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SOLIDS AND LIQUIDS

COHERENT STATES IN THERMAL QUANTUM TRANSPORT

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Abstract. This paper focuses on describing energy transfer by coherent thermal excitations in dielectrics, metamaterials, and nanoscale systems. Using the second quantization technique, a general formalism of thermal conductivity is proposed, considering both the model of free phonons in heat transfer and the formation of coherent Schrödinger states of the oscillator system. A general form of the time-dependent problem solution with arbitrary initial conditions is obtained. An exact solution is analytically derived for the heat flux carried by coherent phonons created by an electronic wave packet produced by a laser pulse effecting a nanomaterial. The obtained exact form of solution in quadratures provides a basis for quantitative description of coherent phonons with various initial conditions, as well as taking into account thermal distributions, which allows for evaluation of thermal properties of nanocrystals. It is shown that under certain ratios of constants characterizing the interaction of phonons with the electronic subsystem, a time-independent heat flux can be established in the crystal.

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1. INTRODUCTION

Theoretical and experimental studies of recent years have shown that the transfer of thermal energy in dielectrics and metamaterials at nano- and microscale often has a quantummechanical nature of coherence. The quantum nature of energy transfer leads to new physical effects, such as phonon coherence, thermal superconductivity [1], thermal echo, ballistic resonance, and others.

In the classical approach to describing thermal processes, based on phenomenologically introduced relatios that define transport coefficients, thermal conductivity in solids is determined by Fourier's law. Within this hypothesis, a linear dependence of heat flows on thermodynamic parameters is usually postulated [2, 3]. In kinetic theory, it is assumed that an set of moving quasiparticles (Bose or Fermi type) [4] carries heat. The motion of quasiparticles (evolution of their distribution function) is described both by the Boltzmann transport equation in the quasi-classical case and by a more rigorous apparatus of temperature Green's functions. Free quasi-classical motion of quasiparticles corresponds to the ballistic mode of heat transfer, which is realized in harmonic crystals. The influence of nonlinearity and lattice defects, interatomic interactions on heat exchange is modeled by interactions (collisions) of quasiparticles; in particular, such effects arise in systems like planar semiconductor nanostructures during the interaction of optically excited excitons with acoustic phonons [5]. As a result of collisions, quasiparticles can perform Brownian motion or Lévy walks. The former corresponds to the classical Fourier mode of heat exchange, while the latter corresponds to anomalous heat exchange [6-8]. In [9], it is shown that the quasiparticle distribution function is a Wigner function rather than a Planck function, as for free phonons. The equation describing the evolution of the Wigner function for harmonic crystals was obtained by Milke [10], and generalization to the weakly anharmonic case was made in [11].

Coherent heat transfer, including minimal thermal conductivity and Anderson localization, has been intensively observed in various nanophononic crystals. Nanophononic crystals are artificial materials in which the wave nature of lattice vibrations is explicitly manifested in the thermal

properties of these materials [12-14]. Phonon coherence has been established as the main source of various unique thermal transport phenomena [12-14], such as coherent heat transfer and phonon confinement effect. Recent studies have found that phonon coherence has a significant impact on phonon-phonon scattering, phonon modal correlations, and interfacial phonon propagation, which differ from the picture of "pure" particles [15-17].

In paper [18], as well as in [5], the connection between Bloch oscillations and longitudinal optical phonons is investigated, for example, in a narrow-well superlattice $In_{0,53}Ga_{0,47}As/In_{0,52}Al_{0,48}As$, where a strong increase in the amplitudes of coherent phonons was observed when Bloch oscillations were subsequently tuned into resonance with various optical phonon modes [18]. Most manifestations of thermal phonon coherence in experimental studies are based on measuring thermal conductivity and its characteristic changes [13, 14]. For instance, the existence of coherent phonons is indirectly evidenced by the experimental observation of non-monotonic dependence of thermal conductivity on the superlattice period [15, 16, 17, 19, 20]. In study [14], phonon excitation coherence is investigated by calculating thermal conductivity κ based on the Green-Kubo approach as a heat flux autocorrelation function $S(t)$, assuming that the expression for specific heat capacity per mode reduces to classical C^{class}, if the correlation term (phonon number autocorrelation), accounting for the number of phonons in a given mode, simply equals $N_\lambda = T / \hbar\omega_\lambda$, where T — is temperature in the energy scale. In the case of predominant "particle-like" behavior, the correlation factor $Cor(t)$ follows an exponential decay law with lifetime $\tau^{(p)}$ (particle), in accordance with the usual single-mode relaxation time approximation

