Anharmonicity, weak localization, and the decay rate of phonons in the long-wave limit

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Specific interference effects taking place in the weak-localization regime cause considerable renormalization of the group velocity and decay rate of phonons in an anharmonic lattice. The renormalization of the quasiparticle lifetime is especially marked. This effect may be stronger than Rayleigh scattering and conventional lattice anharmonicity mechanism. © *1996 American Institute of Physics.* [S1063-7761(96)01902-1]

1. INTRODUCTION

Currently the issue of weak localization of phonons, as well as of acoustic and optical waves, in disordered system is being discussed extensively.[1–5] Note that phonon systems with the diagonal disorder have been investigated in detail in the coherent-potential approximation relatively recently.[6] Akkermans and Maynard[7] focused their attention on specific localization effects which may take place in anharmonic systems.

The aim of our study was to investigate how phonon-density fluctuations (second sound) in the weak-localization regime affects the anharmonic interaction among phonons. Specifically, our purpose was to determine the effect of quantum interference corrections on the basic parameters of the phonon spectrum, namely the group velocity and decay rate in the long-wave limit. For simplicity we consider only the processes due to the cubic anharmonicity, since the fourth-order anharmonicity in the limit $\mathbf{k}\to 0$ has little effect on the phonon spectrum.[8]

Investigations of phonon localization are often applied to the qualitative analysis of the dynamic properties of amorphous systems. We use our results to interpret the anomaly in the temperature dependence of the reciprocal ultrasound attenuation length Γ, which is commonly observed in the temperature interval where the thermal conductivity is a flat function of temperature.

Our theory can be applied to other objects, including, first, doped quantum crystals, in which the anharmonicity is strong. These include, for example, solid solutions of neon and argon in parahydrogen at an impurity concentration of $\sim 0.1\%$. Anomalies in their thermal conductivity have been observed quite recently.[9] Second, there are single crystals of a very high purity, but composed of different isotopes (for example, the natural mixture of germanium isotopes).

2. GENERAL EQUATIONS FOR THE MASS OPERATOR

Consider a crystal with isolated impurity atoms. We shall describe its dynamic properties by the Hamiltonian

$$H=H_0+H_{\rm im}+H_{\rm int}=H'+H_{\rm int},$$

where

$$H_0=\frac{1}{2M_0}\sum_{\mathbf{n},\alpha}(p_{\mathbf{n}}^{\alpha})^2+\frac{1}{2}\sum_{\substack{\mathbf{n},\mathbf{n}'\\ \alpha\beta}}\Phi_{\mathbf{nn}'}^{(0)\alpha\beta}u_{\mathbf{n}}^{\alpha}u_{\mathbf{n}'}^{\beta},$$

$$H_{\rm im}=\frac{1}{2}\left(\frac{1}{M}-\frac{1}{M_0}\right)\sum_{\mathbf{n},\alpha}c_{\mathbf{n}}(p_{\mathbf{n}}^{\alpha})^2+\frac{1}{2}\sum_{\substack{\mathbf{n},\mathbf{n}'\\ \alpha\beta}}\Delta\Phi_{\mathbf{nn}'}^{\alpha\beta}u_{\mathbf{n}}^{\alpha}u_{\mathbf{n}'}^{\beta}, \tag{1}$$

$$H_{\rm int}=\frac{1}{3!}\sum_{\substack{\mathbf{nn}'\mathbf{n}''\\ \alpha\beta\gamma}}\Phi_{\mathbf{nn}'\mathbf{n}''}^{\alpha\beta\gamma}u_{\mathbf{n}}^{\alpha}u_{\mathbf{n}'}^{\beta}u_{\mathbf{n}''}^{\gamma},$$

$$\Delta\Phi_{\mathbf{nn}'}^{\alpha\beta}=\Phi_{\mathbf{nn}'}^{\alpha\beta}-\Phi_{\mathbf{nn}'}^{(0)\alpha\beta}.$$

Here H_0 denotes the hamiltonian of the pure harmonic lattice, $H_{\rm im}$ is the perturbation due to impurities, and H' denotes the hamiltonian of the harmonic doped lattice. The term $H_{\rm int}$ describes the dynamic anharmonic interaction of ions. As usual, the parameters $u_{\mathbf{n}}^{\alpha}$ and $p_{\mathbf{n}}^{\alpha}$ are Cartesian components of the displacement and momentum of an atom at the site $\mathbf{n}$, M and M_0 are the masses of the impurity and host atom, respectively (we assume that the impurity is heavier, i.e., $M\gg M_0$), $\Phi_{nn'}$ and $\Phi_{nn'n''}$ are elements of dynamic matrices of second and third order. In what follows the label "0" denotes parameters of the host lattice. The factor $c_{\mathbf{n}}$ equals zero if a host atom is at the site $\mathbf{n}$ and unity if there is an impurity at the site. The configurational average $\langle c_{\mathbf{n}}\rangle_c$ equals the impurity concentration c.

For simplicity we assume that the dynamic matrices are diagonal with respect to Cartesian indices. For brevity, the combination of the site ($\mathbf{n}$) and Cartesian (α) indices is denoted by n.

In our calculations described in Sec. 3 we presume that the disorder is diagonal, i.e., the impurities are considered as isotopic defects, and the dynamic matrices $\Phi_{nn'n''}$ and $\Phi_{nn'n''}^{(0)}$ are identical. Thus, only the anharmonicity of the host lattice is taken into account, and it is fairly weak. Our results can be generalized for the case of nondiagonal disorder, when $\Delta\Phi_{nn'}=0$ (see the discussion at the end of this section).

