SOVIET PHYSICS JETP VOLUME 34, NUMBER 5 MAY 1972

LOCAL PHONON STATE DENSITY IN A SEMI-INFINITE CRYSTAL OR PLATE

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Submitted April 28, 1971

Zh. Eksp. Teor. Fiz. 61, 2006–2017 (November, 1971)

The space-frequency distribution function for acoustic phonons is found for a semi-infinite solid and a plate of arbitrary thickness with free boundaries. It is shown that this function has an oscillating "tail" of the type $(\sin 2\xi)/2\xi$, where $\xi = \omega x/c$ (c is the characteristic sound velocity, x the distance to the boundary) and, consequently, it very slowly approaches the value corresponding to an unbounded medium.

1. INTRODUCTION

A calculation of the function for the local density of states of acoustic phonons in a half-space and in a plate, to which the present work is devoted, is of significant interest for two reasons. First, the actual value of this function is necessary for the study of a whole series of phenomena in the surface layer of the specimen, in particular, kinetic phenomena and processes of interaction of the solid with external radiation or with a flux of particles incident on its surface. Second, the resolution of this problem allows us to answer the question as to how the density of states, which is practically independent of the form of the boundary conditions, is formulated in terms of the distance from the boundaries in a macroscopic specimen, where each atom oscillates completely differently, depending on the specific dimensions and the shape of the crystal. Here it is appropriate to recall that in the calculation of the averaged spectral functions of the sample as a whole, the spectrum of elementary excitations and, in particular, the spectrum of phonons, is approximated by cyclic boundary conditions. The possibility of such an approximation is substantiated by Ledermann's well known theorem on the density of eigenvalues of a Hermitian matrix.[1] However, the content of this theorem in no way touches on the amplitude of oscillations of the individual atoms and, consequently, on the local density of states as a function of their coordinates, which can differ considerably from the average over the sample. It must also be emphasized that a boundary with a vacuum is a special case of an extended defect in a crystal,[2,3] and therefore the study of the local density of states for this case can give some idea of the spectral distribution of the oscillations in the vicinity of extended defects of more complicated form. Moreover, the method of [3,4], which we shall use in the construction of the local spectral function, is precisely based on the exact solution of the equation for the Green's phonon function of the Dyson type (compare with [5]) and the interpretation of the boundaries as two-dimensional defects.

2. THE HALF-SPACE

The acoustic asymptote of the distribution function $G^{ik}(\mathbf{r};\ \omega^2)$ of the distribution of the squares of the frequencies ω^2 of the oscillations of the matrix or of an impurity atom of mass M_r, located at the point $\mathbf{r}$ of an elasto-isotropic half-space $x > 0$ or plate $0 < x < d$, normalized over the entire phonon spectrum to δ^{ik} (for arbitrary $\mathbf{r}$), has the form[1)]

$$G^{ik}(\mathbf{r};\ \omega^2) = M_r M^{-1} g^{ik}(x;\ \omega^2), \tag{2.1}$$

according to [4]. Here

$$g^{ik}(x;\ \omega^2) = \delta^{ik}[\delta^{i1} g_\perp(x;\ \omega^2) + (\delta^{i2} + \delta^{i3}) g_\parallel(x;\ \omega^2)],$$
$$g_\perp(x;\ \omega^2) = g^{1'1'}(x;\ \omega^2),\ g_\parallel(x;\ \omega^2) = {}^1\!/_2[g^{2'2'}(x;\ \omega^2) + g^{3'3'}(x;\ \omega^2)]; \tag{2.2}$$

$$g^{i'i'}(x;\ \omega^2) = (2\pi)^{-2} M \lim_{\varepsilon\to+0} \operatorname{Im} \int_0^\infty D^{i'i'}(x, x;\ f, \omega^2 - i\varepsilon)\, df^2. \tag{2.3}$$

Here $D^{i'k'}(x, x_0;\ f, w)$ is the two-dimensional Fourier transform of the dynamic Green's function of the corresponding system (see the Appendix), f the modulus of the projection $\mathbf{f}_\parallel$ of the wave vector on the boundary plane, w the square of the complex frequency, M the mean mass per atom. The primed and unprimed superscripts denote the projections on the axes of two different cartesian coordinate systems; the planes y'z' and yz, which are coincident with one another, also coincide with one of the boundaries of the plate or with the single boundary of the halfspace, and the axis $x' = x - c$ is the interior normal to this boundary; the axis is oriented along the vector $\mathbf{f}_\parallel$, the orientation of the y axis is arbitrary. Summation is not carried out over repeated indices in (2.2) and (2.3). The region of applicability of expressions (2.1)–(2.3) is limited above in frequency by the condition which, in particular, guarantees the mirror reflection of elastic waves from the boundary, viz.,

$$\omega \ll \omega_m a_0 / a_s,$$

where ω_m is the upper limit of the phonon spectrum, a_0 the interatomic distance, a_s the characteristic thickness of the surface layer, within the limits of which the lattice parameter and the matrix of force constants reach values corresponding to an unbounded system (usually $a_s \sim (3-4)a_0$).

