Exact solution of the problem of the Green's function and of the distribution function of the frequencies of polar optical phonons in the diffusion region of the energy spectrum of solid solution of uniaxial crystals

I. P. Ipatova and V. A. Shchukin

Ioffe Physicotechnical Institute, USSR Academy of Sciences

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We consider the spectrum of polar optical phonons in solid solutions of uniaxial crystals. The presence of directional dispersion in the spectrum of the polar optical phonons leads to a state density of the same form as in cubic $4D$ and $5D$ crystals. The method of asymptotic summation of perturbation-theory series (the Lipatov–Brezin–Parisi method) is used to find the Green's function of the polar optical phonons $G(\omega^2,\mathbf{q})$ and the frequency distribution function $\rho(\omega^2)$. It is established that through localization suppression in such $4D$ and $5D$ systems the instanton solution of the nonlinear equations of the effective field theory determines the asymptotic behavior of the effective perturbation-theory series for $G(\omega^2,\mathbf{q})$ for all frequencies, both on "tail" $\rho(\omega^2)$ and in the continuous spectrum, as well as in the diffusion region. It is shown that, compared with the single-instanton contribution to the phonon self-energy part $\Sigma(\omega^2,\mathbf{q})$ that describes multiple scattering of phonons by isolated fluctuations, the many-instanton contributions to the phonon self-energy part $\Sigma(\omega^2,\mathbf{q})$, which describe the interference of scattering of various phonons by various fluctuations turn out to be small at all frequencies, including the diffusion region. Under conditions when the interference effects are suppressed in the diffusion region, an exact solution is obtained in the $5D$ case and a solution with logarithmic accuracy for $4D$ systems. It is shown that the dependence of the line width for absorption or scattering of light by optical phonons on the composition of the solid solution has an exponentially sharp maximum. It is established that the width of the optical phonon line depends on the phonon-propagation direction, i.e., has directional dispersion.

The energy spectrum of three-dimensional ($3D$) disordered systems, such as crystals with impurities or solid solutions, contain between the region of the continuous quasiparticle spectrum and the "tail" of the density of state an intermediate diffusion part of the spectrum, in which the mean free path of the quasiparticle and its de Broglie wavelength are of the same order, and the quasiparticle diffuses rather than propagates freely.[1] In the same region of the spectrum a transition takes place from delocalized and localized states, i.e., a localization threshold is located. In the diffusion region, important roles are played simultaneously by single scattering of the quasiparticles by one fluctuations and by multiple scattering of quasiparticles by various fluctuations. As a rule, therefore, it is impossible to obtain in the $3D$ case an analytic expression for the Green's function $G(\omega,\mathbf{q})$ of quasiparticles and for the state density $\rho(\omega)$ in the diffusion region in the $3D$ case.[1]

There exist, however, low-symmetry (uniaxial and biaxial) crystals in which the density of states for dipole-active excitations (polar optical phonons, excitons, plasmons) the density of states has the same form as in cubic $4D$ and $5D$ crystals.[2] In Refs. 3 and 4 was investigated the formation of state-density tails of dipole-active excitations in solid solutions of low-symmetry crystals, and the same suppression of fluctuations that would occur in cubic $4D$ and $5D$ crystals would take place was observed. In this sense one can say that low-symmetry crystals have effective dimensionalities $D=4$ and 5.

Let us consider polar optical phonons whose dispersion law in uniaxial crystals is of the form[5–7]

$$\omega^2(\mathbf{q})=\omega_{LO}^{\parallel 2}+\beta(qa)^2+\alpha\sin^2\vartheta, \quad (1)$$

where ω_{LO}^2 is the frequency of a longitudinal optical phonon polarized along the optical axis, β is the phonon dispersion coefficient over the dispersion zone, α is the directional dispersion coefficient, ϑ is the angle between the wave vector $\mathbf{q}$ of the phonon and the optical axis of the crystal, a is the lattice constant. For $\alpha<0$ and $\beta<0$ the frequency $\omega_{LO}^{\parallel}$ is the edge of the continuous spectrum.

Let us examine the laws of localization of the vibrations near the edge $\omega_{LO}^{\parallel}$ of the continuous spectrum, using as an example the solid solution $A_{1-x}B_xC$, where the localization takes place on fluctuations of the composition x. The "binding energy" $\Delta\omega^2$ of a localized vibration is equal to the difference is equal to the difference between the "phonon kinetic energy" $\beta(qa)^2+\alpha\sin^2\vartheta$ and its "potential" energy $V_0\Delta x(\mathbf{r})$, resulting from the excess fraction of the heavy component B in the volume of the fluctuation. (Here V_0 is the total concentration shift of the square of the frequency on going from outer component of the solid solution to the other: $V_0=\omega_{LO}^{\parallel 2}(\mathrm{AC})-\omega_{LO}^{\parallel 2}(\mathrm{BC})$.) The shift of the square of the frequency of the local vibration relative to the edge of the continuous spectrum $\tilde\omega_{LO}^{\parallel 2}=\omega_{LO}^{\parallel 2}(\mathrm{AC})-xV_0$ is equal to

$$\Delta\omega^2\equiv\omega^2-\tilde\omega_{LO}^{\parallel 2}=\langle\beta(qa)^2\rangle+\langle\alpha\sin^2\vartheta\rangle-\langle V_0\Delta x(\mathbf{r})\rangle, \quad (2)$$

where $\langle...\rangle$ means averaging over the localized vibrational state.

It follows from (2) that formation of a local vibration with a specified $\Delta\omega^2$ in the presence of directional dispersion calls for a fluctuation with a larger value $\langle V_0\Delta x(\mathbf{r})\rangle$ than in the case when there is no directional dispersion. This increase of $\langle V_0 \Delta x(\mathbf{r}) \rangle$ lowers the probability of fluctuation formation and consequently decreases, compared with the $3D$ case, the frequency distribution function,[3,4] and the localization turns out to be suppressed. It is shown in Ref. 4 that for $\alpha \ll V_0$ the tail of the frequency distribution $\rho(\omega^2)$ has no Gaussian section and the entire tail is determined by the Fermi fluctuations of the composition. It was established in Ref. 3 that at

$$\Omega_0 \ll \alpha \ll V_0 \tag{3}$$

(Ω_0 is the characteristic width of the three-dimensional diffusion region) the tail of the function $\rho(\omega^2)$ contains a Gaussian section, but in this case the frequency distribution function

$$\rho(\omega^2) \propto \exp\left\{ -\left[\frac{C_1\alpha + C_2 |\omega^2 - \omega_{LO}^{\parallel 2}|}{\Omega_0} \right]^{1/2} \right\} \tag{4}$$

turns out to be exponentially suppressed with the $3D$ case on account of the frequency-independent exponentially small factor

$$\exp\{-S(0)\} = \exp\{-[C_1\alpha/\Omega_0]^{1/2}\}.$$

Suppression of the localization points to the possibility of obtaining exact analytic expressions for the phonon Green's function $G(\omega^2,\mathbf{q})$ and the frequency distribution function $\rho(\omega^2)$ in the diffusion region of the spectrum. In the present paper we solve the problem of the Green's function of optical phonons in a solid solution with directional dispersion, i.e., in $4D$ and $5D$ disordered systems, for the simplest case corresponding to an exponentially suppressed Gaussian tail of the function (4). Exact expressions are obtained for the $G(\omega^2,\mathbf{q})$ and $\rho(\omega^2)$ of the phonons in a wide range of the energy spectrum, including the diffusion region. The solution is obtained by the method of Lipatov,[8] Brezin, and Parisi,[9,10] based on asymptotic summation of high orders of perturbation theory and separating the instanton contributions into a Green's function.