Let us introduce a one-particle retarded Green's function G^{+} constructed from the atomic displacement operators u_n. We have

$$G_{nn'}^{+}(t-t')=-i\theta(t-t')\langle[u_n(t),u_{n'}(t')]\rangle.$$

One can prove that the Green's function averaged over impurity configurations is approximately determined by an equation of the form[8]

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$$\langle G^+_{nn'}(\omega)\rangle_c \approx \bar{G}^+_{nn'}(\omega) + \sum_{\substack{n_1n_2n_3\\ n_4n_5n_6}} \bar{G}^+_{nn_1}(\omega)\Phi_{n_1n_2n_3}\Phi_{n_4n_5n_6} \times \int d\omega_1 \langle K_{n_2n_4}(\omega_1) G^+_{n_3n_5}(\omega - \omega_1)\rangle_c \bar{G}^+_{n_6n'}(\omega). \quad (2)$$

In Eq. (2) the symbol $\langle \ldots \rangle_c$ denotes the configurational average, and $\bar{G}^+$ is the one-particle function corresponding to the total harmonic Hamiltonian averaged over impurity configurations. We also define

$$K_{n_1n_2}(\omega) = \frac{1}{i}\frac{1}{1-\exp(-\beta\omega)}[G^+_{n_1n_2}(\omega) - G^-_{n_1n_2}(\omega)], \quad (2')$$

where G^- is the advanced Green's function, and $\beta = 1/T$.

Note that $\langle K\bar{G}^+\rangle \sim \langle \bar{G}^+\bar{G}^-\rangle_c$ is the two-particle Green's function. We also emphasize that the second term on the right of Eq. (2) is a product of the components of the anharmonic dynamic matrix and the one-particle and two-particle Green's functions. This product, in particular, determines the anharmonic coupling between single-phonon excitations and fluctuations of the phonon density near defects.

Note that the spatial Fourier component of the one-particle Green's function $\bar{G}$ in the momentum representation can be expressed as

$$\bar{G}^+_{\mathbf{k}}(\omega) = \frac{Q(\omega)}{\omega^2 - \tilde{\omega}^2_{\mathbf{k}} - i\omega/\tau'_i}, \quad (3)$$

where $\tilde{\omega}_{\mathbf{k}}$ is the quasiparticle dispersion law and τ'_i is their lifetime.

The parameters $\tilde{\omega}_{\mathbf{k}}$ and τ'_i, and the factor Q can be expressed in terms of the real and imaginary parts of the impurity mass operator responsible for elastic scattering, $P_i(\omega)$ and ω/τ_i, respectively (see for details Ref. 10):

$$\tau'_i = Q^{-1}\tau_i, \quad Q(\omega) = \left[1 - \frac{\partial P_i(\omega)}{\partial\omega^2}\right]^{-1}.$$

As for the two-particle Green's function G_2 in Eq. (2), we determine it neglecting the anharmonic interatomic interaction. Then in the momentum representation in the general case G_2 satisfies a Bethe–Salpeter equation of the form

$$G_2(\mathbf{k},\mathbf{k}',\omega) = \lim_{\Omega\to 0}\langle \bar{G}^+_{\mathbf{k},\mathbf{k}'}(\omega)\bar{G}^-_{\mathbf{k},\mathbf{k}'}(\omega-\Omega)\rangle_c = \lim_{\Omega\to 0}\langle \bar{G}^+_{\mathbf{k}}(\omega)\bar{G}^-_{\mathbf{k}}(\omega-\Omega)(\delta_{\mathbf{k}\mathbf{k}'} + \sum_{\mathbf{k}_1} U(\mathbf{k},\mathbf{k}_1;\omega,\Omega)G_2(\mathbf{k}_1,\mathbf{k}',\omega,\Omega))\rangle_c. \quad (4)$$

In the limit of small $\mathbf{q} = \mathbf{k} + \mathbf{k}'$ and $\omega \to 0$, the vertex part U is determined by "fan" diagrams.[2,11,12] In the case of a lattice with point defects, the summation of such diagrams for a generalized vertex yields an expression of the form[13]

$$U(\mathbf{k},\mathbf{k}';\omega,\Omega) = \frac{L}{N}\left[1 - \frac{L}{N}\sum_{\mathbf{k}_1}\bar{G}^+_{\mathbf{k}_1}(\omega)\bar{G}^-_{\mathbf{k}_1-\mathbf{q}}(\omega-\Omega)\right]^{-1}.$$

If the initial vertex V_i is defined neglecting the probability of multiple occupation of one lattice site (i.e., when two or more impurities are generated at one site in the formal model), then

$$L = V_i = \frac{\omega}{\pi\tau_i(\omega)g(\omega^2)}, \quad g(\omega^2) = Q\tilde{g}(\omega^2).$$

Here

$$\tilde{g}(\omega^2) = N^{-1}\sum_{\mathbf{k}}\delta(\omega^2 - \tilde{\omega}^2_{\mathbf{k}})$$

is the density of quasi-particles with a momentum $\mathbf{k}$ and energy $\tilde{\omega}_{\mathbf{k}}$. If the effect of multiple occupation is taken into account,

$$L = V_i(1 + V_i\bar{G}^+_{nn}\bar{G}^-_{nn})^{-1}.$$

Now we give an expression for the vertex U under the conditions

$$ql(\omega) \ll 1, \quad \Omega\tau_i \ll 1. \quad (5)$$

Here $l(\omega) = v(\omega)\tau_i(\omega)$ is the quasiparticle free path due to elastic scattering and v is the group velocity of the quasiparticles. The corresponding expression for U has the standard form:[13]

$$U(q;\omega,\Omega) \approx \frac{\omega}{\pi\tau_i^2}\frac{Q(\omega)}{g(\omega^2)}\frac{1}{D_0q^2 - i\Omega}, \quad (6)$$

where $D_0 = v^2\tau_i/3$ is the diffusion coefficient.