We first consider the half-space. Then, following [3], we have (see the Appendix)

$$D^{i'i'}(x, x;\ f, w) = D_0^{i'i'}(0;\ f, w) - B^{i'i'}(x, x;\ f, w), \qquad x > 0, \tag{2.4}$$

where

$$D_0^{1'1'}(0) = \frac{u_0 - f^2}{2\rho w u_t^{1/2}}, \quad D_0^{2'2'}(0) = \frac{u_0 - f^2}{2\rho w u_l^{1/2}}, \quad D_0^{3'3'}(0) = -\frac{1}{2\rho c_t^2 u_t^{1/2}},$$

1) There are several technical misprints in [4]: one should have $\vartheta(x) = \frac{1}{2}(1 + \operatorname{sign} x)$ in (2.9), $w = \pi^2 n^2 c_\alpha^2 d^{-2}$ in (3.10), $fd \ll 1$ in (3.11) and $S_t(d)$ in place of $S_l(d)$ in the last formula of (A.11).

$$B^{1'1'}(x,x) = -(2\rho w u_t^{1/2} U_-)^{-1}[U_+ F_{lt}(x) - E(x)],$$
$$B^{2'2'}(x,x) = -(2\rho w u_l^{1/2} U_-)^{-1}[U_+ F_{tl}(x) - E(x)], \quad (2.5)$$
$$B^{3'3'}(x,x) = (2\rho c_t^2 u_t^{1/2})^{-1} e_t(2x),$$

and the following shorthand notation is used:

$$U_{\mp} = u_*^2 \mp u_0 f^2, \quad F_{\alpha\beta}(x) = u_0 e_\alpha(2x) + f^2 e_\beta(2x),$$
$$E(x) = 4u_* u_0 f^2 e_t(x) e_l(x), \quad e_\alpha(x) = \exp(-u_\alpha^{1/2}|x|),$$
$$u_* = f^2 - \frac{w}{2c_t^2}, \quad u_0 = u_t^{1/2} u_l^{1/2}, \quad u_\alpha = f^2 - \frac{w}{c_\alpha^2}, \quad (2.6)$$
$$\operatorname{Re} u_\alpha^{1/2} > 0, \quad \{\alpha,\beta\} = \{t,l\},$$

$D_0^{i'k'}(x;\ f,\ w)$ is the two-dimensional Fourier transform of the dynamical Green's function of the unbounded con-continuum, c_t and c_l the velocities of transverse and longitudinal sound, respectively, and ρ the density.

Further calculations are materially simplified if $B^{i'i'}(x,\ x;\ f,\ w)$ (2.5) is written in the form

$$B^{i'i'}(x,x;f,w) = P^{i'i'}(x;f,w) + Q^{i'i'}(x;f,w), \quad (2.7)$$

where

$$P^{1'1'}(x) = (2\rho c_t^2 u_t\ )^{-1} e_{lt}^{(0)}(2x), \quad P^{2'2'}(x) = (2\rho c_t^2 u_l^{1/2})^{-1} e_{tl}^{(0)}(2x),$$
$$P^{3'3'}(x) = B^{3'3'}(x,x), \quad Q^{1'1'}(x) = -(\rho w U_-)^{-1} u_l^{1/2}[e_{lt}^{(1)}(x)]^2,$$
$$Q^{2'2'}(x) = -(\rho w U_-)^{-1} u_t^{1/2}[e_{tl}^{(1)}(x)]^2 \quad Q^{3'3'}(x) = 0, \quad (2.8)$$

and

$$e_{\alpha\beta}^{(0)}(x) = u_0 e_\alpha(x) - f^2 e_\beta(x), \quad e_{\alpha\beta}^{(1)}(x) = u_* e_\alpha(x) - f^2 e_\beta(x). \quad (2.9)$$

In order to establish the validity of Eqs. (2.7)–(2.9), we first consider the quantity $B^{i'i'}$ (2.5) and, with the help of the identity $U_+ \equiv 2u_0 f^2 + U_-$ (see (2.6)) we represent the first term in the square brackets in the form of a sum of two terms—respectively containing and not containing U_- in the denominator. We write the coefficient u_0 for $e_l(2x)$ in the second of these by means of (2.6) in the form $u_0 \equiv f^{-2}(u_* - U_-)$ and, by the same token, we isolate another term not containing U_- in the denominator. Grouping terms of the same type, we obtain the given expression for $B^{1'1'}(x,\ x)$. The expression for $B^{2'2'}(x,\ x)$, in accord with (2.5), is obtained from $B^{1'1'}(x,\ x)$ by formal permutation of the subscripts $t \rightleftarrows l$.

Substituting (2.4) in (2.3), with account of (2.7), we get

$$g^{i'i'}(x;\omega^2) = g_0^{i'i'}(\omega^2) + p^{i'i'}(x;\omega^2) + q^{i'i'}(x;\omega^2), \quad (2.10)$$

where

$$g_0^{i'i'}(\omega^2) = (2\pi)^{-2} M \lim_{\varepsilon\to+0} \operatorname{Im} \int_0^\infty D_0^{i'i'}(0;f,\omega^2 - i\varepsilon)\,df^2,$$
$$p^{i'i'}(x;\omega^2) = -(2\pi)^{-2} M \lim_{\varepsilon\to+0} \operatorname{Im} \int_0^\infty P^{i'i'}(x;f,\omega^2 - i\varepsilon)\,df^2. \quad (2.11)$$

