quad \gamma=\frac{\varepsilon-\varepsilon_m}{\varepsilon_m}\ll 1. \tag{3.5}$$

The relationship (3.5) gives $G_\varepsilon(0)$ in two limiting cases:

$$G_\varepsilon(0)=\frac{1}{\varepsilon_m\sqrt{\gamma}}\left[1+O\left(\frac{\omega_1}{\sqrt{\gamma}}\right)\right],\quad \omega_1^2\ll\gamma\ll 1, \tag{3.6}$$

$$G_\varepsilon(0)=\frac{2}{\pi\varepsilon_m\omega_1}A-\frac{2\sqrt{\varepsilon_m}}{\pi\omega_1^2}\sqrt{\gamma},\quad 0<\gamma\ll\omega_1^2. \tag{3.7}$$

Here,

$$A=\lim_{\omega_1\to 0}\left[\omega_1\int_0^{1/2}\frac{\varphi(x)\,dx}{x^2}\right] \tag{3.8}$$

is a number of the order of unity depending on the nature of the function $g(\epsilon)$. We note that a finite contribution to A is made not only by the square-root singularity of the function $g(\epsilon)$ near the upper limit of the spectrum but also by a narrow region in the vicinity of the point $\epsilon=\epsilon_m$. Therefore, the number A cannot be expressed simply in terms of the vibration density $g_0(\epsilon)$ of the corresponding linear chain.

In view of the finite value of $G_\varepsilon(0)$ at the point $\epsilon=\epsilon_m$, there is a threshold for the appearance of local vibrations:

$$|U_0|>U_{\text{th}},\quad U_{\text{th}}=\pi\omega_1/2A,\quad U_0<0, \tag{3.9}$$

which is a manifestation of the three-dimensional nature of the crystal. The "low-demensional" effect is demonstrated by a strong reduction in the threshold value of U_{th} compared with that for an isotropic crystal.

Formulas (3.6) and (3.7) give the frequency of local vibrations in two limiting cases:

$$\varepsilon_l-\varepsilon_m=\varepsilon_m U_0^2,\quad \omega_1^2\ll\varepsilon_l-\varepsilon_m\ll\varepsilon_m; \tag{3.10}$$

$$\varepsilon_l-\varepsilon_m=\omega_1^2\frac{A^2}{\varepsilon_m^2}\left(1-\frac{U_{\text{th}}}{|U_0|}\right)^2,\quad 0<\varepsilon_l-\varepsilon_m\ll\omega_1^2. \tag{3.11}$$

Formula (3.10), valid in the case when ϵ_l is sufficiently far from the limit of the continuous spectrum, has the form typical of the one-dimensional case and known from quantum mechanics.[6] In the immediate vicinity of the limit of the continuous spectrum, we have Eq. (3.11), which is typical of the three-dimensional situation[6] and reflects the existence of a threshold for the appearance of local vibrations.

We shall now consider the shape of the region where vibrations are localized. The dependence of the amplitude $u(\mathbf{r})$ of local vibrations on the distance $\mathbf{r}$ from a point defect is given by the familar expression

$$u(\mathbf{r})=u(0)U_0\varepsilon_l\frac{V_0}{(2\pi)^3}\int d^3k\,\frac{\exp(i\mathbf{kr})}{\omega^2(\mathbf{k})-\varepsilon_l}, \tag{3.12}$$

where V_0 is the volume of a unit cell. Hence, we find that, in a plane transverse relative to the direction of chains, the vibration amplitude decreases with the increase of the distance ρ from a defect in the same plane in accordance with the law typical of an isotropic crystal, irrespective of the dependence of the value of ϵ_l:

$$|u(\rho)|=u(0)|U_0|\frac{\sqrt{\varepsilon_l}}{\pi\omega_1}\frac{b}{\rho}\exp\left(-\frac{\rho}{l_\perp}\right),\quad \rho\gg b. \tag{3.13}$$

The transverse size of the localization region

$$l_\perp=b\frac{\omega_1}{2(\varepsilon_l-\varepsilon_m)^{1/2}} \tag{3.14}$$

is governed by the ratio of the frequency representing the coupling in the direction considered to the distance (along the frequency axis) from the limit of the continuous spectrum.