Using the expressions for G_2, i.e., Eqs. (4) and (6), we can prove that the spatial Fourier component of the one-particle Green's function G^+ in Eq. (2) in the momentum representation is described by the following chain of equations:

$$G^+_{\mathbf{k}}(\omega) \approx \bar{G}^+_{\mathbf{k}}(\omega) + [\bar{G}^+_{\mathbf{k}}(\omega)]^2\Sigma_A(\mathbf{k},\omega), \quad \Sigma_A = \Sigma^{(a)}_A + \Sigma^{(b)}_A.$$

The individual terms in the equation for the anharmonic mass operator Σ_A are defined as

$$\Sigma^{(a)}_A(\mathbf{k},\omega) = \int_0^\infty d\omega_1 \sum_{\mathbf{q}_1\mathbf{q}_2}\Phi^2_{-\mathbf{q}\mathbf{q}_1,\mathbf{q}_2}K_{\mathbf{q}_1}(\omega_1)\bar{G}^+_{\mathbf{q}_2}(\omega-\omega_1), \quad (7)$$

$$\Sigma^{(b)}_A(\mathbf{k},\omega) = i\int_0^\infty d\omega_1 \frac{1}{1-\exp(-\beta\omega_1)} \times \sum_{\mathbf{q}\mathbf{q}_1}\Phi_{\mathbf{k},\mathbf{q}_1,-(\mathbf{q}_1+\mathbf{k})}\bar{G}^-_{\mathbf{q}_1+\mathbf{k}}(\omega_1)\bar{G}^-_{\mathbf{q}_1+\mathbf{q}}(\omega_1) \times U(q,\omega_1,\omega)\bar{G}^+_{\mathbf{q}_1}(\omega-\omega_1)G^+_{\mathbf{q}_1+\mathbf{q}+\mathbf{k}} \times (\omega-\omega_1)\Phi_{\mathbf{k}+\mathbf{q}_1+\mathbf{q},-\mathbf{q}_1-\mathbf{q},-\mathbf{k}}, \quad (8)$$

where $\Phi_{\mathbf{k}\mathbf{k}_1\mathbf{k}_2}$ and $K_{\mathbf{q}}$ are the spatial Fourier components of $\Phi_{nn'n''}$ and the K-correlator in Eq. (2′).

Equation (7) is standard, whereas Eq. (8), which contains the diffusion vertex U, describes the specific anharmonic interaction between virtual phonons and fluctuations

of the phonon density in a disordered system. Below we shall discuss only processes involving two-phonon coherent states. In other terms, we take into account only the "coherent backscattering." It is well known that they control the weak localization. We shall also prove that such processes may lead to a considerable renormalization of the basic phonon parameters in the acoustic limit at $\mathbf{k}\to 0$.

If only the coherent backscattering is taken into account, we have instead of Eq. (8) the following equation for the nonstandard part of the anharmonic operator:

$$\Sigma_A^{(b)}(\mathbf{k},\omega)=i\int_{-\infty}^{\infty}d\omega_1\frac{1}{1-\exp(-\beta\omega_1)}\times\sum_{\mathbf{q}\leqslant\mathbf{q}_c}\sum_{\mathbf{q}_1}\Phi_{\mathbf{k},-\mathbf{q}_1,-(\mathbf{k}-\mathbf{q}_1)}\tilde{G}^-_{\mathbf{q}_1+\mathbf{k}}(\omega_1)\tilde{G}^-_{\mathbf{q}_1}(\omega_1)\times U(q,\omega,\omega_1)\tilde{G}^+_{\mathbf{q}_1}(\omega-\omega_1)\tilde{G}^+_{\mathbf{k}+\mathbf{q}_1}\times(\omega-\omega_1)\Phi_{\mathbf{k}+\mathbf{q}_1,-\mathbf{q}_1,-\mathbf{k}}. \quad (8')$$

Here the summation over $\mathbf{q}$ is limited to the small parameter $q_c=\pi/l(\omega)$, where $l(\omega)$ is the phonon free path due to elastic scattering.

In order to proceed with our derivation, we must explicitly express the anharmonic vertex $\Phi_{\mathbf{k}\mathbf{k}_1\mathbf{k}_2}$. We present it in the conventional form, i.e.,

$$\Phi_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3}=-i\tilde{\gamma}_3\omega_{\mathbf{k}_1}\omega_{\mathbf{k}_2}\omega_{\mathbf{k}_3},\quad \tilde{\gamma}_3=\gamma_3/\gamma_2^{3/2}, \quad (9)$$

where γ_2 and γ_3 are the effective harmonic and anharmonic dynamic constants. The following relationships among these dynamic parameters hold approximately:

$$\frac{\gamma_4\omega_D}{\gamma_2^2}\approx\frac{\gamma_3^2\omega_D}{\gamma_2^3}\approx 10\frac{\langle u^2\rangle}{a^2}=10\delta_A,$$

where $\langle u^2\rangle$ is the averaged square of the atomic displacements, ω_D is the Debye frequency, a is the typical interatomic separation, and δ_A is the anharmonicity parameter. This parameter may range between 10^{-2} and 10^{-1}, but cannot be 10^{-3} (Ref. 14).