A similar problem with suppression of fluctuations was solved by Larkin and Khmel'nitskiĭ for a second-order phase-transition in uniaxial ferroelectrics.[11]

1. FORMULATION OF PROBLEM

For an ideal crystal, the energy spectrum of polar optical phonons having directional dispersion is of the form shown schematically in the figure. The frequency distribution function near the edge of the continuous spectrum $\omega_{LO}^{\parallel}$ is determined mainly by the contribution of the branch (1).

In the solid solution $A_{1-x}B_xC$ with uncorrelated distribution of the atoms A and B over the sites of one of the sublattices, the composition fluctuations produce for an optical phonon, near the edge of the continuous spectrum, a "Gaussian random potential" $V(\mathbf{r})$. If the edge of the continuous spectrum of the solid solution is chosen to be the edge of the spectrum of the so-called virtual crystal $\tilde{\omega}_{LO}^{\parallel 2} = \omega_{LO}^{\parallel 2}(AC) - xV_0$, then $\langle V(\mathbf{r}) \rangle = 0$, and

$$\langle V(\mathbf{r}) V(\mathbf{r}') \rangle = x(1-x) V_0^2 a^3 \delta(\mathbf{r}-\mathbf{r}'). \tag{5}$$

The phonon Green's function averaged over the random potential $V(\mathbf{r})$, just as the electron Green's function,[12]

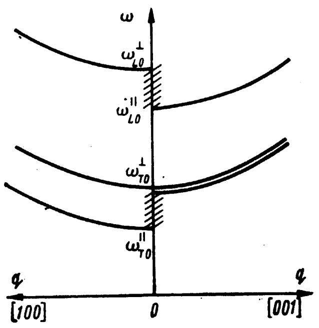

FIG. 1. Scheme of the spectrum of polar optical phonons in uniaxial crystal with directional dispersion. The shaded areas are the areas of directional dispersion. The double-degenerated branch is shown by the double line.

can be expressed with the aid of the replica method in the form of a functional integral

$$G(\omega^2,\mathbf{q}) = -\frac{1}{\alpha} \lim_{N\to 0} \int D\Psi_j(\mathbf{r}) \int d^3\mathbf{r}\, \Psi_N(\mathbf{r}) \Psi_N(0) \times \exp\{-i\mathbf{q}r_0\mathbf{r}\} \exp\{-S[\Psi]\}, \tag{6}$$

where the action $S[\Psi]$ for an N-component phonon field is equal to

$$S[\Psi] = \frac{1}{2} \int \sum_{i=1}^{N} \Psi_i(\mathbf{r}) (\hat{T} - \varepsilon) \Psi_i(\mathbf{r}) d^3\mathbf{r} - \frac{g}{4} \int \left[\sum_{i=1}^{N} \Psi_i^2(\mathbf{r}) \right]^2 d^3\mathbf{r} - \frac{1}{2\alpha} \mathrm{Re}\,\Sigma(\varepsilon=0) \int \left[\sum_{i=1}^{N} \Psi_i^2(\mathbf{r}) \right] d^3\mathbf{r}. \tag{7}$$

In (7), $\hat{T}$ is the "phonon kinetic energy" operator, $(\hat{T}\exp(i\mathbf{q}r_0\mathbf{r}) = \alpha^{-1}[\omega^2(\mathbf{q}) - \tilde{\tilde{\omega}}_{LO}^{\parallel 2}]\exp(i\mathbf{q}r_0\mathbf{r}))$. The dimensionless coordinates r in (6) and (7) are expressed in units of the characteristic dimension $r_0 = a(\beta/\alpha)^{1/2}$ of the optimal fluctuation,[3] and the dimensionless shift of the square of the frequency $\varepsilon = \alpha^{-1}[\omega^2 - \tilde{\tilde{\omega}}_{LO}^{\parallel 2}]$ is written in units of the directional-dispersion coefficient α. The second term in (7) is the result of averaging the Green's function over the random potential; g is a dimensionless coupling constant and its value for the solid solution $A_{1-x}B_xC$ is equal to

$$g = -\frac{x(1-x)V_0^2}{\beta^{3/2}\alpha^{1/2}} = -\left(\frac{\Omega_0}{\alpha}\right)^{1/2}. \tag{8}$$

The last term in (7) takes into account the fluctuation shift of the edge of the continuous spectrum of the solid solution relative to the edge of the spectrum in the virtual-crystal approximation:

$$\tilde{\tilde{\omega}}_{LO}^{\parallel 2} = \omega_{LO}^{\parallel 2}(AC) - xV_0 - \mathrm{Re}\,\Sigma(\omega = \tilde{\tilde{\omega}}_{LO}^{\parallel});$$

where ε in (7) is now measured from the renormalized edge.

The action $S[\Psi]$ [see (7)] has the same form as the effective Hamiltonian in the problem of the second-order phase transition.[13] In contrast to Ref. 13 we have here $g<0$ and the integral (6) formally diverges. Nonetheless, the Green's function (6) exists as an analytic continuation of a similar integral from the semi-axis $g>0$ on the complex g plane with a cut along the semi-axis $g<0$.[12,14] To make this analytic continuation, we use the method of calculating functional integrals of type (6), developed in the papers by Lipatov,[8] Brezin, LeGouillou and Zinn-Justin,[15] and Brezin and Parisi.[9,10]

2. LOCALIZED VIBRATIONS OF THE TAIL OF THE DISTRIBUTION OF THE FREQUENCIES OF LONGITUDINAL OPTICAL PHONONS

In Secs. 2–4 below we calculate the Green's function of the optical phonons of branch (1) for a solid solution, i.e., the Green's function of phonons in a quasi-5D-disordered system. Expansion of the Green's function (6) in powers of the coupling constant g

$$G(\alpha\varepsilon,\mathbf{q})=\sum_{K=0}^{\infty}(-g)^{K}G^{(K)}(\alpha\varepsilon,\mathbf{q}) \tag{9}$$

corresponds uniquely to the perturbation-theory diagram series. At frequencies lower than the energy-spectrum gap, however, i.e., at $\omega<\tilde{\omega}_{LO}^{\parallel}$ or $\varepsilon<0$, all these diagrams turn out to be real and make no contribution to the frequency distribution function

$$\rho(\alpha\varepsilon)=-\frac{1}{\pi}\int \operatorname{Im} G(\alpha\varepsilon,\mathbf{q})\frac{d^3\mathbf{q}}{(2\pi)^3}. \tag{10}$$

It is known, on the other hand, that inside the gap the frequency distribution function has a tail corresponding to $\rho(\varepsilon)>0$.[3,4] The cause of this seeming contradiction is that Green's-function series similar to expression (9) are asymptotic.[8-10,15] Such a series is analyzed by breaking it up into two parts:

$$G(\alpha\varepsilon,\mathbf{q})=\sum_{K=0}^{\infty}(-g)^{K}G^{(K)}(\alpha\varepsilon,\mathbf{q})=\tilde{G}(\alpha\varepsilon,\mathbf{q})+\tilde{\tilde{G}}(\alpha\varepsilon,\mathbf{q}), \tag{11}$$

where

$$\tilde{G}(\alpha\varepsilon,\mathbf{q})=\sum_{K=0}^{K_0-1}(-g)^{K}G^{(K)}(\alpha\varepsilon,\mathbf{q}), \tag{12}$$

$$\tilde{\tilde{G}}(\alpha\varepsilon,\mathbf{q})=\sum_{K=K_0}^{\infty}(-g)^{K}G^{(K)}(\alpha\varepsilon,\mathbf{q}). \tag{13}$$

The first part of the series (11), $\tilde{G}(\alpha\varepsilon,\mathbf{q})$, is obtained by direct summation of a finite number of diagrams and turns out to be pure real at $\varepsilon<0$. It makes no contribution to $\rho(\alpha\varepsilon)$. The Borel asymptotic method is used for the second part of the series, $\tilde{\tilde{G}}(\alpha\varepsilon,\mathbf{q})$.