In the case of atoms in the same chain as a point defect the dependence of the local vibration amplitude on the distance z from the defect is sensitive to the position of ϵ_l relative to the limit of the continuous spectrum. If ϵ_l lies sufficiently far from this limit, so that $\epsilon_l-\epsilon_m\gg\omega_1^2$, the law describing the fall $u(z)$ is typical of a one-dimensional crystal:

$$|u(z)|=u(0)|U_0|\frac{\varepsilon_\pi}{(\varepsilon_l-\varepsilon_m)^{1/2}}\exp\left(-\frac{z}{l_\parallel}\right),\quad z\gg a,\quad \varepsilon_l-\varepsilon_m\gg\omega_1^2. \tag{3.15}$$

The size $l_\parallel$ of the localization region along the chains is governed, like the transverse size given by Eq. (3.14), by the ratio of the frequency representing the coupling of atoms in a chain to the distance from the limit of the continuous spectrum:

$$l_\parallel=a/2(\varepsilon_l-\varepsilon_m)^{1/2}. \tag{3.16}$$

If the vibration frequency lies in the direct vicinity of the limit of the spectrum, $\epsilon_l-\epsilon\ll\omega_1^2$, the change in the vibration amplitude becomes the same as in an isotropic crystal:

$$|u(z)|=u(0)|U_0|\frac{\varepsilon_l}{\omega_1^2}\frac{a}{z}\exp\left(-\frac{z}{l_\parallel}\right),\quad z\gg a,\quad \varepsilon_l-\varepsilon_m\ll\omega_1^2 \tag{3.17}$$

and the value of $l_\parallel$ remains the same. A comparsion of Eqs. (3.13) and (3.17) shows that the amplitude of local vibrations of atoms in the same chain as a point defect exceeds by a factor of $\sqrt{\epsilon_l}/\omega_1\gg 1$ the amplitude of vibrations of atoms in neighboring planes.

It follows from the above that the localization region is the cigar-shaped, being greatly elongated along the direction of the strong interaction parallel to the chain of atoms containing a defect; the ratio of the transverse dimensions to the longitudinal is $\omega_1\ll 1$.

4. CHAIN CRYSTAL. QUASIFLEXURAL BRANCH

Near the lower limit of the spectrum the dispersion law $\omega^2(\mathbf{k})$ of flexural vibrations in a chain crystal has the familiar expansion[1] which we shall write in the form

$$\omega^2(\mathbf{k})={}^1/_{16}a^4k_z^4+{}^1/_4\omega_3^2a^2k_z^2+{}^1/_4\omega_2^2b^2(k_x^2+k_y^2),\quad \omega_2\ll 1,\quad \omega_3\ll 1, \tag{4.1}$$

where ω_2 and ω_3 are small parameters of the same order of magnitude, describing the weak coupling between the chains.

In the absence of the coupling between the chains ($\omega_2 = \omega_3 = 0$), it follows from Eq. (4.1) that the density of flexural vibrations $g_0(\epsilon)$ in the corresponding linear chain has a power-law singularity in the limit $\epsilon \to 0$:

$$g_0(\varepsilon) = \varepsilon^{-3/4}/2\pi, \quad \varepsilon \ll 1, \tag{4.2}$$

which is stronger than for the vibrations polarized along the chains. Near the upper limit of the spectrum the behavior of $g_0(\epsilon)$ for flexural vibrations in a linear chain is essentially the same as in the case of vibrations polarized along the chains.

Bearing in mind the weak coupling between the chains, we find from Eq. (4.1) that in the case of a chain crystal the density $g(\epsilon)$ in a quasiflexural branch is a small square-root quantity near the lower limit of the spectrum, of the same kind as in the case of an isotropic crystal:

$$g(\varepsilon) = 2\sqrt{\varepsilon}/\pi^2\omega_2^2\omega_3, \quad \varepsilon \ll \omega_3^4/4. \tag{4.3}$$

However, away from the limit even for very small values of ϵ the dependence $g(\epsilon)$ changes to

$$g(\varepsilon) = 4\varepsilon^{1/4}/\pi^2\omega_2^2, \quad \omega_3^4/4 \ll \varepsilon \ll \omega_2^2. \tag{4.4}$$

The first critical point $\epsilon = \epsilon_1 \sim \omega_2^2$ is associated with a transition from closed constant-frequency surfaces to open surfaces at type 1 points on the boundary of the Brillouin zone (Fig. 1). In the vicinity of such a point, we have

$$\omega^2(\mathbf{k}) = \varepsilon_1 + {}^1/_{16}a^4\varkappa_z^4 + {}^1/_4\omega_3^2a^2\varkappa_z^2 + {}^1/_4\omega_2^2b^2(\varkappa_x^2 - \varkappa_y^2), \tag{4.5}$$

where $\varkappa = \mathbf{k} - \mathbf{k}_1$ is the vector in the $\mathbf{k}$ space measured from a singularity corresponding to $\mathbf{k} = \mathbf{k}_1$.