Now let us discuss the standard expression (7) for the mass operator. It is important that the quasi-momentum is conserved at its vertices. In the limit $\mathbf{k}\to 0$ we have[10,15]

$$\mathrm{Re}\,\Sigma_A^{(a)}(\omega_k)\approx-\tilde{\gamma}_3^2\omega_k^2\sum_{\mathbf{q}_1}\left(n_{q_1}+\frac{1}{2}\right)=\omega_k^2\Delta_1^{(a)}(T), \quad (10)$$

$$\mathrm{Im}\,\Sigma_A^{(a)}(\omega_k)\approx\tilde{\gamma}_3^2(\omega_k/\omega_D)^6 f(T), \quad (10')$$

where $n_q=[\exp(\beta\omega_q)-1]^{-1}$ and $f(T)$ is a function of temperature which is finite at $T=0$.

Thus, the velocity of sound is renormalized by the cubic anharmonicity, and it becomes a function of temperature. As for the effect of the anharmonicity on the sound damping, it is, generally speaking, negligible in comparison to the Rayleigh scattering from impurities.

Consider the nonstandard expression for the mass operator in Eq. (8′). Note that the diffusion vertex part in it describes the specific interference between phonons with quasimomenta $\mathbf{k}+\mathbf{q}_1$ and $\mathbf{q}_1$. Given these interference processes, limitations on the value of the vector $\mathbf{q}$ can be ignored.

In the limiting case of interest to us defined by Eq. (5) the real component $\Sigma_A^{(b)}$, taking into account Eq. (9), is presented in the form

$$\mathrm{Re}\,\Sigma_A^{(b)}\approx\mathrm{Re}\left[\tilde{\gamma}_3^2\omega_k^2\int_{-\infty}^{+\infty}d\omega_1\frac{1}{1-\exp(-\beta\omega_1)}\times F(\omega_1)\sum_{\mathbf{q}\leqslant\mathbf{q}_c}U(q,\omega_1,\omega)\right]$$

$$\approx\tilde{\gamma}_3^2\omega_k^2\int_0^{\infty}d\omega_1\bar{n}(\omega_1)\omega_1^2 v^2(\omega_1)\tau_{i'}(\omega_1)\times\left[1-\frac{P_i(\omega_1)}{\omega_1^2}\right]\sum_{\mathbf{q}\leqslant\mathbf{q}_c}\frac{\omega}{[D_0(\omega)q^2]^2+\omega^2},$$

$$\bar{n}(\omega)=\frac{1}{e^{\beta\omega}-1}+\frac{1}{2}.$$

One can easily show that

$$\sum_{\mathbf{q}\leqslant\mathbf{q}_c}\frac{\omega}{[D_0(\omega)q^2]^2+\omega^2}\approx\pi\frac{\sqrt{\omega}}{\sqrt{D_0^3(\omega)}}.$$

As a result we have

$$\mathrm{Re}\,\Sigma_A^{(b)}\approx-\tilde{\gamma}_3^2\omega_k^2\sqrt{\omega}\int_0^{\infty}d\omega_1\bar{n}(\omega_1)\omega_1^2\frac{1-P_i(\omega_1^2)/\omega_1^2}{v(\omega_1)\sqrt{\tau(\omega_1)}}=\omega_k^2\Delta_1^{(b)}(\omega,T). \quad (11)$$

The imaginary part $\Sigma_A^{(b)}$ in the same approximation for $\omega,\mathbf{k}\to 0$ is determined by the equation

$$\mathrm{Im}\Sigma_A^{(b)}(\omega_k)\approx i\tilde{\gamma}_3^2\omega_k^2\int_{-\infty}^{+\infty}d\omega_1 F(\omega_1)\sum_{\mathbf{q}\leqslant\mathbf{q}_c}U(q,\omega_1,0),$$

where

$$F(\omega_1)=\sum_{\mathbf{q}_1}[\omega_{q_1}\tilde{G}^-_{\mathbf{q}_1}(\omega_1)\tilde{G}^+_{q_1}(\omega_1^2)]^2.$$

From this it follows that, first,

$$F(\omega_1)=\int d\omega_{q_2}^2\tilde{g}(\tilde{\omega}_{q_2})\omega_{q_2}^4\times\frac{Q^4(\omega_1)}{(\omega_1^2-\tilde{\omega}_{q_2}^2-i\omega_1/\tau_{i'})^2(\omega_1^2-\tilde{\omega}_{q_2}^2+i\omega_1/\tau_{i'})^2}\approx\pi\omega_1\tilde{g}(\omega_1^2)Q^4(\omega_1)\tau_{i'}^3(\omega_1)\left[1-\frac{P_i^2(\omega_1^2)}{\omega_1^2}\right]^2,$$

and second,

$$\sum_{\mathbf{q}\leqslant\mathbf{q}_c}\frac{1}{D_0(\omega)q^2}\approx\frac{3}{2\pi^2}\frac{1}{l(\omega)v^2(\omega)\tau_{i'}(\omega)}.$$