To carry out the asymptotic summation, we calculate the coefficient of the series (9) with the larger number K. By analogy with Refs. 8, 9, and 15, we have

$$G^{(K)}(\alpha\varepsilon,\mathbf{q})=-\frac{1}{\alpha}\lim_{N\to0}\frac{1}{2\pi i}\oint\frac{dg}{(-g)}\int D\Psi_i(\mathbf{r})\int d^3\mathbf{r}$$
$$\times\Psi_N(\mathbf{r})\Psi_N(0)\exp\{-i\mathbf{q}r_0\mathbf{r}\}\exp\{-K\ln(-g)-S[g;\Psi_i(\mathbf{r})]\}. \tag{14}$$

For $K\gg1$, the integral (14) is calculated by the saddle-point method with respect to g and by a functional saddle point with respect to $\Psi_i(\mathbf{r})$. The conditions for the determination of the saddle point [9] yield for $\Psi_i(\mathbf{r})$ a nonlinear equation, a nonzero (so-called instanton) solution of which can be represented in the form[9,16]

$$\Psi_i^{INST}(\mathbf{r})=\left[\frac{4K}{I_4(\varepsilon,0)}\right]^{1/2}u_i\Phi(\varepsilon,\mathbf{r}), \tag{15}$$

where u_i is a unit vector in the replica space, $\Phi(\varepsilon,\mathbf{r})$ is the nonzero solution of the equation for the optimal fluctuation

$$\hat{T}\Phi(\varepsilon,\mathbf{r})-\Phi^3(\varepsilon,\mathbf{r})=\varepsilon\Phi(\varepsilon,\mathbf{r}), \tag{16}$$

and

$$I_n(\varepsilon,\mathbf{q})=\int\Phi^n(\varepsilon,\mathbf{r})\exp(-i\mathbf{q}r_0\mathbf{r})\,d^3\mathbf{r}. \tag{17}$$

It is shown in Ref. 3 that, owing to directional dispersion in the phonon spectrum (1), and hence in the "phonon kinetic energy operator" $\hat{T}$ from (16), the function $\Phi(\varepsilon,\mathbf{r})$ in the phonon spectrum (16) is almost independent of ε as $\varepsilon\to0$ at distances of the order of the dimension of the optimal fluctuation. The integration over g in (14) and over $\Psi_i(\mathbf{r})$ in the vicinity of the saddle point is practically independent of ε as $\varepsilon\to0$. The integration in (14) over $\mathbf{g}$ and over $\Psi_i(\mathbf{r})$ in the vicinity of the saddle point is carried out at $\varepsilon<0$ in a manner similar as used by Berezin and Parisi[9] and yields

$$G^{(K)}(\alpha\varepsilon,\mathbf{q})=\frac{C_0(\varepsilon)\,|I_3(\varepsilon,\mathbf{q})|^2}{\alpha[\varepsilon-\varepsilon(\mathbf{q})]^2}KK!\left[\frac{4}{I_4(\varepsilon,0)}\right]^{K}. \tag{18}$$

Here, in contrast to Ref. 9, the functions $I_4(\varepsilon,0)$, $I_3(\varepsilon,\mathbf{q})$ and $C_0(\varepsilon)$ in the limit as $\varepsilon\to0$ are independent of ε. An expression for $C_0(\varepsilon)$ is given in the Appendix.

It follows from (18) that the asymptotic behavior of the series (11) for the phonon Green's function is monitored by the instanton solution (15) with constant action

$$S[\Psi^{INST}]=\frac{1}{-4g}\int\Phi^4(\varepsilon,\mathbf{r})\,d^3\mathbf{r}=\frac{1}{-4g}I_4(\varepsilon,0)<\infty.$$

Under the constraint (3) on the directional-dispersion coefficient α, the coupling constant g of (8) is small, and consequently the instanton action is large:

$$S(\varepsilon)\equiv S[\Psi^{INST}(\varepsilon)]=\frac{I_4(\varepsilon,0)}{-4g}\gg1. \tag{19}$$

Note that owing the weak dependence of $I_4(\varepsilon,0)$ on ε the action $S(\varepsilon)$ remains large also in the limit as $\varepsilon\to0$.

The condition (19) means that the terms $(-g)^K G^{(K)}(\alpha\varepsilon,\mathbf{q})\sim K![S(\varepsilon)]^{-K}$ of the series (9) with numbers K that are not too large ($1\ll K\ll\tilde{K}=S(\varepsilon)$) decrease in succession, and later begin to increase at $K\gtrsim\tilde{K}$. The function $\tilde{\tilde{G}}(\alpha\varepsilon,\mathbf{q})$ from (13) is obtained by substituting $G^{(K)}(\alpha\varepsilon,\mathbf{q})$ from (18) in (13) and by asymptotic Borel summation (see Ref. 10). As a result we have

$$\tilde{\tilde{G}}(\alpha\varepsilon, \mathbf{q}) = \frac{C_0(\varepsilon)\,|I_3(\varepsilon, \mathbf{q})|^2}{\alpha[\varepsilon-\varepsilon(\mathbf{q})]^2}\left[\frac{I_4(\varepsilon, 0)}{-4g}\right]$$

$$\times \int_0^\infty \frac{e^{-t}[-4gt/I_4(\varepsilon, 0)]^{K_0+1}}{1+[4gt/I_4(\varepsilon, 0)]}\,dt. \qquad (20)$$

An estimate of the real part of the integral (20) shows that it is best to break up the initial series (9) for $G(\varepsilon,\mathbf{q})$ into two components with K_0 in the initial section of the asymptotic series, i.e., at $1 \ll K_0 \ll \tilde{\tilde{K}} = S(\varepsilon)$. $\mathrm{Re}\tilde{\tilde{G}}(\varepsilon,\mathbf{q})$ is then smaller than the last, largest term of $\tilde{G}(\varepsilon,\mathbf{q})$ [see Eq. (12)]. The integral (20), which converges and is real at $g>0$, has after analytic continuation on the complex plane g with a cut along the $g<0$ axis, on the upper edge of the cut, an imaginary part

$$\mathrm{Im}\, G(\alpha\varepsilon, \mathbf{q}) = -\frac{\Gamma(\varepsilon, \mathbf{q})}{\alpha^2[\varepsilon-\varepsilon(\mathbf{q})]^2}, \qquad (21)$$

where

$$\Gamma(\varepsilon, \mathbf{q}) = \pi C_0(\varepsilon)\left[\frac{I_4(\varepsilon, 0)}{4|g|}\right]^2 |I_3(\varepsilon, \mathbf{q})|^2 \exp\{-S(\varepsilon)\}\alpha. \qquad (22)$$

In (21) the imaginary part of $G(\alpha\varepsilon,\mathbf{q})$ is calculated in the single-instanton approximation corresponding to allowance for multiple scattering of the phonons into isolated fluctuations (optimal and close to optimal). The quantity $\Gamma(\varepsilon,q)$ contains an exponentially small factor $\exp\{-S(\varepsilon)\}$, proportional to the small density of the fluctuations capable of localizing the vibration.