The quantities $q^{i'i'}(x,\ \omega^2)$ are expressed in terms of $Q^{i'i'}(x;\ f,\ \omega^2 - i\epsilon)$ by means of a formula similar to (2.11), which is conveniently written in the form

$$q^{i'i'}(x;\omega^2) = \sum_{p=0}^{2} q_p^{i'i'}(x;\omega^2), \quad (2.12)$$

where

$$q_p^{i'i'}(x;\omega^2) = -(2\pi)^{-2} M \lim_{\varepsilon\to+0} \operatorname{Im} \int_{f_{p+1}^2}^{f_p^2} Q^{i'i'}(x;f^2,\omega^2 - i\varepsilon)\,df^2,$$

$$f_0^2 = \infty, \quad f_1^2 = \frac{\omega^2}{c_t^2}, \quad f_2^2 = \frac{\omega^2}{c_l^2}, \quad f_3^2 = 0. \quad (2.13)$$

$$u_\alpha^{1/2}(\omega^2 - i\varepsilon) = \left[1 + \frac{i\varepsilon}{2c_\alpha^2 u_\alpha(\omega^2)} - \cdots\right] u_\alpha^{1/2}(\omega^2)$$

Setting $u_\alpha \equiv u_\alpha(w)$ and $w = \omega^2 - i\epsilon$, we find from the expression

$$\lim_{\varepsilon\to+0} u_\alpha^{1/2}(\omega^2 - i\varepsilon) = \begin{cases} \sqrt{u_\alpha(\omega^2)}, & \text{if } u_\alpha(\omega^2) > 0, \\ i\sqrt{|u_\alpha(\omega^2)|}, & \text{if } u_\alpha(\omega^2) < 0, \end{cases} \quad (2.14)$$

(see (2.6)) that only the following of the two values of the function satisfies the condition $\operatorname{Re} u_\alpha^{1/2} > 0$ in the limiting case $\epsilon \to +0$, where the square roots are taken in the sense of their arithmetic values.

The integrals (2.11), with account of (2.5), (2.6), (2.8), (2.9) and (2.14), are computed in elementary fashion (thanks to the Im sign, only the contributions to them in the region $(0,\ \omega^2/c_t^2)$ are included), so that we have, finally,

$$g_0^{1'1'}(\omega^2) = \frac{\omega}{3\omega_*^3}(2 + r^{3/2}), \quad g_0^{2'2'}(\omega^2) = \frac{\omega}{3\omega_*^3}(1 + 2r^{3/2}), \quad g_0^{3'3'}(\omega^2) = \frac{\omega}{\omega_*^3},$$
$$p^{1'1'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\left[-\left(1 + \frac{\partial^2}{\partial\xi_t^2}\right)\frac{\sin\xi_t}{\xi_t} + r^{3/2}\frac{\partial^2}{\partial\xi_l^2}\frac{\sin\xi_l}{\xi_l}\right],$$
$$p^{2'2'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\left[\frac{\partial^2}{\partial\xi_t^2}\frac{\sin\xi_t}{\xi_t} - r^{3/2}\left(1 + \frac{\partial^2}{\partial\xi_l^2}\right)\frac{\sin\xi_l}{\xi_l}\right] \quad (2.15)$$
$$p^{3'3'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\frac{\sin\xi_t}{\xi_t},$$

where

$$\omega_*^3 = \frac{4\pi^2 c_t^3}{a_0^3}, \quad a_0^3 = \frac{M}{\rho}, \quad r = \frac{c_t^2}{c_l^2}, \quad \xi_\alpha = \frac{2\omega x}{c_\alpha},$$
$$0 < r < 1/2, \quad \alpha = t, l, \quad (2.16)$$

a_0^3 is the mean volume per atom. So far as the values $q_p^{i'i'}(x;\ \omega^2)$ (2.12) are concerned, these are also materially simplified when account is taken of (2.6), (2.8), (2.9), (2.14) and (2.16), and can be written in the form

$$q_0^{1'1'}(x;\omega^2) = \frac{\pi\omega}{\omega_*^3}\sqrt{\varphi_0 - r}\,|V_0'(\varphi_0)|^{-1}\Big[\left(\varphi_0 - \frac{1}{2}\right)\exp(-\xi\sqrt{\varphi_0 - r})$$
$$- \varphi_0 \exp(-\xi\sqrt{\varphi_0 - 1})\Big]^2,$$
$$q_0^{2'2'}(x;\omega^2) = \frac{\pi\omega}{\omega_*^3}\sqrt{\varphi_0 - 1}\,|V_0'(\varphi_0)|^{-1}[(\varphi_0 - 1/2)\exp(-\xi\sqrt{\varphi_0 - 1})$$
$$- \varphi_0 \exp(-\xi\sqrt{\varphi_0 - r})]^2; \quad (2.17)$$

$$q_1^{1'1'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\int_r \sqrt{\varphi - r}\,|V_1(\varphi)|^{-2} \operatorname{Im}\Big\{V_1^*(\varphi)\Big[\left(\varphi - \frac{1}{2}\right)\cdot$$
$$\cdot \exp(-\xi\sqrt{\varphi - r}) - \varphi\exp(-i\xi\sqrt{1-\varphi})\Big]^2\Big\}d\varphi,$$

$$q_1^{2'2'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\int_r \sqrt{1-\varphi}\,|V_1(\varphi)|^{-2}\cdot$$
$$\times \operatorname{Re}\Big\{V_1^*(\varphi)\Big[\left(\varphi - \frac{1}{2}\right)\exp(-i\xi\sqrt{1-\varphi}) - \varphi\exp(-\xi\sqrt{\varphi - r})\Big]^2\Big\}\,d\varphi,$$