With due account of the latter two approximate equations, we finally have

$$\mathrm{Im}\Sigma_A^{(b)}(\omega_k)\approx\gamma_3^2\omega_k^2\int_0^{\infty}d\omega_1\bar{n}(\omega_1)\omega_1^2\frac{1-P_i(\omega_1^2)/\omega_1^2}{v(\omega_1)\tau_{i'}(\omega_1)}=\omega_k^2\Delta_2^{(b)}(T). \quad (11')$$

Note that the parameters $\Delta_1^{(a)}$, $\Delta_1^{(b)}$, and $\Delta_2^{(b)}$ are defined by Eqs. (10), (11), and (11′). It is essential for our further analysis that $\Delta_1^{(a)}$ and $\Delta_1^{(b)}$ are independent of frequency, and $\Delta_2^{(b)} \propto \sqrt{\omega}$.

Now we shall discuss the derived expressions for the mass operator Σ_A of the quasiparticles. Comparing the frequency dependence in Eqs. (10), (10′), and (11), (11′), we can see immediately that in the long-wave limit the interference effects in the phonon scattering from impurities due to the anharmonicity may lead to a considerable renormalization of Σ_A. Its imaginary component can vary more rapidly. The decay of phonons due to the nonstandard anharmonic processes may be faster than those due the Rayleigh and standard anharmonic scattering. The real component of Σ_A should also change considerably. In order of magnitude

$$\mathrm{Re}\,\Sigma_A^{(b)}/\mathrm{Re}\,\Sigma_A^{(a)} \sim \sqrt{c\omega_{\mathbf{k}}}/\omega_D .$$

Note that in our calculation we assumed that all the defect were isotopic, i.e., the interatomic interaction parameters are equal for the host and impurity atoms: $\gamma_2 = \gamma_2^{(0)}$. A question arises whether our results can be generalized to the case in which host and impurity atoms have different interaction parameters. Our answer is positive. First, the one-particle Green's function in the basic equations of the theory presents no difficulty and is described by Eq. (3) with different parameters. Second, the vertex part of the two-particle Green's function equation should be modified. It turns out that for $\gamma_2 \neq \gamma_2^{(0)}$ the structure of the equation for the vertex V is the same. Naturally, the parameters g, τ_i, and Q in the equation for the Green's function and the vertex part, which are functions of $M - M_0$ and $\gamma_2 - \gamma_2^{(0)}$ (see for details Ref. 13), should be redefined. Taking this into account, we can analyze the more general case.

Let us summarize our discussion. We have considered the processes in which the anharmonic interaction couples acoustic phonons to fluctuations of the phonon density around a defect in the weak-localization regime. We have found that if the conditions (5) are satisfied, specific interference processes may lead to a considerable renormalization of the phonon mass operator.

3. PARAMETERS OF THE PHONON SPECTRUM AND ACOUSTIC ATTENUATION FACTOR IN THE ULTRASOUND LIMIT

Let us start with a harmonic lattice. First we consider the dispersion equation, which defines the effective frequency $\tilde{\omega}_k$ and the damping of acoustic modes. It is written as follows:

$$\tilde{\omega}_k^2 - \omega_k^2 - P_i(\tilde{\omega}_k^2) - i\frac{2\tilde{\omega}_k}{\tau_{i'}(\omega_k)} = 0.$$

Assume that

$$\tilde{\omega}_k(k \to 0) = vk^*, \quad k^* = k + i\Delta k.$$

Given that for $\omega \to 0$ we have

$$Q^{-1} = 1 - \frac{\partial P_i(\omega)}{\partial \omega^2} \approx 1 - \frac{P_i(\omega^2)}{\omega^2},$$

we can prove that

$$v(\omega) = v_0\left[1 - \frac{P_i(\omega^2)}{\omega^2}\right]^{-1/2}, \quad \Delta k = \lim_{\omega \to 0} \frac{1}{v(\omega)\tau_{i'}(\omega)}. \tag{12}$$

Here v_0 is the phonon group velocity in the host lattice, $\tau_{i'} = d/\omega^4$ is the phonon lifetime due to the Rayleigh scattering (d is independent of frequency).

It is known that the sound damping factor is defined as

$$\Gamma = \mathrm{Im}|\mathbf{k}^*|,$$

where $\mathbf{k}$ is the complex wave vector of a mode propagating across a crystal.[16] Note that, according to Eq. (12), the factor $\Gamma = \Delta k$ is proportional to ω^4 and does not depend on temperature.

Now let us consider an anharmonic crystal. The corresponding dispersion equation is

$$\tilde{\omega}_k^2 - \omega_k^2 - P_i(\tilde{\omega}_k^2) - i\frac{2\tilde{\omega}}{\tau_{i'}(\tilde{\omega}_k)} - \omega_k^2 \times[\Delta_1^{(a)}(T) + \Delta_1^{(b)}(T) + \Delta_2^{(b)}(T)] = 0.$$

Using our equations derived above, we can easily prove that in the long-wave limit the sound velocity and phonon decay rate are determined by the approximate equations

$$\bar{v}(\omega) \approx v_0\sqrt{\frac{1 + \Delta_1^{(a)}(T) + \Delta_1^{(b)}(T)}{1 - P_i(\omega^2)/\omega^2}}, \tag{13}$$

$$\frac{1}{\tau(\omega)} = \frac{\omega^4}{d} + \frac{\omega\Delta_2^{(b)}(T)}{\sqrt{1 + \Delta_1^{(a)}(T) + \Delta_1^{(b)}(T)}}. \tag{13′}$$

From this it follows that in an anharmonic crystal specific interference effects lead to substantial renormalizations of the parameters v and $1/\tau$. Since the parameter $\Delta_2^{(b)}$ is constant with the frequency, the quasiparticle decay rate may be controlled by the interference effects, which are stronger than both the Rayleigh and standard anharmonic scattering.