The frequency distribution function $\rho(\alpha\varepsilon)$ in the very same single-instanton approximation is determined by the contribution of the vibrations localized on the isolated fluctuations, and is obtained by substituting $\mathrm{Im}G(\alpha\varepsilon,\mathbf{q})$ from (21) in (10). Just like $\Gamma(\varepsilon,q)$, the quantity $\rho(\alpha\varepsilon)$ is proportional to $\exp\{-S(\varepsilon)\}$. Owing to the weak dependence of S on ε as $\varepsilon \to 0$, the quantity $\rho(\alpha\varepsilon)$ is proportional to $\exp\{-S(\varepsilon)\}$. Owing to the weak dependence of S on ε as $\varepsilon \to 0$, the quantity $\rho(\alpha\varepsilon)$ contains in this limit a frequency-independent exponentially small factor $\exp\{-S(0)\}$ that reflects suppression of the localization in the $5D$ system compared with the $3D$ case.

The expression obtained in the single-instanton approximation for $G(\alpha\varepsilon,q)$, is subject to many-instanton corrections corresponding to phonon scattering by two, three, and more fluctuations, and due to contributions made to the integral (6) can generally speaking be represented, with allowance for such corrections, in the form of a series in powers of the powers of the concentration of the fluctuations capable of localize the phonons (see, e.g., Refs. 17 and 18);

$$G(\alpha\varepsilon, \mathbf{q}) = G_0(\alpha\varepsilon, \mathbf{q}) + G_1(\alpha\varepsilon, \mathbf{q}) + G_2(\alpha\varepsilon, \mathbf{q}) + G_3(\alpha\varepsilon, \mathbf{q}) + \dots, \qquad (23)$$

where

$$G_0(\alpha\varepsilon, \mathbf{q}) = \tilde{G}(\alpha\varepsilon, \mathbf{q}) + \mathrm{Re}\,\tilde{\tilde{G}}(\alpha\varepsilon, \mathbf{q})$$

does not contain the exponential factor $\exp\{-S(\varepsilon)\}$, $G_1(\alpha\varepsilon, \mathbf{q}) = i\,\mathrm{Im}\,\tilde{\tilde{G}}(\alpha\varepsilon, \mathbf{q}) \propto \exp\{-S(\varepsilon)\}$, $G_2(\alpha\varepsilon, \mathbf{q}) \propto \exp\{-2S(\varepsilon)\}, \dots$

The exponential factors in $G_n(\alpha\varepsilon,\mathbf{q})$ ($n = 2,3,\dots$) ensure exponential suppression of these contributions relative to $G_1(\alpha\varepsilon,\mathbf{q})$ in terms of the parameter

$$\frac{\exp\{-2S(\varepsilon)\}}{\exp\{-S(\varepsilon)\}} = \exp\{-S(\varepsilon)\} \ll 1. \qquad (24)$$

Since $S(0)$ is finite, the parameter (24) is small at arbitrarily distance from the edge of the continuous spectrum.

To make clear the physical meaning of $\Gamma(\varepsilon,\mathbf{q})$, let us compare the expression that follows from (11), (12), and (13) for the Green's function $G(\alpha\varepsilon,\mathbf{q})$ with the general expression for the phonon Green's function

$$G(\alpha\varepsilon, \mathbf{q}) = [\alpha[\varepsilon-\varepsilon(\mathbf{q})] - \Sigma(\varepsilon, \mathbf{q})]^{-1}, \qquad (25)$$

where $\Sigma(\varepsilon,\mathbf{q})$ is the phonon self-energy part due to phonon scattering by the fluctuations of the solid-solution composition. The quantity $\Sigma(\varepsilon,\mathbf{q})$ can be expressed as a series in powers of the density of the fluctuations that are capable of localizing the phonons, i.e., in powers of $\exp\{-S(\varepsilon)\}$:

$$\Sigma(\varepsilon, \mathbf{q}) = \Sigma_0(\varepsilon, \mathbf{q}) + \Sigma_1(\varepsilon, \mathbf{q}) + \Sigma_2(\varepsilon, \mathbf{q}) + \dots, \qquad (26)$$

where $\Sigma_0(\varepsilon,\mathbf{q})$ does not contain as a factor $\exp\{-S(\varepsilon)\}$, $\Sigma_1(\varepsilon,\mathbf{q}) \propto \exp\{-S(\varepsilon)\}$, $\Sigma_2(\varepsilon,\mathbf{q}) \propto \exp\{-2S(\varepsilon)\}$, etc. All the contributions to $\Sigma(\varepsilon,\mathbf{q})$, starting with $\Sigma_2(\varepsilon,\mathbf{q})$, are small compared with $\Sigma_1(\varepsilon,\mathbf{q})$ relative to the parameter (24). Retaining then only Σ_0 and Σ_1 in (26), substituting the sum $\Sigma = \Sigma_0 + \Sigma_1$ in (25), and expanding the Green's function in powers of Σ_1, we get

$$G(\alpha\varepsilon, \mathbf{q}) = \frac{1}{\alpha[\varepsilon-\varepsilon(\mathbf{q})] - \Sigma_0(\varepsilon, \mathbf{q})} + \frac{\Sigma_1(\varepsilon, \mathbf{q})}{\{\alpha[\varepsilon-\varepsilon(\mathbf{q})] - \Sigma_0(\varepsilon, \mathbf{q})\}^2} + \frac{\{\Sigma_1(\varepsilon, \mathbf{q})\}^2}{\{\alpha[\varepsilon-\varepsilon(\mathbf{q})] - \Sigma_0(\varepsilon, \mathbf{q})\}^3} + \dots \qquad (27)$$

The third and all succeeding terms in the expansion (27) can be neglected to the extent that the parameter (24) is small. In the second term, which contains the small factor $\Sigma_1(\varepsilon,\mathbf{q}) \propto \exp\{-S(\varepsilon)\}$, the denominator can be expanded in powers of $\Sigma_0 \propto g$ and (27) can be represented in the form

$$G(\alpha\varepsilon, q) = \frac{1}{\alpha[\varepsilon-\varepsilon(\mathbf{q})] - \Sigma_0(\varepsilon, \mathbf{q})} + \frac{\Sigma_1(\varepsilon, \mathbf{q})}{\alpha^2[\varepsilon-\varepsilon(\mathbf{q})]^2}\left\{1 + \frac{2\Sigma_0(\varepsilon, \mathbf{q})}{\alpha[\varepsilon-\varepsilon(\mathbf{q})]} + \dots\right\}. \qquad (28)$$

Since only the principal contributions with respect to g were taken into account in the calculation of the coefficients of the asymptotic series (13) and its asymptotic summation, it is necessary to neglect in the curly brackets of (28) to the same approximation all the terms but the first.

On the tail of the frequency distribution function $\rho(\alpha\varepsilon)$, i.e., at $\varepsilon<0$, the quantity $\Sigma_0(\varepsilon,\mathbf{q})$ in (28), just as $G(\alpha\varepsilon,\mathbf{q})$ in (12), is pure real, and only the second term of (28) contributes to the value of $\mathrm{Im}G(\alpha\varepsilon,\mathbf{q})$:

$$\mathrm{Im}\, G(\alpha\varepsilon, \mathbf{q}) = \mathrm{Im}\,\Sigma_1(\varepsilon, \mathbf{q})/\alpha^2[\varepsilon-\varepsilon(\mathbf{q})]^2. \qquad (29)$$

Comparing this expression with (21), we see that

$$\Gamma(\varepsilon, \mathbf{q}) = -\operatorname{Im} \Sigma_1(\varepsilon, \mathbf{q}). \tag{30}$$

Relation (30) means that the quantity $\Gamma(\varepsilon,\mathbf{q})$ in (22) is the phonon damping due to their scattering by the exponentially rare fluctuations capable of localized vibrations (i.e., by optimal or near-optimal fluctuations).