Substituting the expansion (4.5) of the dispersion law into the definition of the density of states

$$g(\varepsilon) = \frac{V_0}{(2\pi)^3}\int d^3k\,\delta(\varepsilon - \omega^2(\mathbf{k})), \tag{4.6}$$

we find that the behavior of $g(\epsilon)$ in the vicinity of the first cirtical point is given by the integral

$$g(\varepsilon) = \frac{2}{\pi^3}\iint\limits_D d\varphi\,d\psi\,\frac{[{}^1/_2\omega_3^2 + ({}^1/_4\omega_3^4 + \Delta - \omega_2^2\varphi^2 + \omega_2^2\psi^2)^{1/2}]^{1/2}}{(\Delta - \omega_2^2\varphi^2 + \omega_2^2\psi^2)^{1/2}({}^1/_4\omega_3^4 + \Delta - \omega_2^2\varphi^2 + \omega_2^2\psi^2)^{1/2}}, \tag{4.7}$$

where $\Delta = \epsilon - \epsilon_1$ denotes here (and later) the distance along the frequency axis from the corresponding critical point. The integration domain D in the (φ, ψ) plane consists of that part of the square defind by $0 \leqslant \varphi \leqslant \pi/2$, $0 \leqslant \psi \leqslant \pi/2$ in which all the expressions in the radicals of the integrand are simultaneously nonnegative.

The function $g(\epsilon)$ given by Eq. (4.7) has a characteristic square-root kink only in a very narrow range of frequencies near the point $\epsilon = \epsilon_1$:

$$g(\varepsilon) = \frac{8\sqrt{2}}{\pi^3}K\left(\frac{1}{\sqrt{2}}\right)\frac{1}{\omega_2^{3/2}} - \frac{2}{\pi^2}\frac{\sqrt{|\Delta|}}{\omega_3\omega_2^2}\theta(-\Delta), \qquad \Delta = \varepsilon - \varepsilon_1, \quad |\Delta| \ll \omega_3^4/4, \tag{4.8}$$

where $\theta(x) = 1$ for $x > 0$ and $\theta(x) = 0$ for $x < 0$; $K(1/\sqrt{2})$ is a complete elliptic integral of the first kind. Outside this narrow range of frequencies but still close to the critical point the dependence of $g(\epsilon)$ on Δ is different:

$$g(\varepsilon) = \frac{8\sqrt{2}}{\pi^3}K\left(\frac{1}{\sqrt{2}}\right)\frac{1}{\omega_2^{3/2}}\left[1 - \frac{|\Delta|^{1/4}}{\omega_2^{1/2}}\nu_\Delta\left(2E\left(\frac{1}{\sqrt{2}}\right) - K\left(\frac{1}{\sqrt{2}}\right)\right)\right], \qquad \omega_3^4/4 \ll |\Delta| \ll \omega_2^2, \tag{4.9}$$

where $\nu_\Delta = \sqrt{2}$ for $\Delta > 0$ but $\nu_\Delta = 1$ for $\Delta < 0$; $E(1/\sqrt{2})$ is a complete integral of the second kind.

Consequently, in a relatively wide range of frequencies the expansion of $g(\epsilon)$ is in powers of $|\Delta|^{1/4}$ of the difference $\Delta = \epsilon - \epsilon_1$. It is clear from Eqs. (4.8) and (4.9) that near the first critical point ϵ_1 the density of quasiflexural vibrations has a sharp tooth-like peak.

The second critical point, $\epsilon_2 > \epsilon_1$, $\epsilon_2 \sim \omega_2^2$, is due to a transition from open constant-frequency surfaces to closed at type 2 points (Fig. 1). In the vicinity of these points, we have

$$\omega^2(\mathbf{k}) = \varepsilon_2 + {}^1/_{16}a^4\varkappa_z^4 + {}^1/_4\omega_3^2a^2\varkappa_z^2 - {}^1/_4\omega_2^2b^2(\varkappa_x^2 + \varkappa_y^2), \quad \varkappa = \mathbf{k} - \mathbf{k}_2. \tag{4.10}$$