In the ultrasound limit, we can derive an equation for the reciprocal attenuation length Γ of ultrasound using our previous equations and neglecting the Rayleigh term $\tau_{i'}^{-1}$:

$$\Gamma = \lim_{\omega \to 0} \frac{\omega\sqrt{1 - P_i(\omega^2)/\omega^2}}{\sqrt{1 + \Delta_1^{(a)}(T) + \Delta_1^{(b)}(T)}}\Delta_2^{(b)}(T). \tag{14}$$

It follows from Eq. (14) that in an anharmonic lattice with impurities the factor Γ is proportional to the frequency ω and is a function of temperature. The phonon decay rate is determined by specific anharmonic effects, including fluctuations of the phonon density around defects (recall that the temperature in this case is quite low, $T \approx 10\ \mathrm{K} \ll \Theta_D$). These specific processes control both the frequency and the temperature dependence of the reciprocal ultrasound attenuation length. Note that in our model the velocity of sound is determined by standard anharmonic processes.

Below we consider a specific example—a lattice with low-frequency resonant scatterers.

4. A MODEL OF A NONIDEAL LATTICE WITH LOW-FREQUENCY ANTICROSSING SPLITTING OF ACOUSTIC SPECTRUM

Let us determine the density of states g, group velocity v, and the lifetime τ of quasi-particles in a harmonic lattice when the acoustic spectrum has an anticrossing with a low-frequency quasi-local resonance. These parameters characterize the phonon-spectrum renormalization due to anharmonicity.

Let us consider a simple cubic lattice with a scalar interaction between neighboring atoms. According to the statement of the problem , heavier impurity atoms are placed at some of its sites. We assume that the dynamic parameters of the interaction between impurity atom and host atoms may differ from the dynamic parameters of the host lattice, namely

$$\varepsilon=\left|1-\frac{M}{M_0}\right|\geqslant 1, \quad f=1-\frac{\gamma_2}{\gamma_2^{(0)}}.$$

The impurity concentration is relatively low, i.e., $c\ll 1$. We only take into account pair dynamic interaction between the impurities.

It is known that the scattering t-matrix has a resonant singularity around the frequency $\omega_R\ll\omega_D$. If variations in the local dynamic parameters are included, then[13,17]

$$\frac{\omega_R^2}{\omega_D^2}\approx\frac{1}{-3\varepsilon+2f(1-\varepsilon)/(1-f)}=\frac{\rho}{-\varepsilon}, \quad \rho=\frac{1-f}{3-f}. \tag{15}$$

On the other hand,

$$\tau_{i'}^{-1}=\frac{c\rho^2x^2}{(x-x_R)^2+c\rho x_R}\left[1+\frac{c\rho}{2(x_R-x)}\right], \tag{16}$$

$$v(x)=\frac{1-P_i(x)/x}{1-\partial P_i/\partial x}v_0(x)$$

$$=\frac{(x_R-x)^2}{(x_R-x)^2+c\rho x_R}\sqrt{1+\frac{c\rho}{x_R-x}}v_0(x),$$

$$\tilde{g}(x)=\frac{2x}{\pi}\sqrt{1+\frac{c\rho}{x_R-x}}. \tag{17}$$

For brevity, we have introduced the dimensionless parameters

$$x=\frac{\omega^2}{\omega_D^2}, \quad x_k=\frac{\omega_k^2}{\omega_D^2}, \quad x_R=\frac{\omega_R^2}{\omega_D^2}.$$

Now let us determine the reciprocal ultrasound attenuation length in this model. To this end, we express the factors $\Delta_{1,2}^{(b)}$ in Eq. (14) for Γ using the explicit expressions for $\tau_{i'}$ [Eq. (16)] and v [Eq. (17)]. The main contributions to the integrals in equations for $\Delta_{1,2}^{(b)}$ come from the frequency band corresponding to the lower branch. One can prove that

$$\Gamma\approx\omega\delta_A\sqrt{x_R}c^2\bar{n}(\omega_R). \tag{18}$$

Now we shall comment about Eq. (18). First, in the absence of cross splitting (anticrossing) and in the presence of a resonant local mode we have

$$\Gamma_*\approx\omega\delta_A x_R c\bar{n}(\omega_R). \tag{18'}$$

Since in the case of anticrossing the parameters c and x_R satisfy the condition $c\geqslant x_R^{3/2}$, the attenuation factor Γ in Eq. (18) is, generally speaking, larger than Γ_* in Eq. (18'). Second, note the temperature dependence of the reciprocal ultrasound attenuation length. At very low temperatures it is constant, and at higher temperatures it grows linearly with the temperature.

5. COMPARISON WITH EXPERIMENTAL DATA

5.1. Amorphous systems

Studies of the phonon weak localization are often applied to the qualitative analysis of dynamic properties of amorphous systems. We use our results to interpret an anomaly in the temperature dependence of the reciprocal ultrasound attenuation length Γ, which is commonly observed in amorphous systems in the temperature range where a plateau in thermal conductivity is observed.