3. LONGITUDINAL OPTICAL PHONONS OF CONTINUOUS SPECTRUM

To find the Green's function of the phonons of the continuous spectrum of a solid solution, it is simplest to consider the phonon self-energy part $\Sigma_0(\varepsilon,\mathbf{q})$ due to phonon scattering by all possible composition fluctuations and representable in the form of a series in powers of the coupling constant g:

$$\Sigma_0(\varepsilon, \mathbf{q}) = \Sigma(-g)^K \Sigma_0^{(K)}(\varepsilon, \mathbf{q}). \tag{31}$$

Each term in (31) can be represented by a diagram. The imaginary part, which describes the phonon damping, of each diagram contains, in at least one section, the integral

$$2|g| \operatorname{Im} \int [\varepsilon - \varepsilon(\mathbf{q})]^{-1} (2\pi)^{-3} d^3\mathbf{q} = 2|g| \rho_0(\alpha\varepsilon)$$

[here $\rho_0(\alpha\varepsilon)$ is the frequency distribution function in an ideal crystal], and the integrals in all the remaining cross sections remain finite. Since the function $\rho_0(\alpha\varepsilon)$ in an ideal crystal has for the phonon branch with the spectrum (1) a quasi-$5D$ form and is proportional to $(\alpha\varepsilon)^{3/2}$ (Ref. 2), the phonon reciprocal lifetime calculated by perturbation theory is equal to $\gamma(\varepsilon) = |g|\alpha\varepsilon^{3/2}/6\pi$ and satisfies, in contrast to the $3D$ case, the weak-damping condition

$$\gamma(\varepsilon) \ll \alpha\varepsilon \tag{32}$$

for all ε arbitrarily close to zero, and tends to zero as $\varepsilon \to 0$.

Finite damping of the phonons near the edge of the continuous spectrum can be obtained by taking into account additionally the multiple scattering of the phonons by composition fluctuations capable of producing quasilocal vibrations in the continuous spectrum. Such multiple scattering can be considered by analogy with multiple scattering of phonons by fluctuations capable of producing local vibrations of the frequency distribution-function tail. To obtain the phonon Green's function $G(\alpha\varepsilon,\mathbf{q})$ for the continuous-spectrum frequencies, we continue analytically the instanton solution (15) of the equation $\delta S/\delta\Psi_i(\mathbf{r}) = 0$ with $\varepsilon < 0$ to the complex ε plane with a cut along the semi-axis $\varepsilon > 0$. As noted in Sec. 1, at short distances from the optimal fluctuation, the solution $\Phi(\varepsilon,\mathbf{r})$ of Eq. (16) is independent of ε as $\varepsilon \to -0$. All that depends on ε is the asymptote $\Phi(\varepsilon,\mathbf{r})$ at large distances. For the solution continued into the region $\varepsilon > 0$ of the solution, such an asymptote is equal to

$$\Phi(\varepsilon, \mathbf{r}) = \int \frac{I_3(\varepsilon, \mathbf{q}) \exp[i\mathbf{q}(r_0\mathbf{r})] r_0^3}{\varepsilon + i0 - (r_0 q)^2 - (q_x^2 + q_y^2) q^{-2}} \frac{d^3\mathbf{q}}{(2\pi)^3}$$
$$= -\frac{\varepsilon I_3(\varepsilon, 0)}{4\pi|z|} \exp\left[i\left(\varepsilon^{1/2}|z| - \frac{\varepsilon^{3/2}\rho^2}{2|z|}\right)\right]. \tag{33}$$

The normalization integral $\int |\Phi(\varepsilon,\mathbf{r})|^2 d^3\mathbf{r}$ for the function $\Phi(\varepsilon,\mathbf{r})$ (33) diverges, as it should for the amplitude of a quasilocal vibration.

However, the action integral

$$S(\varepsilon) = (4|g|)^{-1} \int \Phi^4(\varepsilon, \mathbf{r}) d^3\mathbf{r}$$

converges at short distances of the order of the size of the optimal fluctuation. Therefore at $\varepsilon > 0$, i.e., in the continuous spectrum, the action $S(\varepsilon)$, remains first finite:

$$S(\varepsilon) < \infty, \tag{34}$$

and second, large in value:

$$S(\varepsilon) \gg 1. \tag{35}$$

As $\varepsilon \to 0$ the action S is practically independent of S: $S(\varepsilon) \approx S(0)$.

It follows from (34) that for $\varepsilon > 0$ there exists a single-instanton contribution of form (21) to the phonon Green's function; in this contribution the phonon damping $\Gamma(\varepsilon,\mathbf{q})$ is described by an equation of type (22). It is shown in the Appendix that the pre-exponential factors $I_3(\varepsilon,\mathbf{q})$ and $C_0(\varepsilon)$ in (2) are practically independent of ε as $\varepsilon \to +0$. Consequently, phonon damping $\Phi(\varepsilon,\mathbf{q})$ is also independent of ε in the limit as $\varepsilon \to +0$:

$$\Gamma(\varepsilon, \mathbf{q}) \approx \Gamma(0, \mathbf{q}). \tag{36}$$

According to (30), $-i\Gamma(\varepsilon,\mathbf{q}) = i \operatorname{Im} \Sigma_1(\varepsilon,\mathbf{q})$ is the one-instanton contribution to the phonon self-energy part. It follows from (35) that the many-instanton corrections to $\Gamma(\varepsilon,\mathbf{q}) = -\operatorname{Im}\Sigma(\varepsilon,\mathbf{q})$ are small in terms of the parameter (24).

The frequency distribution function $\rho(\alpha\varepsilon)$ is obtained by substituting $\Gamma(\omega,\mathbf{q})$ from (36) in (21) and then in (10). Just as in the tail, $\rho(\alpha\varepsilon)$ is proportional to the parameter $\exp\{-S(\varepsilon)\}$ and remains finite as $\varepsilon \to 0$. The quantity $\rho(\alpha\varepsilon)$ calculated in this manner has the meaning of the distribution function of the frequencies of quasilocal vibrations coupled on isolated composition fluctuations, both optimal and close to optimal.

4. DIFFERENTIAL REGION OF LONGITUDINAL-OPTICAL-PHONON SPECTRUM

In a narrow frequency region near the edge of the continuous spectrum, when $\alpha\varepsilon \lesssim \Gamma(0,0)$, the weak-damping condition (32) is violated. The phonon damping become strong, and the phonon mean free path is of the same order as its wavelength. In this sense the behavior of the phonons can be called diffusive, and this spectrum region called diffusive. The $5D$ scattering by phonon fluctuations having frequencies in the diffusion region, however, differs in principle from the $3D$ case.

In the $3D$ case we have $S(\omega) = [-C_3(\omega^2 - \omega_0^2)/\Omega_0]^{1/2}$ (Ref. 19), therefore at $-(\omega^2 - \omega_0^2) \lesssim \Omega_0$ the one-instanton parameter $\exp\{-S(\omega)\}$ is no longer small and all many-instanton contributions to $\Sigma(\omega^2,\mathbf{q})$ describing interference effects in phonon scattering become substantial. The analogous parameter of the perturbation-theory series on moving from the direction of the continuous spectrum, which takes into account phonon scattering by all possible composition fluctuations in the $3D$ case, is equal to $[\Omega_0/(\omega^2 - \omega_0^2)]^{1/2}$ (Ref. 20) and becomes large at $|\omega^2 - \omega_0^2| \lesssim \Omega_0$, likewise reflecting the substantial role of interference effect. Therefore the diffusion part $|\omega^2 - \omega_0^2| \lesssim \Omega_0$ turns out in the $3D$ case to be inaccessible to an analytical description.[1,20]