The density of vibrations near the point $\epsilon = \epsilon_2$ is given by Eq. (4.7) where we have to reverse the sign in front of φ^2 and regard Δ as equal to $\epsilon - \epsilon_2$. An analysis of this function shows that in the vicinity of the second critical point $\epsilon = \epsilon_2$ the function $g(\epsilon)$ has a square-root kink again in a very narrow range of frequencies:

$$g(\varepsilon) = \frac{2}{\pi^2}\frac{1}{\omega_2^{3/2}}\left[1 - \frac{\Delta^{1/2}}{\omega_3\omega_2^{1/2}}\theta(\Delta)\right], \qquad \Delta = \varepsilon - \varepsilon_2, \quad |\Delta| \ll \frac{\omega_3^4}{4}. \tag{4.11}$$

Outside this narrow range the expansion of $g(\epsilon)$ is in powers of $|\Delta|^{1/4}$ on the high-frequency side ($\Delta > 0$) and in integral powers of Δ on the low-frequency side ($\Delta < 0$):

$$g(\varepsilon) = \frac{2}{\pi^2}\frac{1}{\omega_2^{3/2}}\left[1 - \frac{\Delta^{1/4}}{\omega_2^{1/2}}\theta(\Delta) + \frac{\Delta}{4\omega_2^2}\theta(-\Delta)\right], \quad \frac{\omega_3^4}{4} \ll |\Delta| \ll \omega_2^2. \tag{4.12}$$

Far from the limits of the spectrum, $\epsilon \gg \omega_2^2$, $\epsilon_m - \epsilon \gg \omega_2^2$, i.e., throughout most the frequency range, the density $g(\epsilon)$ is equal to the density of flexural vibrations $g_0(\epsilon)$ of a linear chain, whereas in the vicinity of the upper limit of the spectrum there are singularities fully analogous to those exhibited in the same range by the density of vibrations of a quasilongitudinal branch.

It follows that an important feature of quasiflexural vibrations, which distinguishes them from quasilongitudinal branches, is the occurrence near the lower limit of the spectrum and in the vicinity of the first two critical points of several frequency intervals in which $g(\epsilon)$ behaves differently. The familiar square-root Van Hove kink occurs only in a very narrow range (of width of the order of $\omega_3^4 \ll \omega_2^2 \ll 1$) near the critical points ϵ_1 and ϵ_3. Outside this range the behavior of $g(\epsilon)$ is quite different. It should also be noted that although in the vicinity of the critical points ϵ_1 and ϵ_2 there is no definite polarization, nevertheless all the important features of the behavior of $g(\epsilon)$ are still governed by vibrations with the flexural polarization in a quasiflexural branch, as deduced in Sec. 2. Vibrations of other polarizations of the frequencies in the quasiflexural branch dominate the value of $g(\epsilon)$. The general appear-

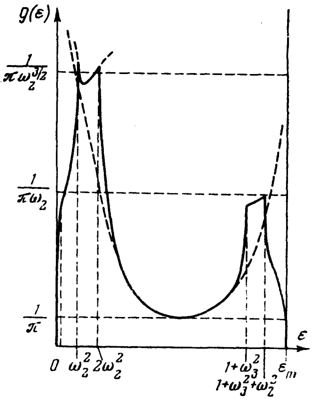

FIG. 3. Density of quasiflexural vibrations in a chain crystal ($\omega_2^2 \ll 1$). The dashed curve represents the results for a linear chain.

ance of the density of quasiflexural vibrations is shown schematically in Fig. 3.

The equality of the densities of quasiflexural and quasilongitudinal vibrations near the upper limit of the spectrum allows us to apply to a quasiflexural branch all the results (without significant changes) of the preceding section on the conditions of appearance of local vibrations, values of local frequencies, and shape of the localization region.

5. LAYER CRYSTAL. QUASILONGITUDINAL BRANCH

In considering the phonon spectrum of layer crystals we shall, as before, assume that they have a simple tetragonal lattice and that the direction of weak binding between the layers coincides with the fourfold axis z. A schematic representation of the density of states of a quasilongitudinal branch obtained for this case is given in Fig. 4. There are four Van Hove critical points, two of which are near the limits of the spectrum and the other two near its midpoint. At all critical points the density $g(\epsilon)$ has the standard square-root kink.