$$q_2^{1'1'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\int_0^r \sqrt{r-\varphi}\,V_2^{-1}(\varphi)\operatorname{Re}\Big[\left(\varphi - \frac{1}{2}\right)$$
$$\times \exp(-i\xi\sqrt{r-\varphi}) - \varphi\exp(-i\xi\sqrt{1-\varphi})\Big]^2 d\varphi, \quad (2.18)$$

$$q_2^{2'2'}(x;\omega^2) = \frac{\omega}{\omega_*^3}\int_0^r \sqrt{1-\varphi}\,V_2^{-1}(\varphi)$$
$$\times \operatorname{Re}[(\varphi - 1/2)\exp(-i\xi\sqrt{1-\varphi}) - \varphi\exp(-i\xi\sqrt{r-\varphi})]^2 d\varphi,$$

where

$$V_n(\varphi)=\left(\varphi-\frac{1}{2}\right)^2-\left[\exp\left(\frac{i\pi n}{2}\right)\right]\varphi\sqrt{|(\varphi-1)(\varphi-r)|},\quad n=0,1,2;$$
$$\varphi=\omega^{-2}c_t^2f^2,\quad \xi\equiv{}^1/_2\,\xi_t=\omega x\,/\,c_t,\qquad (2.19)$$

and all the square roots are taken in the sense of their arithmetic values, the prime indicates differentiation, $\varphi_0>1$ is the real root of the equation $V_0(\varphi)=0$, which is equivalent to $U_-(f,\omega^2)=0$.

The quantities (2.17) appear from integration over the interval $\omega^2/c_t^2<f^2<\infty$ (i.e., $1<\varphi<\infty$), where

$$\lim_{\varepsilon\to+0}\operatorname{Im}U_-^{-1}(f,\omega^2-i\varepsilon)=\pi\delta(U_-(f,\omega^2)).$$

Inasmuch as the root $\omega^2=c_s^2f^2$ of the equation $U_-(f,\omega^2)=0$, which satisfies the inequality $\omega^2<c_t^2f^2$, and which constitutes a simple pole of the half-space Green's function, corresponds to Rayleigh waves[6] (c_s is their velocity, $c_s<c_t$, $\varphi_0\equiv c_t^2/c_s^2>1$), the stated quantities determine the statistical weight of the surface modes. On the other hand, the quantities (2.15) and (2.18) were obtained as a result of integration over the interval $0<f^2<\omega^2/c_t^2$ (i.e., $0<\varphi<1$) and, consequently, determine the statistical weight of the volume modes. Here we mean by the statistical weight of the specified normal vibrations for an atom located at the point **r**, we mean their contribution to the function (2.1).

Substituting the quantities (2.12), with account of (2.17)–(2.19) and (2.15) in (2.10), we can represent the function $g^{ik}(x;\omega^2)$ (2.2) in the form

$$g^{ik}(x;\,\omega^2)=\delta^{ik}g_0(\omega^2)+p^{ik}(x;\,\omega^2)+q^{ik}(x;\,\omega^2),\qquad (2.20)$$

where

$$g_0(\omega^2)=g_0^{1'1'}(\omega^2)={}^1/_2[g_0^{2'2'}(\omega^2)+g_0^{3'3'}(\omega^2)]={}^3/_2\Omega^{-3}\omega,$$
$$\Omega^{-3}=\frac{a_0^3}{18\pi^2c_t^3}(2+r^{3/2}),\qquad (2.21)$$

while for $p^{ik}(x;\omega^2)$ and $q^{ik}(x;\omega^2)$, we obtain formulas similar to (2.2), with only the difference that, by definition (see (2.8)),

$$q^{3'3'}(x;\,\omega^2)=0.\qquad (2.22)$$

The quantity $\delta^{ik}g_0(\omega^2)$, with accuracy to within the factor M_rM^{-1}, (see (2.1)), is the distribution function of the acoustic oscillations of the individual atoms, located in an unbounded elasto-isotropic solid, since Ω is their Debye frequency.

Setting $x=0$, we get[2)]

$$g^{ik}(0;\,\omega^2)={}^3/_2\,(\hat{\Omega}^{-3})^{ik}\omega,\qquad (2.23)$$

where

$$(\hat{\Omega}^{-3})^{ik}=\delta^{ik}[\delta^{i1}\Omega_\perp^{-3}+(\delta^{i2}+\delta^{i3})\Omega_\parallel^{-3}]\qquad (2.24)$$

is the tensor of the inverse cubes of the Debye frequencies of the surface atoms (summation over repeated indices has not been carried out). Here the dimensionless quantities

$$Z_\perp=\frac{a_0}{c_t}\Omega_\perp,\quad Z_\parallel=\frac{a_0}{c_t}\Omega_\parallel,\quad Z=\frac{a_0}{c_t}\Omega\qquad (2.25)$$

are functions of a single parameter r (2.16) and are tabulated as such in [7].

In the general case ($x\neq 0$), one can introduce the dimensionless tensor spectral function

$$\psi^{ik}(\xi,r)=\frac{c_t^3}{a_0^3\omega}g^{ik}(x;\,\omega^2),\qquad (2.26)$$

which is expressed in terms of its eigenvalues

$$\psi_\perp(\xi,r)=\frac{c_t^3}{a_0^3\omega}g_\perp(x;\,\omega^2),\quad \psi_\parallel(\xi,r)=\frac{c_t^3}{a_0^3\omega}g_\parallel(x;\,\omega^2)\qquad (2.27)$$

with the help of a formula similar to (2.2). The quantities (2.26) and (2.27) obviously depend only on the two variables ξ and r (see (2.16), $\xi_t=2\xi$, $\xi_l=2\sqrt{r}\,\xi$), and the latter figures in the elastic properties of the solid.