The main feature of $5D$ systems is that the parameter $\exp\{-S(\varepsilon)\}$ remains small as $\varepsilon \to 0$ both from the side of the tail [see (19)], and on the side of the continuous spectrum [see (35)], thus ensuring smallness of the many-instanton contributions to $\Sigma(\varepsilon,\mathbf{q})$ for all ε that tend to zero. As shown in Sec. 3, the perturbation-theory-series parameter for $\Sigma_0(\varepsilon,\mathbf{q})$ also turns out to be small in the $3D$ case for all ε [see (32)] in the entire frequency region near the edge of the spectrum, including also the diffusion region. Therefore it suffices to retain in expression (26) for $\Sigma(\varepsilon,\mathbf{q})$ only $i\,\mathrm{Im}\Sigma_1(\varepsilon,\mathbf{q}) = -i\Gamma(\varepsilon,\mathbf{q})$ and one can neglect both the multi-instanton contributions $\Sigma_n(\varepsilon,\mathbf{q}) \propto \exp\{-nS(\varepsilon)\}$ $(n=2,3,...)$, and the contributions $\Sigma_0(\varepsilon,\mathbf{q}) \propto g\alpha\varepsilon$ and $\mathrm{Re}\Sigma_1(\varepsilon,\mathbf{q}) \sim \alpha\varepsilon\exp\{-S(\varepsilon)\}$, which vanish as $\varepsilon\to 0$. The final expression for the exact Green's function of the phonons $G(\alpha\varepsilon,\mathbf{q})$ is obtained by making the substitution $\Sigma(\varepsilon,\mathbf{q}) = -i\Gamma(\varepsilon,\mathbf{q})$ in (25).

Suppression of the multi-instanton contributions in $\Sigma(\varepsilon,\mathbf{q})$ relative to the parameter (24) means suppression of the interference of phonon scattering by various fluctuations at all frequencies, including also the diffusion regions, something that does not occur in the $3D$ case. The question of the localization threshold of the vibrational states is not considered in the present paper.

To obtain the frequency distribution function $\rho(\alpha\varepsilon)$ in a wide frequency range including the tail, the diffusion region, and the continuous spectrum we obtain $\mathrm{Im}G(\alpha\varepsilon,\mathbf{q})$ from (25) and substitute in (10). Using expression (2) for $\Gamma(\varepsilon,\mathbf{q})$ and taking into account the relation

$$\int |I_3(0,\mathbf{q})|^2\varepsilon^{-2}(\mathbf{q})(2\pi)^{-3}r_0^3\,d^3\mathbf{q}=I_2(0,0),$$

which is obtained by the Fourier transform (16), we get for $\rho(\alpha\varepsilon)$

$$\rho(\alpha\varepsilon)=\frac{\alpha^{1/2}}{(\beta a^2)^{3/2}}C(0)\left[\frac{I_4(0,0)}{4|g|}\right]^2 I_2(0,0)\exp\left\{-\frac{I_4(\varepsilon,0)}{4|g|}\right\}$$
$$+\frac{1}{12\pi^2(\beta a^2)^{3/2}\alpha}\left\{\left(\frac{[(\alpha\varepsilon)^2+\Gamma^2(0,0)]^{1/2}+\alpha\varepsilon}{2}\right)^{1/2}\alpha\varepsilon\right.$$
$$\left.-\left(\frac{[(\alpha\varepsilon)^2+\Gamma^2(0,0)]^{1/2}-\alpha\varepsilon}{2}\right)^{1/2}\Gamma(0,0)\right\}. \qquad (37)$$

In the diffusion region of the spectrum, at $|\alpha\varepsilon|\sim\Gamma(0,0)$, the second term in (37) is of the order of $\Gamma^{3/2}(0,0)\propto\exp\{-\frac{3}{2}S(0)\}$, and is small compared with the first term of order $\exp\{-S(0)\}$.

In the continuous spectrum at $\alpha\varepsilon\gg\Gamma(0,0)$ the second term in (37) yields for the distribution function of the frequencies of the freely propagating phonons of an ideal crystal

$$\rho(\alpha\varepsilon)=(12\pi^2)^{-1}(\beta a^2)^{-3/2}\alpha^{1/2}\varepsilon^{3/2}.$$

In this case the total distribution function is a sum of contributions of quasilocal and free vibrational states: $\rho(\alpha\varepsilon)=\rho_{\mathrm{qu}}(0)+\rho_{\mathrm{fr}}(\alpha\varepsilon)$. The contribution of the free states to $\rho(\alpha\varepsilon)$ becomes predominant in the continuous spectrum at, $\varepsilon\gtrsim|g|-{}^{4/3}\exp\{-\frac{4}{3}S(0)\}$, i.e., far beyond the limits of the diffusion region.

On the tail at $\varepsilon<0$, $|\alpha\varepsilon|\gg\Gamma(0,0)$, the second term in (37) is equal to $-(12\pi^2)^{-1}(\beta^2)^{-3/2}\cdot\frac{3}{2}\Gamma(0,0)\alpha^{1/2}|\varepsilon|^{1/2}$, and $\rho(\alpha\varepsilon)$ takes the form

$$\rho(\alpha\varepsilon)=\frac{\alpha^{1/2}}{(\beta a^2)^{3/2}}C(0)\left[\frac{I_4(0,0)}{4|g|}\right]^2$$
$$\times\exp\left\{-\frac{I_4(\varepsilon,0)}{4|g|}\right\}\left[I_2(0,0)-\frac{|\varepsilon|^{1/2}}{8\pi}\right]. \qquad (38)$$

For $|\varepsilon|\lesssim g^2$ the main dependence of $\rho(\alpha\varepsilon)$ on ε is determined by the correction $\sim|\varepsilon|^{1/2}$, while at larger values of $|\varepsilon|$ the principal role is assumed by the exponential decrease of $\rho(\alpha\varepsilon)$ due to the exponential decrease of the probability of optimal fluctuation, which follows, according the Ref. 3, the law

$$\exp\left\{-\frac{1}{4|g|}I_4(\varepsilon,0)\right\}$$
$$=\exp\left\{-\frac{1}{4|g|}[I_4(0,0)+I_2(0,0)\,|\varepsilon|]\right\}.$$

Green's function and the frequency distribution function of the prolonged optical phonons near the frequency $\omega_{LO}^{\parallel}$. The quantity $\mathrm{Im}\{-\varepsilon_{zz}^{-1}(\omega)\}$ observed in the optical experiments, the maxima of which correspond to the frequencies of the longitudinal phonons, and also the cross section for Raman scattering of light, are proportional to the spectral density of the phonons $\mathscr{A}(\omega^2,\mathbf{q}) = -\pi^{-1}\,\mathrm{Im}G(\omega^2,\mathbf{q})$, (Refs. 21, 22). From the expression for $\mathrm{Im}\,G(\alpha\varepsilon,\mathbf{q})$ it follows that the optical phonon line near $\omega_{LO}^{\parallel}$ has a Lorentz form, and its width Γ_{opt} is equal to $(2\tilde{\bar{\omega}}_{LO}^{\parallel})^{-1}\Gamma(0,0)$. Substituting g from (8) in (22) we obtain in explicit form the dependence of the width of the optical phonon line Γ_{opt} on the parameters of the phonon spectrum and on the composition of the solid solution x:

$$\Gamma_{\mathrm{opt}}(x)$$
$$=\mathrm{const}\cdot\frac{\alpha}{2\tilde{\bar{\omega}}_{LO}^{\parallel}}\frac{\alpha\beta^3}{x^2(1-x)^2V_0^4}\exp\left\{-\frac{I_4(0,0)\alpha^{1/2}\beta^{3/2}}{2x(1-x)V_0^2}\right\}.$$
$$(39)$$