As in the case of a chain crystal, the Green function $G_\epsilon(0)$ of vibrations in a layer crystal has the characteristic (of the three-dimensional case) finite limit as ϵ tends to the maximum frequency of the spectrum from above. The "low-dimensional" effect is manifested by an increase in the limit:

$$G_\varepsilon(0)=g_0(\varepsilon_m)\ln\frac{1}{\omega_1}-\frac{2\sqrt{\varepsilon_m}}{\pi\omega_1}\sqrt{\gamma},\quad 0\leqslant\gamma\leqslant\omega_1^2,\quad \gamma=\frac{\varepsilon-\varepsilon_m}{\varepsilon_m},\tag{5.1}$$

where, as before, $g_0(\epsilon)$ denotes the density of vibrations of the corresponding planar lattice:

$$g_0(\varepsilon)=\lim g(\varepsilon),\quad \omega_1\to 0;\qquad g_0(\varepsilon)=1/\pi,\quad \varepsilon\ll 1.\tag{5.1a}$$

Further away from the limits of the spectrum, we have

$$G_\varepsilon(0)=g_0(\varepsilon_m)\ln(1/\gamma)+O(\omega_1^2/\gamma),\quad \omega_1^2\ll\gamma\ll 1.\tag{5.2}$$

Since $G_\epsilon(0)$ is finite at $\epsilon=\epsilon_m$, there is a threshold of appearance of local vibrations near a point defect in a layer crystal:

$$|U_0|>U_{\text{th}},\quad U_{\text{th}}=\frac{\pi}{2B\ln(1/\omega_1)},\quad U_0<0,\quad B=\pi\varepsilon_m g_0(\varepsilon_m),\tag{5.3}$$

which is lower than for an isotropic crystal.

It follows from Eqs. (5.1) and (5.2) that under conditions such that the frequency of local vibrations is sufficiently far from the limit of the continuous spectrum, $\epsilon_l-\epsilon_m \gg \omega_1^2$, the value of ϵ_l is given by the standard quantum-mechanics formula for the two-dimensional case:

$$\varepsilon_l-\varepsilon_m=\varepsilon_m\exp[-1/\varepsilon_m g_0(\varepsilon_m)|U_0|],\quad \omega_1^2\ll\varepsilon_l-\varepsilon_m\ll\varepsilon_m.\tag{5.4}$$

However, sufficiently close to the limit of the continuous spectrum the local frequency is given by the typical "three-dimensional" formula reflecting the existence of the threshold:

$$\varepsilon_l-\varepsilon_m=\left(\omega_1\ln\frac{1}{\omega_1}\right)^2\frac{B^2}{\varepsilon_m^2}\left(1-\frac{U_{\text{th}}}{|U_0|}\right)^2,\quad 0<\varepsilon_l-\varepsilon_m\ll\omega_1^2.\tag{5.5}$$

The localization region of vibrations is strongly anisotropic in shape. If the frequency of local vibrations is sufficiently far from the limit of the continuous spectrum, $\epsilon_l-\epsilon_m \gg \omega_1^2$, the dependence of the vibration amplitude $u(\rho)$ of atoms in a layer containing a defect on the distance ρ from the defect in the plane of the layer is the same as in the two-dimensional case:

$$|u(\rho)|=u(0)|U_0|\frac{2}{\pi}K_0\left(\frac{\rho}{l_\parallel}\right),\quad \rho\gg b,\ \omega_1^2\ll\varepsilon_l-\varepsilon_m,\tag{5.6}$$

where $K_0(x)$ is a modified Hankel function of the first kind. The size of the localization region in the plane of the layer is governed, as before, by the ratio of the coupling frequency in the plane of the layer to the distance from the upper limit of the continuous spectrum:

$$l_\parallel=b/2(\varepsilon_l-\varepsilon_m)^{1/2}.\tag{5.7}$$

On approach of ϵ_l to the upper limit of the continuous spectrum, the expression for $u(\rho)$ assumes the "three-dimensional" form:

$$|u(\rho)|=u(0)|U_0|\frac{2\sqrt{\varepsilon_l}}{\pi\omega_1}\frac{b}{\rho}\exp\left(-\frac{\rho}{l_\parallel}\right),\quad 0<\varepsilon_l-\varepsilon_m\ll\omega_1^2,\quad \rho\gg b.\tag{5.8}$$

In a direction normal to the plane of the layer the amplitude of local vibrations is always expressed in the form typical of an isotropic crystal:

$$|u(z)|=u(0)|U_0|\varepsilon_l\frac{a}{z}\exp\left(-\frac{z}{l_\perp}\right),\quad z\gg a,\quad l_\perp=a\frac{\omega_1}{2(\varepsilon_l-\varepsilon_m)^{1/2}}.\tag{5.9}$$

The last result is to be expected because the presence of more than one layer of atoms makes a crystal three-dimensional. It should be noted that in a layer crystal the amplitude of vibrations of atoms in a layer containing a defect is much greater than the amplitude of vibrations in neighboring layers. Thus, the region of localization of vibrations in a layer crystal is pancake-

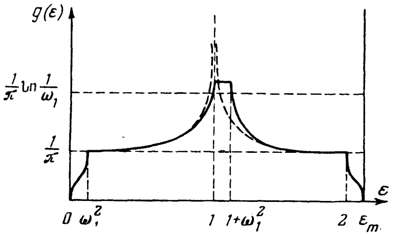

FIG. 4. Density of quasilongitudinal vibrations in a layer crystal ($\omega_1^2 \ll 1$). The dashed curve represents the density of longitudinal vibrations in a planar lattice.

shaped and it is located in the plane of the layer containing a defect; the ratio of the thickness of this pancake to its diameter is of the order of $\omega_1 \ll 1$.