Present-day concepts of the temperature dependence of Γ are based on the models of structural defects[18] (see also the review by Gol'danskii and Flerov[19]), soft atomic configurations,[20,21] and localized excitations like fractons.[22,23] Note that all these models are in fact phenomenological. We propose a microscopic model to interpret the temperature dependence of Γ (other possible microscopic models were discussed by Yu and Leggett[24]).

We must stress that a model of localized modes in amorphous systems with energies of 1–3 meV can be constructed using the available experimental data. First, there are regions of a higher density with a typical dimension of several tens of angstroms. It is generally accepted that they contain a lot of interstitial defects. The effective local dynamic lattice parameters in these regions are stringent. Hence the low-frequency branch of the phonon spectrum can be modelled using a lattice with interstitial defects of a large effective mass.[25,26] Second, the dynamic parameters of interaction between the host lattice and defects have some distribution. It is due to fluctuations in the field of static displacements and is, naturally, a function of the structural disorder, which depends on the growth technique and annealing regime.

We therefore assume that there are localized modes with a typical energy $\omega_R\approx 1$ meV in a lattice with defects (for simplicity we presume that the distribution function of local dynamic parameters is a Lorentzian centered at ω_R). Corresponding to this is $x_R\approx 10^{-3}$. According to experimental data (neutron-scattering measurements given in Refs. 27–29), the concentration of localized modes is $c\approx 0.5\cdot 10^{-2}$. In this situation, we must describe the material with defects using the model with an anticrossing between the phonon branch and localized modes.

In this case, according to Eq. (18),

$$\Gamma\approx 10^{-5}\delta_A\omega\bar{n}(\omega_R). \tag{19}$$

It is clear that Eq. (19) gives a qualitatively correct description of the temperature dependence of the ultrasound attenuation length in a temperature range where the thermal conductivity is approximately constant (beyond this range the thermal conductivity grows linearly with T). This result can

be compared to experimental data on the amorphous material SiO, in which the attenuation length was measured at a frequency $\omega = 2 \cdot 10^7$ Hz.[22,30] If we assume $\delta_A = 10^{-2} - 10^{-1}$, the agreement with the experiment is quite reasonable.

5.2. Quantum crystals

As was noted in Introduction, our results can be applied to low-temperature properties of quantum crystals, such as dilute solutions of neon and argon in parahydrogen. The samples have a concentration of chemical impurities of about 10^{-8} and a concentration of very heavy defects $c \approx 10^{-6}$ (1 ppm) or higher. The typical sample dimension is 6 mm. The thermal conductivity of such samples has been measured,[9] and the decay rate of phonons due to scattering from boundaries in pure crystals (without Ne and Ar impurities) was estimated to be $\tau_B^{-1} = 5 \cdot 10^5$ s^{-1}.

According to experimental data, Ne atoms behave as isotopic defects, whereas the change in the local dynamic parameters for Ar atoms is essential. In both cases, the effective frequency of the resonant mode is determined by Eq. (15). Since the concentration of defects is low, the anticrossing effects can be neglected and the standard theory can be employed. According to Eq. (18a), the decay rate of phonons due to the quantum interference can be estimated as

$$\frac{1}{\tau_{qn}} \sim c\delta_A \frac{1}{|\varepsilon|}\omega,$$

and if $\omega \leqslant \omega_R$ ($\leqslant 10^{12}$ Hz) this estimate is correct within an order of magnitude.

Only the low-frequency band is essential in integrals which determine the low-temperature thermal conductivity.[10] Although the defect concentration is very small ($c \approx 10^{-6}$–10^{-4}), the decay rates $1/\tau_B$ and $1/\tau_{qn}(\omega)$ ($\omega \approx \omega_R$) may be comparable because the anharmonism parameter δ_A is large. As a result, the contribution of specific interference processes may be finite. (We discuss the complicated behavior of the thermal conductivity in dilute solutions of neon and argon in parahydrogen in another publication[31].)

The effects of anharmonicity and weak localization may take place in chemically pure crystals composed of several isotopes. The anharmonicity is weak in this case, but, on the other hand, the effective parameter of squared atomic mass fluctuations ΔM^2 inserted in Eq. (18) instead of the concentration c is quite large; as a result, these effects may be important in such systems, for example, in ultrasound damping and low-temperature thermal conductivity.

6. CONCLUSION

First, let us compare our results to the conclusions by Akkermans and Maynard,[7] who were the first to study the anharmonic effect taking into account fluctuations of the phonon density on the spectrum of quasiparticles. They analyzed peculiarities of the quasi-particle spectrum near the localization threshold in a hypothetical situation with unspecified parameters of the theory. We have studied the case $\mathbf{k} \to 0$, i.e., far from expected localization thresholds, using a realistic microscopic model. Exact solutions can be derived in this model. We must stress that the low-frequency characteristics of phonons and parameters of the anharmonic interaction are steep functions of frequency, therefore models that yield exact solutions are necessary for our study.