At $x=0.5$ the line width Γ_{opt} has an exponentially sharp maximum, substantially sharper than in a hard $3D$ solution, where $\Gamma_{\mathrm{opt}}(x)=\Gamma_{\mathrm{opt}}^{(0)}x^2(1-x^2)$ (Ref. 23). The experimental data on the optical spectra of the solid solutions $Pb(MoO_4)_{1-x}(WO_4)_x$, which have the Scheelite structure, confirm qualitatively the conclusion that the dependence of Γ_{opt} on x has an exponentially sharp maximum.[24]

5. GREEN'S FUNCTION AND FREQUENCY DISTRIBUTION FUNCTION OF TRANSVERSE OPTICAL PHONONS

The dispersion law of the transverse optical phonons in uniaxial crystals near the edge $\omega_{TO}^{\parallel}$ of the spectrum is[8-10]

$$\omega^2(\mathbf{q})=\omega_{TO}^{\parallel 2}+\beta(qa)^2+\alpha\cos^2\vartheta, \qquad (40)$$

and the frequency distribution function $\rho(\omega^2)$, equal to[2]

$$\rho(\omega^2)=[32\pi\alpha^{1/2}(\beta a^2)^{3/2}]^{-1}(\omega^2-\omega_{TO}^{\parallel 2})\,\theta(\omega^2-\omega_{TO}^{\parallel 2}), \qquad (41)$$

has a quasi-$4D$-dependence on $\varepsilon=(\omega^2-\omega_{TO}^{\parallel 2})/\alpha$ (here

$\theta(y)$ is the Heaviside step function). The main difference between quasi-4D systems and the 5D case considered above is that the perturbation-theory series for the phonon self-energy part $\Sigma_0(\varepsilon,\mathbf{q})$ describing phonon scattering by all possible solid-solution composition fluctuations is now alongside the parameter $g\ln(\alpha/-\varepsilon)$ (Refs. 25, 26), which becomes larger as $\varepsilon\to 0$. Summation of series of this type in the parquet approximation, which yields a sum with logarithmic accuracy, was carried out by Larkin and Khmel'nitskiĭ[11] for the problem of a second-order phase transitions in uniaxial ferroelectrics.

For phonons in a solid solution, besides scattering, described by perturbation theory, for all possible composition fluctuations, there is also another scattering mechanism—multiple scattering by composition fluctuations, capable of producing local and quasilocal vibrations. This mechanism corresponds to the instanton contribution to $\Sigma(\varepsilon,\mathbf{q})$. The single-instanton approximation parameter (24) turns out in the 4D system, just as in the 5D case, to be small for arbitrary $\varepsilon\to 0$. This makes it possible to take into account, in a wide frequency range that includes the tail, the diffusion region, and the continuous spectrum, both scattering mechanisms: the perturbation-theory series sum calculated with logarithmic accuracy in Ref. 11 for $\Sigma(\varepsilon,\mathbf{q})$, and the single-instanton contribution $\Sigma_1(\varepsilon,\mathbf{q}) = -i\Gamma(\varepsilon,\mathbf{q})$. The obtained phonon Green's function is

$$G(\alpha\varepsilon,\mathbf{q})=\left\{[\alpha\varepsilon+i\Gamma(\varepsilon,0)]\left[1-\frac{|g|}{8\pi}\ln\frac{\alpha}{-\alpha\varepsilon-i\Gamma(\varepsilon,0)}\right]^{-1/4}-i\Gamma(\varepsilon,0)+i\Gamma(\varepsilon,\mathbf{q})-\alpha\varepsilon(\mathbf{q})\right\}^{-1}. \quad (42)$$

Substituting $\mathrm{Im}G(\alpha\varepsilon,\mathbf{q})$ of (42) in (10) we obtain, with the same logarithmic accuracy the frequency distribution function

$$\rho(\alpha\varepsilon)=\left\{1-\frac{|g|}{8\pi}\ln\frac{\alpha}{[(\alpha\varepsilon)^2+\Gamma^2(\varepsilon,0)]^{1/2}}\right\}^{1/4}[32\pi\alpha^{1/2}(\beta a^2)^{3/2}]^{-1}\times\left\{\Gamma(\varepsilon,0)\ln\frac{\alpha}{[(\alpha\varepsilon)^2+\Gamma^2(\varepsilon,0)]^{1/2}}+\alpha\varepsilon\,\mathrm{arctg}\frac{-\alpha\varepsilon}{\Gamma(\varepsilon,0)}\right\}. \quad (43)$$

In the diffusion region of the spectrum, at $|\alpha\varepsilon|\sim\Gamma(0,0)$, the second term in the last curly brackets in (43) is of the order of $\Gamma(0,0)$ and is small compared with the first term, which is $\sim\Gamma(0,0)/|g|$.

In the continuous spectrum, however, at $\alpha\varepsilon\gg\Gamma(0,0)/|g|$, i.e., far beyond the limits of the diffusion region, it is precisely the second term which becomes principal, and expression (43) for $\rho(\alpha\varepsilon)$ goes over into expression (41) for $\rho(\alpha\varepsilon)$ of the ideal crystal. On the tail, at $\varepsilon<0$, we have $|\alpha\varepsilon|\gg\Gamma(0,0)$, and the expression (43) for $\rho(\alpha\varepsilon)$ goes over into

$$\rho(\alpha\varepsilon)=\frac{1}{32\pi\alpha^{1/2}(\beta a^2)^{3/2}}\Gamma(\varepsilon,0)\ln\frac{1}{|\varepsilon|}. \quad (44)$$

Substituting in $\Gamma(\varepsilon,0)\propto\exp\{-S(\varepsilon)\}$ the $S(\varepsilon)$ dependence, which takes according to Ref. 3 the form

$$S(\varepsilon)=\frac{1}{4|g|}\left\{I_4(0,0)+\frac{1}{4\pi}I_3^2(0,0)\,|\varepsilon|\ln\frac{1}{|\varepsilon|}\right\},$$

we can verify that at $|\varepsilon|\lesssim|g|(\ln|g|^{-1})^{-2}$ the main frequency dependence of $S(\varepsilon)$ is due to the pre-exponential factor $\ln|\varepsilon|^{-1}$, and still farther from the edge of the continuous spectrum, at $|\varepsilon|\gtrsim|g|(\ln|g|^{-1})^{-2}$, to the exponential decrease of the probability of the optimal fluctuation in proportion to $\exp\{-S(\varepsilon)\}$.

From (42) it follows for the phonon Green's function that the characteristic width of the optical phonon line is equal to $(2\omega_{TO}^{\parallel})^{-1}\Gamma(0,0)$. The dependence of the width on the composition of the solid solution, just as in the 5D case, has an exponential sharp maximum at $x=0.5$.

We have considered above phonons that are close in frequency either to the edge $\omega_{LO}^{\parallel}$ of the continuous spectrum or to the edge $\omega_{TO}^{\parallel}$ of the continuous spectrum. These phonons propagate respectively at angles $\vartheta=0$ and $\pi/2$ to the optical axis and correspond to the edges of the directional-dispersion region. For phonons propagating at angles $\vartheta\neq 0$ and $\pi/2$ to the optical axis, however, the frequencies lie inside the directional dispersion region, i.e., inside the continuous spectrum, where the frequency distribution function is not small. The damping of such phonons, due to scattering by composition fluctuations, can be calculated by perturbation theory. The result is:

$$\Gamma_{opt}=\frac{1}{2\omega(\vartheta)}x(1-x)V_0^2\rho(\omega^2(\vartheta))=\Gamma_{opt}(\vartheta). \quad (45)$$

The damping (45) determines also the width of the corresponding optical phonon line. For a branch with directional frequency dispersion, i.e., with a dependence of ω on ϑ, the width Γ_{opt} (45) also depends on ϑ, i.e., also has directional dispersion.