$$\mathrm{Cor}_\lambda = e^{-t/\tau^{(p)}}.$$

As the coherence effect increases in describing phonon decay, a correction is considered here that includes the modal coherence time τ_λ^c (coherent) as follows:

$$\mathrm{Cor}_\lambda = \exp\left[\frac{t}{\tau^{(p)}}\right]\exp\left[-4\ln(2)\frac{t^2}{(\tau_\lambda^c)^2}\right].$$

It was expected that coherence would have a decisive effect on phonon decay and its propagation, phonon decay should follow a generalized law, as shown in [14] for the thermal conductivity coefficient

$$\kappa \propto \frac{1}{3}\sum_{\alpha,\lambda} C_\lambda^{class}\upsilon_{\lambda\alpha}^2\tau_\lambda^c \exp\left[\frac{(\tau_\lambda^c)^2}{128(\tau_\lambda^p)^2}\right].$$

However, experimentally obtained dependencies of accumulative classical and quantum thermal conductivity for Tl_3VSe_4 at temperatures of 50 and 300 K show good agreement between molecular dynamics (MD) calculations and experiment for high temperature, when the classical limit "works," while for temperature 50 K, when the expected quadratic (Gaussian-type) decay in calculations shows significant divergence from experiment. The evaluation of this generalized thermal conductivity was implemented by introducing wavelet transformation of MD values, which provides phonon excitation coherence time as well as their lifetime.

Coherent effects in heat transfer also manifest themselves in a recently emerged direction – semiconductor optomechanics based on the use of exciton polaritons [21, 22]. Polaritons are a mixture of photons and material excitations [5]. In study [5], the interaction of optically excited excitons with acoustic waves in planar semiconductor nanostructures was theoretically investigated. This interaction leads to strong nonlinearity in sound propagation in quantum well arrays, or in planar semiconductor Bragg microresonators supporting exciton-polariton modes.

Taking into account the constant of nonlinear optomechanical interaction between optically pumped excitons and propagating acoustic waves, calculated in study [5], we will show that coherent states during thermal transport indeed form into a wave packet. In the coordinate representation, these states are nothing but an oscillator with a displaced center. These coherent states with Poisson distribution by the number of phonons in a given mode play an important role and lead to characteristic time dependencies of heat flows. At certain phonon decay times in the frequency band associated with this constant, a non-decaying heat flux (spectral flux density in the frequency band) can be formed over time. Such behavior of heat flux resembles superthermal conductivity considered in works [22-27], for which the term "thermal

superconductivity" is sometimes used in literature. Semiconductors, cubic crystals of boron arsenide (BAs), as recently discovered [22-25], possess ultrahigh thermal conductivity compared to most conventional materials and show great promise for thermal management in electronics [25-27].

2. HAMILTONIAN DESCRIBING COHERENT STATES OF PHONONS

As is known, elastic vibrations of a crystal lattice in the classical limit can be considered as a set of plane waves with wave vector k and corresponding frequency

$$\nu = c\left|\mathrm{k}\right| / 2\pi = \omega / 2\pi$$

(where ω — angular frequency) and polarizations, for example linear, λ ($\lambda = 0,1,2,$). In quantum description, assuming wave amplitude quantization $\left|n_{k\lambda}\right\rangle$ — it is a set of $n_{k\lambda}$ phonons with momenta $\mathrm{p} = \hbar\mathrm{k}$ and energies $\varepsilon_k = \hbar\omega_k$ with corresponding distribution function of phonon numbers in a given mode $\mathrm{k}\lambda$:

$$n_{\mathrm{k}\lambda} = \frac{1}{e^{\mathrm{h}\omega_k / T} - 1},$$

where T is temperature in energy scale:

$$T = k_B T^{\circ},$$

k_B — Boltzmann constant, T° — temperature in degrees. The corresponding creation and annihilation operators, $\hat{b}^{\dagger}_{k\lambda}$, $\hat{b}_{k\lambda}$, of a phonon in a given state $\left|n_{k\lambda}\right\rangle$ are defined through generalized coordinate operators $\hat{Q}_{k\lambda}$ and momenta $\hat{P}_{k\lambda}$ as

$$\hat{b}^{\dagger}_{\mathrm{k}\lambda} = \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{Q}_{\mathrm{k}\lambda} + \frac{\hat{P}_{\mathrm{k}\lambda}}{im\omega_k}\right),$$

$$\hat{b}_{\mathrm{k}\lambda} = \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{Q}_{\mathrm{k}\lambda} - \frac{\hat{P}_{\mathrm{k}\lambda}}{im\omega_k}\right),$$

where m is the mass of crystal lattice ion. The corresponding commutation relations for them, $\left[\hat{b}_{\mathrm{k'}\lambda'}, \hat{b}^{\dagger}_{\mathrm{k}\lambda}\right] = \delta_{\mathrm{k'k}}\delta_{\lambda'\lambda}$, are determined by known commutation conditions for coordinate and momentum operators (see Appendix for details). Thus, the displacement vector operator of the nth lattice ion $\hat{\xi}_n(\mathrm{r},t)$ is defined as

$$\hat{\xi}_n(\mathrm{r},t) =$$

$$= \sum_{\mathrm{k},\lambda}\sqrt{\frac{\hbar}{2m\omega_k}}\left[\hat{b}_{k\lambda}e^{-i\omega_k t}A_{\mathrm{k}\lambda}(r) + \hat{b}^{\dagger}_{k\lambda}e^{i\omega_k t}A^{*}_{\mathrm{k}\lambda}(\mathrm{r})\right]. \quad (1)$$

Here

$$A_{\mathrm{k}\lambda}(\mathrm{r}) = \frac{1}{\sqrt{N}}e_{\mathrm{k}\lambda}e^{i\mathbf{k}\cdot\mathbf{r}}$$

— a coordinate part of the harmonic (mode) amplitude $\mathrm{k}\lambda$,

$$\hat{b}_{k\lambda}(t) = \hat{b}_{k\lambda}e^{-i\omega_k t},$$

$$\hat{b}^{\dagger}_{k\lambda}(t) = \hat{b}^{\dagger}_{k\lambda}e^{i\omega_k t}.$$

The corresponding Hamiltonian describing free oscillations of the crystal lattice has the form

$$\hat{H}^0 = \sum_{i=1}^{N}\left\{\frac{m}{2}\hat{\xi}_i^2 + \frac{\gamma}{2}\left(\hat{\xi}_i - \hat{\xi}_{i-1}\right)^2\right\} =$$

$$= \sum_{\mathrm{k}\lambda}\hbar\omega_k\left(\hat{b}^{\dagger}_{\mathrm{k}\lambda}\hat{b}_{\mathrm{k}\lambda} + \frac{1}{2}\right). \quad (2)$$

Here γ — is the lattice "stiffness coefficient" which is determined by the interaction potential of neighboring ions:

$$\gamma = \frac{\partial^2}{\partial x^2}U(x).$$

In an isotropic medium, the deformation potential

$$W_d = -\gamma\mathrm{Sp}\hat{\xi}$$

determines the energy interaction operator of an atom (ion, or any defect having electronic structure) with acoustic phonons [28]:

$$\hat{W}_d \equiv \hat{V}_{eph} = -\gamma\sum_{\mathrm{k},\lambda}\left\{\sqrt{\frac{N}{2m\hbar\omega_k}}\right\}\times$$

$$\times\left(ie_{\mathrm{k}}\cdot\mathrm{k}_{i\to f}\right)\hat{c}^{\dagger}_{f\sigma'}\hat{c}_{i\sigma}\times$$

$$\times\left(b_{\mathrm{k},\lambda}(t)e^{i\mathrm{k}_{\lambda}\cdot\mathrm{r}} - b(t)^{+}_{-\mathrm{k},\lambda}e^{-i\mathrm{k}_{\lambda}\cdot\mathrm{r}}\right)\}, \quad (3)$$