The obtained results graphically illustrate the fact that the relaxation of the function of the local density of phonon states, from the value $g^{ik}(0;\omega^2)$ (2.23) on the surface of the sample to the quantity $\delta^{ik}g_0(\omega^2)$ (2.21) which is smaller by approximately two orders of magnitude takes place as $x\to\infty$ in a different way for the surface and volume oscillations. The statistical weight of the Rayleigh waves tends to zero exponentially, while the statistical weight of the volume oscillations falls off chiefly like $1/x$ and simultaneously oscillates. Moreover, it is seen from (2.18) that in the statistical weight of the volume oscillations, the wave vector of which satisfies the condition $\omega^2/c_l^2<f^2<\omega^2/c_t^2$ (i.e., $r<\varphi<1$), there is also a term which falls off exponentially with increase in the distance to the surface, and the oscillations are superposed on this decay. Finally, we turn our attention to the extremely simple form of the function

$$g^{3'3'}(x;\,\omega^2)=\frac{\omega}{\omega_*^3}\left(1+\frac{\sin\xi_t}{\xi_t}\right),\quad \xi_t\equiv\frac{2\omega x}{c_t}\qquad (2.28)$$

(see (2.10), (2.15), (2.16) and (2.22)) which, in the meaning which follows from the choice of the primed set of coordinates, is a function of the space-frequency distribution of purely transverse oscillations. The functional dependence on the frequency and distance to the surface, described by the expressions (2.28), as is seen from the results obtained, is also typical for the distribution of the other volume oscillations, although the character of the oscillations of the latter is much more complicated.

According to the expression for the complex frequency $\sqrt{\omega^2-i\epsilon}=\omega-i\epsilon/2\omega$, one can associate with ϵ the parameters $\tau=\omega/\epsilon$ and $l=c\omega/\epsilon$, which have the meaning of the time and length, respectively, of the coherent elastic wave in the classical theory, or the lifetime and free path length of the phonon in quantum theory (c is the characteristic value of the sound velocity, for example, $c=c_t$ or c_l). Equation (2.3), in which $\epsilon\to+0$ for fixed x, obviously corresponds to the case $l\gg x$. On the other hand, if $l\ll x$, then x would have to be made initially tend to infinity, and then ϵ to zero, which would lead to a frequency distribution independent of the coordinates and corresponding to an unbounded crystal.

3. THE PLATE

In connection with what has been said above, it is of interest to explain how the local density of phonon states

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2) With the help of (2.15) or (2.11), it is not difficult to establish the fact that

$$p^{i'i'}(0;\,\omega^2)=-g_0^{i'i'}(\omega^2),\quad i'=1',2'.$$

is modified in the case in which the free path length of the phonon exceeds the minimal linear dimension of the specimen. With this purpose, it is convenient to consider an unbounded crystal plate of arbitrary thickness d, for which the formulas (2.1)–(2.3) are preserved (ϵ tends to zero for fixed d, $l \gg d$), and the dynamic Green's function is directly determined by the same method as for the half-space (see the Appendix). The function $g^{ik}(x; \omega^2)$ now describes the gradual transformation of the local density of phonon states from the value $\sim 1/\omega$ at low frequencies $\omega \lesssim \pi c_t/d$, i.e., from the values determined essentially by shear oscillations,[4,8] to very complicated oscillations for $\omega > \pi c_t/d$ and turns out to be extraordinarily cumbersome. Therefore, we illustrate the most typical marks of its behavior using as an example one component, $g^{3'3'}(x; \omega^2)$, which characterizes the spectral distribution of purely transverse oscillations.

By means of the expression (see the Appendix)

$$D^{3'3'}(x, x_0; f, w) = -(2\rho c_t^2 u_t^{1/2})^{-1}\{e_t(x-x_0) + \mathrm{sh}^{-1} u_t^{1/2} d$$
$$\times [e_t(x)\,\mathrm{ch}\, u_t^{1/2}(d-x_0) + e_t(d-x)\,\mathrm{ch}\, u_t^{1/2} x_0]\}, \quad x, x_0 \in (0, d),$$

where the notation (2.6) is used, we write down the integrand in (2.3) for $i' = 3'$ in the form

$$D^{3'3'}(x, x; f, w) = -(2\rho c_t^2)^{-1} F^{-1}(u_t)\Phi(u_t),$$
$$\Phi(u_t) \equiv \mathrm{ch}\, u_t^{1/2}(d-2x) + \mathrm{ch}\, u_t^{1/2} d, \qquad (3.1)$$
$$F(u_t) \equiv u_t^{1/2} \mathrm{sh}\, u_t^{1/2} d.$$

Then, with account of the symbol Im in (2.3), it follows that a nonzero contribution is made to $g^{3'3'}(x; \omega^2)$ only by integration over the ϵ-vicinities of the points

$$u_t = u_{tn} \equiv -\pi^2 n^2/d^2, \qquad 0 \leqslant n \leqslant n_\omega,$$

where

$$n_\omega \equiv [\omega d/\pi c_t], \qquad (3.2)$$

and the square brackets denote the integer part. Inasmuch as $F(u_{tn}) = 0$, we have, in the vicinity of each such point,

$$F(u_t) = F'(u_{tn})(u_t - u_{tn}),$$

where, as is seen from (3.1),

$$F'(0) = d; \quad F'(u_{tn}) = (-1)^n d/2, \quad n \geqslant 1,$$

consequently,

$$\lim_{\epsilon\to+0} \mathrm{Im}\, F^{-1}\left(u_t + \frac{i\varepsilon}{c_t^2}\right) = -\pi \sum_{n=0}^{\infty} \frac{1}{F'(u_{tn})} \delta(u_t - u_{tn}).$$