Investigation of various dependence of the widths of optical phonon lines on the composition x and on the angle make it possible in principle to distinguish all the listed line-broadening mechanisms.

Note that the results pertain not only to polar optical phonons, but also to other dipole-active excitations in low-symmetry crystals (excitons, plasmons).

CONCLUSION

The results of the present paper can be represented by a table that permits a comparison, in various regions of the energy spectrum, of the properties of 3D crystals and of low-symmetry (uniaxial and biaxial) crystals with effective dimensionality 4D and 5D.

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APPENDIX

In the calculation of the functional integral (14), the integration with respect to g and $\Psi_i(\mathbf{r})$ produces in the vicinity of the saddle point a pre-exponential factor $C_0(\varepsilon)$ equal to

$$C_0(\varepsilon)=\frac{4\cdot 3^{3/4}}{\pi^2 I_4^{5/2}(\varepsilon,0)}[\mathscr{L}_x(\varepsilon)\mathscr{L}_y(\varepsilon)\mathscr{L}_z(\varepsilon)]^{1/2}\left[\frac{\bar{D}(\varepsilon,1/3)}{\bar{D}(\varepsilon,1)}\right]^{1/2}, \quad (A1)$$

where

$$\mathscr{L}_x(\varepsilon)=\int\left(\frac{\partial\Phi(\varepsilon,\mathbf{r})}{\partial x}\right)^2\Phi^2(\varepsilon,\mathbf{r})\,d^3\mathbf{r}, \quad (A2)$$

TABLE I. Comparison of the properties of cubic $3D$ crystals and low-symmetry crystals with effective dimensionality $4D$ and $5D$.

Parameters and properties	Dimensionality		
	3D	4D	5D
Born-approximation parameter	$\left(\frac{\Omega_0}{\omega^2-\omega_0^2}\right)^{1/2}$	$g \ln \frac{\alpha}{-(\omega^2-\omega_{TO}^{\parallel 2})}$	g
Small at	$\lvert\omega^2-\omega_0^2\rvert \gg \Omega_0$	$\left\lvert\frac{\omega^2-\omega_{TO}^{\parallel 2}}{\alpha}\right\rvert \gg \exp\left(-\frac{\text{const}}{g}\right)$	arbitrary ω
One-instanton approximation	$\exp\left\{-\left(-C_3\frac{\omega^2-\omega_0^2}{\Omega_0}\right)^{1/2}\right\}$	$\exp\{-S(\omega_{TO}^{\parallel})\}=\exp\{-S(\varepsilon=0)\}$	$\exp\{-S(\omega_{LO}^{\parallel})\}=\exp\{-S(\varepsilon=0)\}$
Small at	$\lvert\omega^2-\omega_0^2\rvert \gg \Omega_0$ $\omega<\omega_0$	arbitrary ω	arbitrary ω
Scattering of phonons from continuous spectrum	Born	Born + multiple	Multiple
Scattering of phonons from diffusion region	multiple + interference	multiple + interference	Multiple
Analytic expressions for $G(\omega^2,\mathbf{q})$ and $\rho(\omega^2)$	none	with logarithmic accuracy	exact

The expressions for $\mathscr{L}_y(\varepsilon)$ and $\mathscr{L}_z(\varepsilon)$ are similar.

The quantities $\bar{D}(\varepsilon,1/3)$ and $\bar{D}(\varepsilon,1)$ in (A1) are equal to

$$\bar{D}(\varepsilon,1/3)=\lim_{z\to 1/3}\frac{D(\varepsilon,z)}{(1-3z)^3},\quad \bar{D}(\varepsilon,1)=\lim_{z\to 1}\frac{D(\varepsilon,z)}{1-z}. \tag{A3}$$

Here $D(\varepsilon,z)$ is the infinite product

$$D(\varepsilon,z)=\prod_{n=1}^{\infty}\left(1-\frac{z}{\lambda_n(\varepsilon)}\right)\exp\left(\frac{z}{\lambda_n(\varepsilon)}\right), \tag{A4}$$

where $\lambda_n(\varepsilon)$ are eigenvalues determined from the equation

$$[\hat{T}-\varepsilon-3\lambda_n\Phi^2(\varepsilon,\mathbf{r})]\chi_n(\varepsilon,\mathbf{r})=0. \tag{A5}$$

Since the integral in (A2), just as the integrals $I_n(\varepsilon,\mathbf{q})$ of (17), converge at short distances on the order of the size of the optimal fluctuation, where $\Phi(\varepsilon,\mathbf{r})$ is practically independent of ε as $\varepsilon\to 0$, the quantities $\mathscr{L}_x(\varepsilon)$, $\mathscr{L}_y(\varepsilon)$, $\mathscr{L}_z(\varepsilon)$ are practically independent of ε as $\varepsilon\to 0$.

The frequency dependence of the eigenvalue $\lambda_n(\varepsilon)$ of (A5) as $\varepsilon\to 0$ can be determined by expanding in a series in ε:

$$\lambda_n(\varepsilon)=\lambda_n(0)+\delta\lambda_n(\varepsilon)=\lambda_n(0)-\int\{\varepsilon+3\lambda_n(0)[\Phi^2(\varepsilon,\mathbf{r})-\Phi^2(0,\mathbf{r})]\}\chi_n^2(0,\mathbf{r})d^3\mathbf{r}\Big/\int 3\Phi^2(0,\mathbf{r})\chi_n^2(0,\mathbf{r})d^3\mathbf{r}. \tag{A6}$$

The correction $\delta\lambda_n(\varepsilon)$ for $\lambda_n(0)$ in (A6) is proportional to ε. With increase of n, the function $\chi_n(9,\mathbf{r})$ becomes more and more oscillating; the integrals in (A6) are determined by the smoothed values of $\overline{\chi_n^2}(0,\mathbf{r})$ and are independent of n as $n\to\infty$.

Substituting $\delta\lambda_n(\varepsilon)$ of (A6) in (A4) we obtain the correction $\delta D(\varepsilon,z)\equiv D(\varepsilon,z)-D(0,z)$ to $D(0,z)$ for small ε:

$$\delta D(\varepsilon,z)=\left\{\sum_{n=1}^{\infty}\frac{z^2\delta\lambda_n(\varepsilon)}{\lambda_n^2(0)[\lambda_n(0)-z]}\right\}D(0,z). \tag{A7}$$

The contribution of large n to the sum (A7) can be represented in integral form

$$\sum_n\ldots=\int n(\lambda)\ldots d\lambda,$$

and the contribution of large n to the infinite product (A4) in the form

$$\prod_n\ldots=\exp\left\{\sum_n\ln\ldots\right\}=\exp\left\{\int n(\lambda)\ldots d\lambda\right\}$$

[here $n(\lambda)$ is the density of the eigenvalues λ_n]. Since the phonon spectrum (1) goes over into a quadratic $3D$ spectrum at large quasimomenta, and the operator $\hat{T}$ of (16) and (A5) becomes a $3D$ Laplace operator, the eigenvalue density $n(\lambda)$ turns out to be as $\lambda\to\infty$ as in the $3D$ case (see Ref. 9): $n(\lambda)\sim\lambda^{1/2}$. Therefore both integrals with respect to λ converge as $\lambda\to\infty$. Consequently, both the infinite product $D(0,z)$ of (A4) itself and the correction to it, described by (A7), turn out to be finite. It follows from (A7) that the correction $\delta D(\varepsilon,z)\sim\varepsilon$ as $\varepsilon\to 0$.

We have proved thus that the pre-exponential numerical factor C_0 that enters into expression (22) for phonon damping and in expression (37) for the frequency distribution $\rho(\alpha\varepsilon)$ tend to a constant as $\varepsilon\to\infty$.

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