6. LAYER CRYSTAL. QUASIFLEXURAL BRANCH

We shall now consider the influence of anisotropy on the position and nature of critical points for quasiflexural vibrations in a layer crystal and we shall largely ignore numerical factors of the order of unity; to simplify the calculations, we shall write down the necessary expansions of the dispersion law of flexural vibrations near singularities in its simpler form which allows for the characteristic properties of flexural vibrations. In the long-wavelength range, we have

$$\begin{gathered}\omega^2(\mathbf{k}) = {}^1/_{16} b^4 (k_x^4 + k_y^4) \\ + {}^1/_4 \omega_3^2 b^2 (k_x^2 + k_y^2) + {}^1/_4 \omega_2^2 a^2 k_z^2. \\ \omega_2 \sim \omega_3 \ll 1.\end{gathered} \tag{6.1}$$

The above form of the dispersion law is simplified by omitting the product $k_x^2 k_y^2$, which is generally of the same order of magnitude as the remaining terms with k_x^4 and k_y^4. This simplification does not alter the topological properties of the constant-frequency surfaces and does not affect the important properties of the vibration density.

If we ignore the interaction between the layers assuming that $\omega_2 = \omega_3 = 0$, we find that the resultant planar lattice is characterized by the density of flexural vibrations $g_0(\epsilon)$ with a square-root singularity near the lower limit of the spectrum:

$$g_0(\varepsilon) = \frac{1}{\pi^2} \mathrm{K}\left(\frac{1}{\sqrt{2}}\right) \frac{1}{\sqrt{\varepsilon}}, \quad \varepsilon \ll 1. \tag{6.2}$$

Moreover, there is a power-law singularity of the function $g_0(\epsilon)$ at $\epsilon = \epsilon_m/2$ and this singularity is stronger than in the case of quasilongitudinal vibrations:

$$g_0(\varepsilon) = \frac{2}{\pi^2} \mathrm{K}\left(\frac{1}{\sqrt{2}}\right) \frac{1}{|\Delta|^{1/4}} [1 + (\sqrt{2} - 1)\theta(-\Delta)], \quad |\Delta| \ll 1, \quad \Delta = \varepsilon - \frac{\varepsilon_m}{2}. \tag{6.3}$$

The function $g_0(\epsilon)$ has no singularities near the upper limit of the spectrum and it tends to a finite limit [the function $g_0(\epsilon)$ is represented by a dashed curve in Fig. 5]. A weak interaction between layers in a crystal limits the vibration density $g(\epsilon)$ and results in truncation of the function $g_0(\epsilon)$ near the limits of the spectrum.

Application of the expansion (6.1) shows that the function $g(\epsilon)$ varies extremely rapidly in the direct vicinity of the lower limit and that it vanishes at $\epsilon = 0$ in accordance with the square-root law:

$$g(\varepsilon) = \frac{2}{\pi^2} \frac{\sqrt{\varepsilon}}{\omega_2 \omega_3^2}, \quad \varepsilon \ll \frac{\omega_3^4}{4}, \tag{6.4}$$

but a short distance away $\epsilon \sim \omega_3^4 \ll \omega_2^2 \ll 1$ it reaches a high value of the order of $1/\omega_2$. Outside this region, but far from the first critical point ϵ_1 the function $g(\epsilon)$ is constant:

$$g(\varepsilon) = \frac{1}{\pi^2} \mathrm{K}\left(\frac{1}{\sqrt{2}}\right) \frac{1}{\omega_2}, \quad \frac{\omega_3^4}{4} \ll \varepsilon \ll \omega_2^2. \tag{6.5}$$

Formulas (6.4) and (6.5) are in full agreement with the results obtained by Kosevich.[2]

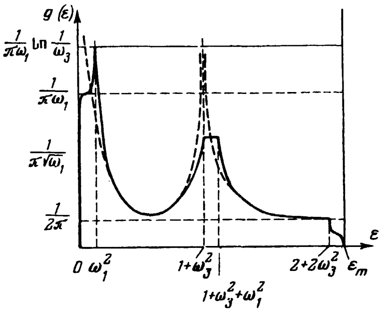

FIG. 5. Density of quasiflexural vibrations in a layer crystal ($\omega_1^2 \ll 1$, $\omega_3^2 \ll 1$). The dashed curve represents the density of flexural vibrations in a planar lattice.