Transforming in (2.3) from integration over f^2 to integration over $u_t = f^2 - \omega^2/c_t^2$ (from $-\omega^2/c_t^2$ to ∞), we thus obtain

$$g^{3'3'}(x; \omega^2) = \frac{a_0^3}{4\pi c_t^2 d}\left\{1 + n_\omega + \frac{\sin(\pi n_\omega x/d)\cos(\pi(n_\omega+1)x/d)}{\sin(\pi x/d)}\right\}, \quad (3.3)$$

where the latter term is obtained as the result of summation of the geometric progression

$$\sum_{n=1}^{n_\omega} \cos\frac{2\pi n x}{d} = \mathrm{Re} \sum_{n=1}^{n_\omega} \exp\left(\frac{2\pi i n x}{d}\right).$$

Inasmuch as integration of the first term of the function $\Phi(u_i)$ (3.1) over x from zero to d, yields zero, the function of the spectral distribution of transverse oscillations, averaged over the thickness of the plate, has the form

$$g^{3'3'}(\omega^2) \equiv \frac{1}{d}\int_0^d g^{3'3'}(x; \omega^2)\,dx = \frac{a_0^3}{4\pi c_t^2 d}(1 + n_\omega). \qquad (3.4)$$

If we do not consider the region of very low frequencies $\omega \lesssim \pi c_t/d$ and assume that $n_\omega \gg 1$ ($\omega \gg \pi c_t/d$), then the last term in (3.3) is always small in comparison with n_ω, with the exception of the regions $x \ll d$ and $d - x \ll d$ and, consequently, neglecting the discrete spectrum, we have

$$g^{3'3'}(x; \omega^2) = g^{3'3'}(\omega^2) = g_0^{3'3'}(\omega^2) \qquad (3.5)$$

(see (2.15)). At the same time, for $x \ll d$ and $d - x \ll d$, Eq. (3.3) transforms into (2.28). The spectral distribution of the remaining eigenoscillations behave in the same fashion, so that the function of the local density of phonon states in the plate for $\omega \gg \pi c_t/d$ does not differ essentially from such a function for the half-spaces $x > 0$ and $x < d$.

4. CONCLUSION

1. The spectral function (2.1) found in the present work makes it possible to compute the temperature dependent parts of the tensors of the mean square fluctuations of position $\langle u_r^i u_r^k \rangle$ and momenta $\langle p_r^i p_r^k \rangle$ of the particles of a solid as functions of $\mathbf{r}$ in the presence of plane free boundaries, at low temperatures and according to the usual formulas (see, for example, [4,5]). These fluctuations are important, in particular, in the study of processes of the incoherent interaction of particles, quasiparticles, or radiation with phonons. For the description of coherent processes, it is necessary to know the correlators of the form $\langle u_r^i u_0^k \rangle$ for $\mathbf{r} \neq \mathbf{r}_0$, which can be found directly with the aid of the corresponding Green's functions given in the Appendix.

2. The essential difference of the function of the local density of phonon states from the mean values at very large distances from the surface should evidently affect kinetic characteristics of the bounded system, in particular, the time of phonon relaxation of the current carriers in thin plates and in the surface layer of a bulk sample under the conditions of the skin effect and also the absorption (scattering) cross section of the flux of external radiation or of particles with the participation of phonons. At liquid helium temperature, the parameter ξ (2.19), which corresponds to the "thermal" frequency of the phonons $\omega_T = kT/\hbar$, can be seen to be equal to unity even for $x \sim \delta$, where δ is the thickness of the skin layer or the penetration depth into the sample of the external flux. Nevertheless, the length of the oscillating "tail" of the spectral distribution can be comparable with δ.

Inasmuch as the density of states of the acoustic phonons in the surface layer is greater than in the bulk, it must be expected, in general, that there will be an increase in the surface phonon electroresistance in comparison with the bulk value. Along with this, the bulk conductivity evidently ought to change in some definite fashion. In principle, because of the formation of electronic wave functions that satisfy the proper boundary conditions, one could have expected strong interference here of the phonon-"defect" scattering of the type considered by Kagan and Zhernov[9] for the case of impurity atoms. However, a highly polished plane boundary, which is an "elementary" extended defect for long-wave phonons, is not such for electrons. Because of the diffuse reflection from the boundary, the latter should generally be described by density matrices, so that the interference effects in the bulk are of low probability.

3. The local density of states of the acoustic phonons in the vicinity of the plane boundary differs from that for electrons[10] by the incommensurably large spatial periods of the oscillations, equal to $\pi c_\alpha/\omega$ ($\alpha = t, l$) instead of π/k_F (k_F is the Fermi momentum) and, as a rule, is greater than the penetration depth. Moreover, for given fixed frequency, the first is maximal on the surface itself ($x = 0$), while the second vanishes.

4. In conclusion, we note again that the free plane boundary of a solid can be regarded as a special case of a two-dimensional defect in an unbounded crystal. This makes it possible to assume that other extensive defects, such as single dislocations, dislocation walls, stacking faults, and so on, ought, at very large distances, to change materially the local density of phonons in comparison with those which correspond to the ideal unbounded crystal.