Here operators $\hat{c}^{\dagger}_{f\sigma'}\hat{c}_{i\sigma}$ — are creation and annihilation operators of electrons in specified, for

example excitonic, states $\left|\eta_{i\sigma}\right\rangle, \left|\eta_{f\sigma'}\right\rangle$ are operators of fermion type. Here vector $|\eta_{i\sigma}\rangle$ denotes the initial state of an electron in excitonic state, which includes electron spin with projection σ. Phonons, whose number in a given mode $k\lambda$ is denoted as $n_{k\lambda}^{(i)}$, interact with the electron in the specified state. Then the initial state of the system "exciton + phonon" will be described as $\left|i\right\rangle = \left|n_{k\lambda}^{(i)}\eta_{i\sigma}\right\rangle$. During interaction with phonons, described by the electron-phonon interaction operator $\hat{V}_{eph}$, the atomic system, or "electronic medium", transitions to the final state f (or $\left|f\right\rangle = \left|n_{k\lambda}^{(f)}\eta_{f\sigma'}\right\rangle$). In this case, we denote the set of all quantum numbers characterizing the electronic system as $\eta_{f\sigma'}$ a coordinate part their spin state σ', and the state of the phonon system with the number of phonons in a given mode $k\lambda$ as $n_{k\lambda}^{(f)}$.

As a result of this interaction, one or more phonons in a specific polarization state and with specific momenta are emitted or absorbed by the "electronic medium." The difference in momentum and polarization of the "electronic medium," initiated by the emission or absorption of phonons, essentially determines the polarization characteristics of the emitted or absorbed phonons. This process is described by the differential transition probability, $dw_{fi}^{(a)}$ (for absorption) and $dw_{fi}^{(e)}$ (for emission). It should be emphasized that, generally speaking, the initial and final excited states of the "electronic medium" are not stationary. They are not only proportional to the corresponding time-oscillating factors,

$$\left|\eta_i\right\rangle \propto \exp(-iE_i t/\hbar), \quad \left|\eta_f\right\rangle \propto \exp(-iE_f t/\hbar),$$

but also are relaxing to their corresponding ground states with relaxation frequencies γ_i and γ_f or so-called relaxation probabilities per unit time:

$$|\eta_i\rangle \propto \exp(-iE_i t/\hbar - \gamma_i t),$$

$$|\eta_f\rangle \propto \exp(-iE_f t/\hbar - \gamma_f t),$$

which determine the spectral line width. Taking into account the relative smallness of the interaction constant between the electronic system and lattice vibrations, this interaction can be consistently described using perturbation theory methods. According to the general formulas of non-stationary perturbation theory with explicitly time-dependent perturbation, the probability $P_{fi}(t)$ of transition from the initial state $\left|i\right\rangle$ of the phonon system + "electronic medium" to the final state $\left|f\right\rangle$ under the influence of perturbation acting in the time interval $[0,t]$, can be represented as an expansion in terms of contributions accounting for single-, two-, three-phonon, etc. transitions.

For a single-phonon transition accompanied by emission (e), or absorption (a) of one phonon characterized by a set of quantum numbers $\pi_\rho \equiv \{k,\lambda,\omega_k\}$, the probability of this process is determined by the following formula:

$$\hat{V}(t') = \hat{V}^{(e)}(\pi_p)e^{i\omega_k t'} + \hat{V}^{(a)}(\pi_p)e^{-i\omega_k t'}, \quad (4)$$

where

$$\begin{aligned}\hat{V}^{(e)}(\pi_p) &= -\gamma\sqrt{\frac{\hbar}{2m\omega_k}}\hat{b}^{\dagger}_{k\lambda}(0)A^{*}_{k\lambda}(r),\\ \hat{V}^{(a)}(\pi_p) &= -\gamma\sqrt{\frac{\hbar}{2m\omega_k}}\hat{b}_{k\lambda}(0)A_{k\lambda}(r).\end{aligned} \quad (5)$$