In this work we have analyzed the effects of fluctuations of the phonon density on the basic characteristics of quasiparticles (group velocity v and decay rate $1/\tau$) in the long-wave limit at low temperatures ($T \ll \Theta_D$). The cubic anharmonism was taken into account in deriving the mass operator. Two-phonon coherent states taking place in the weak-localization regime were also included. We have demonstrated that in the case of cubic anharmonism the specific interference processes lead to a considerable renormalization of phonon-spectrum parameters. The effect of the fourth-order anharmonism is weaker if phonon-density fluctuations are taken into account (see for details Ref. 8). It is important when the frequency is close to the localization threshold.[32] The reciprocal length of ultrasound damping has been calculated. We have discussed a specific microscopic model—a lattice with low-frequency resonant scatterers with a typical frequency $\omega_R \approx 10$ K. Our results may be useful in a qualitative description of the reciprocal length of ultrasound damping in disordered solids and of the low-temperature thermal conductivity. Preliminary results were published in Ref. 8.

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[1] H. Bottger and M. Theuerkauf, Phys. St. Solidi (b) **150**, 73 (1988).
[2] T. R. Kirkpatrik, Phys. Rev. B **31**, 5746 (1985).
[3] J. E. Graebner, B. Golding, and L. C. Allen, Phys. Rev. B **34**, 5696 (1986).
[4] E. Wolf, G. Maret, E. Akkermans, and R. Maynard, J. Phys (Paris) **49**, 63 (1988); **49**, 77 (1988).
[5] M. P. van Albada, M. B. van der Mark, and A. Lagendik, in *Scattering and Localization of Classical Waves in Random Media*, ed. by P. Shjeng, World Scientific, Singapore (1989), p. 97.
[6] Qian-Jin Chu and Zhao-Oing Zhag, Phys. Rev. B **38**, 4906 (1988).
[7] E. Akkermans and R. Maynard, Phys. Rev. B **32**, 7860 (1985).
[8] A. P. Zhernov, Preprint IAE 5805/9 (1994).
[9] T. N. Antsygina, B. Ya. Gorodilov, N. N. Zholonko *et al.*, Fiz. Nizkikh Temp. **18**, 417 (1992) [Sov. J. Low Temp. Phys. **18**, 283 (1992)]; B. Ya. Gorodilov, A. I. Krivchikov, V. G. Manzhelii, and N. N. Zholonko, Fiz. Nizkikh Temp. **20**, 77 (1994).
[10] A. Maradudin, Solid State Phys. **18**, 275 (1966); **19**, 1 (1966).
[11] S. Langer and T. Neel, Phys. Rev. Lett. **16**, 984 (1965).
[12] D. Vollhardta and P. Wolfle, Phys. Rev. B **22**, 4666 (1994).
[13] A. P. Zhernov, E. I. Salamatov, and E. P. Chulkin, Phys. Stat. Solidi (b) **165**, 355 (1991); **168**, 81 (1991).
[14] V. G. Vaks, *Introduction to Microscopic Theory of Ferroelectrics* [in Russian], Nauka, Moscow (1973).
[15] M. A. Krivoglaz, *Theory of X-ray and Thermal Neutrons Scattering by Crystals* Plenum, New York (1969).
[16] A. A. Slutskin and G. P. Sergeeva, Zh. Éksp. Teor. Fiz. **50**, 1649 (1966) [Sov. Phys. JETP **23**, 1097 (1966)].
[17] A. P. Zhernov and G. R. Augst, Fiz. Tverd. Tela **9**, 2196 (1967).
[18] O. L. Anderson and H. E. Bommel, J. Amer. Ceram. Soc. **38**, 125 (1955).
[19] V. I. Gol'danskii and V. N. Flerov, *Tunneling Effects in Chemical Physics* [in Russian], Nauka, Moscow (1986).
[20] M. I. Klinger, Phys. Rep. **165**, 397 (1988).
[21] V. Buchenau, Yu. Al. Galperin, V. L. Gurevich, and H. R. Schober, Phys. Rev. B **43**, 5039 (1991).

[22] J. Jagannathan and R. Orbach, Phys. Rev. B **41**, 3153 (1990).
[23] S. Alexander, C. Laermans, R. Orbach, and H. M. Rosenberg, Phys. Rev. B **28**, 4615 (1983).
[24] C. C. Yu and A. J. Leggett, Comm. Cond. Mat. Phys. **14**, 231 (1988).
[25] P. H. Dederichs and P. Zeller, in *Point Defects in Metals*, Vol. 2, Springer-Verlag (1981).
[26] H. R. Schober and Brian B. Laird, Phys. Rev. Lett. **66**, 636 (1991); Phys. Rev. B **44**, 6746 (1991).
[27] G. F. Syryh, A. P. Zhernov, and N. A. Chernoplekov, Fiz. Tverd. Tela **32**, 2332 (1990) [Sov. Phys. Solid State **32**, 1254 (1990)].
[28] G. F. Syryh, A. P. Zhernov, and N. A. Chernoplekov, Zh. Éksp. Teor. Fiz. **100**, 982 (1991) [Sov. Phys. JETP **73**, 542 (1991)].
[29] J. B. Suck, H. Rubin, H. J. Guntlerodt, and H. Beck, J. Noncryst. Solids **61– 62**, 289 (1986).
[30] S. Hunklinger and W. Arnold, in *Physical Acoustics*, ed. by W. P. Mazon and R. N. Kurston (Academic Press, New York, 1976).
[31] A. P. Zhernov and E. P. Chulkin, Phys. St. Solidi (b) **193** (1996), in press.
[32] A. P. Zhernov and E. P. Chulkin, Fiz. Tverd. Tela **36**, 2302 (1994) [Sov. Phys. Solid State **36**, 1254 (1994)].

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