The author is greatly indebted to I. M. Lifshitz for useful discussion.

APPENDIX

The two-dimensional Fourier transform of the dynamical Green's function of an elasto-isotropic plate of thickness d ($0 < x < d$) in the primed set of coordinates ($x' = x$) satisfies the Dyson equation

$$s(x)D^{i'i_0'}(x,x_0) = s(x_0)D_0^{i'i_0'}(x-x_0) - T^{i'k'}(x)D^{k'i_0'}(0,x_0) + T^{i'k'}(x-d)D^{k'i_0'}(d,x_0), \quad x, x_0 \in (-\infty, \infty), \tag{A.1}$$

where

$$s(x) = {}^1/_2[\operatorname{sign} x - \operatorname{sign}(x-d)] \tag{A.2}$$

is a function of the shape of this plate, while the nonlinear components of the matrices

$$D_0^{i'k}(x) \equiv D_0^{i'k'}(x; f, w), \quad T^{i'k'}(x) \equiv T^{i'k'}(x; f, w) \tag{A.3}$$

have the form

$$D_0^{1'1'}(x) = u_l^{1/2} P_0^{-1} e_{lt}^{(0)}(x), \quad D_0^{2'2'}(x) = u_t^{1/2} P_0^{-1} e_{tl}^{(0)}(x),$$
$$D_0^{1'2'}(x) = D_0^{2'1'}(x) = ifu_0 s_x P_0^{-1}[e_t(x) - e_l(x)],$$
$$D_0^{3'3'}(x) = -(2\rho c_t^2 u_t^{1/2})^{-1} e_t(x); \tag{A.4}$$

$$T^{1'1'}(x) = s_x c_t^2 w^{-1} e_{lt}^{(1)}(x), \quad T^{2'2'}(x) = s_x c_t^2 w^{-1} e_{tl}^{(1)}(x),$$
$$T^{1'2'}(x) = ifc_t^2 (wu_t^{1/2})^{-1} e_{tl}^{(2)}(x),$$
$$T^{2'1'}(x) = -ifc_t^2 (wu_l^{1/2})^{-1} e_{lt}^{(2)}(x), \quad T^{3'3'}(x) = -{}^1/_2 s_x e_t(x). \tag{A.5}$$

We have used here the notation of (2.6) and (2.9), as well as

$$e_{\alpha\beta}^{(2)}(x) = u_* e_\alpha(x) - u_0 e_\beta(x), \quad s_x \equiv \operatorname{sign} x, \quad P_0 = 2\rho w u_0. \tag{A.6}$$

After two alternate substitutions $x = x_-, x_+$, where x_- and x_+ are arbitrary points from the intervals $(-\infty, 0)$ and (d, ∞), respectively, the expression (A.1) transforms into a set of six inhomogeneous linear algebraic equations in $D^{i'i_0'}(0, x_0)$ and $D^{i'i_0'}(d, x_0)$ (i_0' and x_0 are arbitrary but fixed). By calculating these quantities from the formulas of [3], we find that their nonzero components have the form

$$D^{i'k'}(0, x_0; f, w) = D^{i'k'}(d, d-x_0; -f, w); \tag{A.7}$$

$$D^{1'1'}(d,x_0) = -u_l^{1/2} L^{-1}[S_{tl}^{(1)}(d)C_{lt}^{(1)}(x_0) - u_* f^2 C_{lt}^{(2)}(d) S_{tl}^{(2)}(x_0)],$$
$$D^{2'2'}(d,x_0) = -u_t^{1/2} L^{-1}[S_{lt}^{(1)}(d)C_{tl}^{(1)}(x_0) - u_* f^2 C_{tl}^{(2)}(d) S_{lt}^{(2)}(x_0)],$$
$$D^{1'2'}(d,x_0) = ifL^{-1}[S_{tl}^{(1)}(d)S_{lt}^{(2)}(x_0) - u_* u_0 C_{lt}^{(2)}(d) C_{tl}^{(1)}(x_0)],$$
$$D^{2'1'}(d,x_0) = -ifL^{-1}[S_{lt}^{(1)}(d)S_{tl}^{(2)}(x_0) - u_* u_0 C_{tl}^{(2)}(d) C_{lt}^{(1)}(x_0)],$$
$$D^{3'3'}(d,x_0) = -[\rho c_t^2 u_t^{1/2} S_t(d)]^{-1} C_t(x_0), \quad x_0 \in (0, d), \tag{A.8}$$

where

$$D^{i'k'}(d, x_0) = D^{i'k'}(d, x_0; f, w); \tag{A.9}$$

$$S_{\alpha\beta}^{(1)}(x) = u_*^2 S_\alpha(x) - u_0 f^2 S_\beta(x), \quad S_{\alpha\beta}^{(2)}(x) = u_* S_\alpha(x) - u_0 S_\beta(x),$$
$$C_{\alpha\beta}^{(1)}(x) = u_* C_\alpha(x) - f^2 C_\beta(x), \quad C_{\alpha\beta}^{(2)}(x) = C_\alpha(x) - C_\beta(x),$$
$$C_\alpha(x) = \operatorname{ch}(u_\alpha^{1/2} x), \quad S_\alpha(x) = \operatorname{sh}(u_\alpha^{1/2}|x|), \quad \{\alpha, \beta\} = \{t, l\}, \tag{A.10}$$

and the quantity L, which determines the character of the poles of the components $\{i', k'\} = \{1', 2'\}$ of the Green's function, is written as

$$L = 8\rho c_t^2 W_{tl} W_{lt} C_t^2\left(\frac{d}{2}\right) C_l^2\left(\frac{d}{2}\right),$$
$$W_{\alpha\beta} = u_*^2 \operatorname{th}({}^1/_2 u_\alpha^{1/2} d) - u_0 f^2 \operatorname{th}({}^1/_2 u_\beta^{1/2} d), \quad \alpha \neq \beta. \tag{A.11}$$