In contrast to chain crystals, the density of quasiflexural vibrations in a layer crystal has only one critical point $\epsilon = \epsilon_1 \sim \omega_2^2$ in the low-frequency range and at this point the function $g(\epsilon)$ changes from a rising section to a falling one. This circumstance is associated with the possibility that at low frequencies the constant-frequency surfaces of a layer crystal become open along just one direction, which is normal to the plane of the layer (at points of type 3 in Fig. 1).

Expansion of the dispersion law of a quasiflexural branch near a point of type 3 (Fig. 1) can be written in the form

$$\omega^2(\mathbf{k}) = \varepsilon_1 + {}^1/_{16} b^4 (\varkappa_x^4 + \varkappa_y^4) + {}^1/_4 \omega_3^2 b^2 (\varkappa_x^2 + \varkappa_y^2) - {}^1/_4 \omega_2^2 a^2 \varkappa_z^2, \quad \boldsymbol{\varkappa} = \mathbf{k} - \mathbf{k}_3. \tag{6.6}$$

In the vicinity of the first critical point ϵ_1 the dependence $g(\epsilon)$ is given by the integral

$$\begin{aligned}g(\varepsilon) = \frac{2}{\pi^3} \iint_D d\varphi\, d\psi [{}^1/_2 \omega_3^2 + ({}^1/_4 \omega_3^4 + \Delta + \omega_2^2 \psi^2 - \omega_3^2 \varphi^2 - \varphi^4)^{1/2}]^{1/2} \\ \times (\Delta + \omega_2^2 \psi^2 - \omega_3^2 \varphi^2 - \varphi^4)^{-1/2} ({}^1/_4 \omega_3^4 + \Delta + \omega_2^2 \psi^2 - \omega_3^2 \varphi^2 - \varphi^4)^{-1/2},\end{aligned} \tag{6.7}$$

where the integration domain is defined as before. The function (6.7) has its usual square-root kink at the point $\epsilon = \epsilon_1$ but the frequency interval where this occurs is very narrow:

$$g(\varepsilon) = \frac{2}{\pi^2} \mathrm{K}\left(\frac{1}{\sqrt{2}}\right) \frac{1}{\omega_2} \ln \frac{2\omega_2}{\omega_3^2} - \frac{\pi\sqrt{|\Delta|}}{\omega_2 \omega_3^2} \theta(-\Delta), \quad |\Delta| \ll \frac{\omega_3^4}{4}, \quad \Delta = \varepsilon - \varepsilon_1. \tag{6.8}$$

Outside this narrow interval the dependence of $g(\epsilon)$ on Δ changes and become logarithmic and symmetric:

$$g(\varepsilon) = \frac{2}{\pi^2} \mathrm{K}\left(\frac{1}{\sqrt{2}}\right) \frac{1}{\omega_2} \ln \frac{2\omega_2}{|\Delta|^{1/2}} \cdot \quad \frac{\omega_3^4}{4} \ll |\Delta| \ll \omega_2^2. \tag{6.9}$$

Thus, in the vicinity of the lower limit of the spectrum the density of quasiflexural vibrations has a sharp peak whose existence was first pointed out by Kosevich.[2] This peak is asymmetric only in a very narrow frequency interval $\omega_3^4 \ll \omega_2^2 \ll 1$ near its center.

The next two critical points ϵ_2 and ϵ_3 are located near the midpoint of the spectrum $\epsilon = \epsilon_m/2$ and are separated by distances of ω_2^2 from it. Near these points there are again several frequency ranges with different behavior of the function $g(\epsilon)$. For example, near the point ϵ_2, we have

$$g(\varepsilon)=\frac{2\sqrt{2}}{\pi^2}\mathbf{K}\left(\frac{1}{\sqrt{2}}\right)\frac{1}{\sqrt{\omega_2}}-\frac{\pi}{\sqrt{2}}\frac{\sqrt{|\Delta|}}{\omega_2\omega_3},\qquad |\Delta|\ll\frac{\omega_3^4}{4},\qquad \Delta=\varepsilon-\varepsilon_2; \tag{6.10}$$

in a wider range, we find that

$$g(\varepsilon)=\frac{2\sqrt{2}}{\pi^2}\mathbf{K}\left(\frac{1}{\sqrt{2}}\right)\frac{1}{\sqrt{\omega_2}}\left[1-\frac{|\Delta|^{1/2}}{\sqrt{2}\omega_2}\left(2\mathbf{E}\left(\frac{1}{\sqrt{2}}\right)-\mathbf{K}\left(\frac{1}{\sqrt{2}}\right)\right)\right], \quad \frac{\omega_3^4}{4}\ll|\Delta|\ll\omega_2^2. \tag{6.11}$$