Finally, substituting (A.4)–(A.11) in (A.1) and assuming $x, x_0 \in (0, d)$, we obtain the Green's function for the plate for an arbitrary pair of spatial arguments. Special attention must be paid to the condition $\operatorname{Re} u_\alpha^{1/2} > 0$ (2.6), which chooses one each from among the two branches of the functions $u_\alpha^{1/2}$ ($\alpha = t, l$) and excludes the possibility of replacement of u_0 (2.6) by the quantity $(u_t u_l)^{1/2}$.

The transformations which lead from the general formulas of [3] to (A.7)–(A.11) are not very complicated in principle, although they are cumbersome. For the reader who desires to repeat them, we note that the pairs of arguments (x_1, x_2) of the matrices $A^{i'k'}(x_1, x_2)$ and $\Theta^{i'k'}(x_1, x_2)$ from [3], which determine the solution of the problem, satisfy respectively the conditions $\operatorname{sign}(x_1 - x_2) = \operatorname{sign} x_1$ and $\operatorname{sign} x_2 = \operatorname{sign} x_1$. The general formulas[11] for the matrices are greatly simplified from the very beginning with account of these[4] and further calculations are reduced to multiplication of double-row matrices, similar in shape to (A.4) and (A.5).

For satisfaction of the conditions

$$(d-X)\operatorname{Re} u_\alpha^{1/2} \gg 1, \quad X \operatorname{Re} u_\alpha^{1/2} \leqslant 1, \quad X = x, x_0; \quad \alpha = t, l \tag{A.12}$$

the expressions (A.1) and (A.7) (with account of (A.8)–(A.11)) with accuracy to exponentially small quantities like $e_\alpha(d-x)$, $e_\alpha(d-x_0)$ and $e_\alpha(d)$, take the form

$$\vartheta(x)D^{i'i_0'}(x,x_0) = \vartheta(x_0)D_0^{i'i_0'}(x-x_0) - T^{i'k'}(x)D^{k'i_0'}(0,x_0), \quad x, x_0 \in (-\infty, \infty); \tag{A.13}$$

$$D^{1'1'}(0,x_0) = -u_l^{1/2} P^{-1} e_{lt}^{(1)}(x_0), \quad D^{2'2'}(0,x_0) = -u_t^{1/2} P^{-1} e_{tl}^{(1)}(x_0),$$
$$D^{1'2'}(0,x_0) = -ifP^{-1} e_{lt}^{(2)}(x_0), \quad D^{2'1'}(0,x_0) = ifP^{-1} e_{tl}^{(2)}(x_0),$$
$$D^{3'3'}(0,x_0) = -(\rho c_t^2 u_t^{1/2})^{-1} e_t(x_0), \quad x_0 > 0, \tag{A.14}$$

where

$$D^{i'k'}(x, x_0) \equiv D^{i'k'}(x, x_0; f, w), \quad \vartheta(x) = {}^1/_2(1 + s_x), P = 2\rho c_t^2 U_-, \tag{A.15}$$

and the notation of (2.6), (2.9) and (A.6) is used. For $x > 0$ and $x_0 > 0$, these expressions obviously determine the Green's function of the isotropic elastic half-space. They can be obtained also by direct calculation from the general formulas, which refer to an arbitrary anisotropic half-space.[11]

The only zeroes of the expression for L(f, w) (A.11) are the roots of the equations $W_{lt} = 0$ and $W_{tl} = 0$. For $|u^{1/2}|d \ll 1$, they are easily solved relative to w by successive approximations if each of the hyperbolic tangents in (A.11) are expanded in power series, so that

$$W_{lt} = \frac{u_l^{1/2} wd}{8c_t^4}\Big\{w - \frac{d^2}{12}\Big[c_0^2 f^4 - (3-4r)wf^2 - \frac{rw^2}{c_t^2}\Big]$$
$$+ \frac{d^4}{120}\Big[2c_0^2 f^6 - (11 - 8r - 4r^2)wf^4 + 2(2 - r - 2r^2)\frac{f^2w^2}{c_t^2} + \frac{r^2w^2}{c_t^4}\Big] + \ldots\Big\}$$

$$W_{tl} = \frac{u_t^{1/2} wd}{8c_t^4}\Big\{w - c_0^2 f^2 + \frac{d^2}{12}\Big[2c_0^2 f^4 - (5 - 4r^2)wf^2 + \frac{w^2}{c_t^2}\Big] + \ldots\Big\},$$

where $c_0^2 \quad 4(1 - r)c_t^2$. As a result, one can obtain the dispersion law of shear and longitudinal vibrations of the plate in the form of a series in fd.[4] In the opposite limiting case, when $\mathrm{Re}\, u_d^{1/2} \gg 1$, each of the hyperbolic tangents in (A.11) is replaced by unity, so that both the given terms are identical with the dispersion equation $U_-(f, w) = 0$ for surface Rayleigh waves.

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Translated by R. T. Beyer
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