Throughout the frequency range, with the exception of narrow ($\sim\omega_2^2$) intervals near the limits and near the middle of the spectrum the function $g(\epsilon)$ is identical, apart from small corrections of the order of ω_2^2, with the density of flexural vibrations of the corresponding planar lattice. Near the upper limit of the spectrum the behavior of $g(\epsilon)$ is analogous to that of quasilongitudinal vibrations. Figure 5 shows schematically the behavior of $g(\epsilon)$ for a quasiflexural branch.

The properties of local vibrations in a quasiflexural branch are also similar to the properties of vibrations polarized in the plane of a layer. It should be noted that if the difference between the behavior of the densities of vibrations in the limit $\epsilon\to 0$ described by Eqs. (5.1a) and (6.2) had occurred in the optical zone, the conditions for the appearance (below the bottom of the zone) of local flexural vibrations near a heavy impurity would have been quite different from the case of vibrations polarized in the plane of a layer. The difference between the threshold values, due to the different behavior of the vibration density, would have ensured the existence of only local flexural vibrations for a wide range of impurity masses.

It must be stressed that the numbers and positions of the critical points of strongly anisotropic crystals have been obtained above for the simplest most symmetric case. In other situations the number of the critical points may be greater.

We shall conclude by pointing out that all the results obtained above apply equally well to the spectra of other excitations in strongly anistropic crystals provided their dispersion law agrees with one of the types discussed above.

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[1] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. 22, 475 (1952).

[2] A. M. Kosevich, Osnovy mekhaniki kristallicheskoĭ reshetki (Fundamentals of Crystal Lattice Mechanics), Nauka, M., 1972.

[3] I. M. Lifshitz, Zh. Eksp. Teor. Fiz. 17, 1017, 1076 (1947).

[4] I. M. Lifshitz, Adv. Phys. **13**, 483 (1964).

[5] I. M. Lifshitz and A. M. Kosevich, Rep. Prog. Phys. 29, 217 (1966).

[6] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika, Nauka, M., 1974 (Quantum Mechanics: Non-Relativistic Theory, 3rd ed., Pergamon Press, Oxford, 1977).

[7] L. D. Landau and E. M. Lifshitz, Statisticheskaya fizika, Nauka, M., 1976 (Statistical Physics, 3rd ed., Pergamon Press, Oxford, 1978), Part 1.

[8] L. D. Landau and E. M. Lifshitz, Teoriya uprugosti, Nauka, M., 1965 (Theory of Elasticity, 2nd ed., Pergamon Press, Oxford, 1970).

[9] Yu. Kagan and Ya. A. Iosilevskiĭ, Zh. Eksp. Teor. Fiz. 42, 259 (1962); **44**, 1375 (1963) [Sov. Phys. JETP **15**, 182 (1962); **17**, 926 (1963)].

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Quantum oscillations of the magnetoresistance of thin antimony ribbons

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An investigation was made of the dependence of the derivative of the magnetoresistance of antimony whiskers on magnetic fields of 0–80 kOe intensity applied at temperatures of 1.3–4.2°K. These whiskers were broken up into ribbon-shaped samples with the following dimensions: thickness from 0.08 to 0.44 μ, width from 1.1 to 31 μ, and length from 0.2 to 3 mm. The size cutoff of quantum oscillations of the magnetoresistance was observed and investigated. It was also found that quantum oscillations appeared in truncated extremal electron orbits in fields below the cutoff value. These phenomena were predicted by A. M. Kosevich and I. M. Lifshitz in 1955 [Sov. Phys. JETP 2, 646 (1956)]. The experimental results indicated that the probability of specular reflection of conduction electrons from the surface of a sample was close to unity.

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INTRODUCTION

One of the important current problems in the physics of metals is the interaction of conduction electrons with the surface of a sample. The most interesting is the case of specular reflection of electrons from the surface. The possibility of specular reflection has been demonstrated experimentally.[1,2]

The interaction of electrons with a specularly reflec-