The description of the interaction process between phonons and the electronic system with polarization due to the deformation potential is carried out taking into account both the contribution of free thermal oscillations of the crystal, see formula (2), and the electronphonon interaction itself:

$$\hat{H} = \hat{H}^0 + \hat{V}(t') = \sum_{k\lambda}\{\hbar\omega_k\left(\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda} + \frac{1}{2}\right) + \\ + \left(-\frac{i}{\hbar}\right)\left\langle\eta_f\left|(-\gamma)e\sqrt{\frac{\hbar}{2m\omega_k N}}e_{k\lambda}\cdot ik\hat{c}^{\dagger}_f\hat{c}_i\right|\eta_i\right\rangle \times \\ \times\left(\hat{b}^{\dagger}_{k\lambda}(t') + \hat{b}_{k\lambda}(t')\right)\}, \quad (6)$$

The matrix elements $\langle\eta_f \mid \hat{V}_{eph} \mid \eta_i\rangle$, calculated for the initial and final states of the electronic system, can also include effects due to interaction with exciton polarization and described in detail in [5]. Here, the elastic interaction constant γ should be replaced by the constant Ξ, which, in addition to the deformation potential constant γ, approximately equal to 10 eV, also contains the contribution of the polarization potential $\varepsilon|P|^2$, where $\varepsilon = 4\pi\Xi^2/\omega E$, P — is the exciton polarization amplitude, E — is Young's modulus. Calculation of matrix elements $\left\langle\eta_f\left|\hat{V}_{eph}\right|\eta_i\right\rangle$ leads to a Hamiltonian describing lattice vibrations taking into account the influence of the electronic system

on the phonon system, for example, considering excitonphonon interaction:

$$\hat{\mathcal{H}} = \sum_{k\lambda}\hat{\mathcal{H}}_{k\lambda} = \sum_{k\lambda}\left\{\hbar\omega_k\left(\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda} + \frac{1}{2}\right) - \Lambda_{k\lambda}\left\{\hat{b}^{\dagger}_{k\lambda} + \hat{b}_{k\lambda}\right\}\right\},$$

$$\Lambda_{k\lambda} = e\Xi e_{k\lambda k}\sqrt{\frac{1}{2m\hbar\omega_k N}}, \tag{7}$$

$$\Xi = \gamma\left(1 + \frac{4\pi\gamma^2}{\omega E}\mid P\mid^2\right).$$

In its form, the description of the phonon system using Hamiltonian (7) coincides with the description of optical fields interacting with matter (electronic system). For the latter, it is shown that the most acceptable basis is not the basis of "Fock" states with a definite number of photons in a given mode and undefined phase, but the basis of coherent states, which, unlike "Fock" states, has a variable number of particles (photons in the optical sense) but a definite phase [29]. (See Appendix for more details.)

3. COHERENT STATES OF PHONONS

Let's consider in more detail the obtained Hamiltonian (7), or rather its component corresponding to the mode $(k\lambda)$:

$$\hat{\mathcal{H}}_{k\lambda} = \hbar\omega_k\left(\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda} + \frac{1}{2}\right) - \Lambda_{k\lambda}\left\{\hat{b}^{\dagger}_{k\lambda} + \hat{b}_{k\lambda}\right\}. \tag{8}$$

For its diagonalization, we will perform a unitary transformation – one that connects the original (old) creation/annihilation operators of a particle in the oscillator state with new operators of creation and annihilation as follows:

$$\begin{aligned}\hat{b}^{\dagger}_{k\lambda} &= B^{\dagger}_{k\lambda} + u^{*}_{k\lambda},\\ \hat{b}_{k\lambda} &= B_{k\lambda} + u_{k\lambda}.\end{aligned} \tag{9}$$

where $u_{k\lambda}$ is some generally complex function. They also satisfy the bosonic commutation relation:

$$\left[B_{k'\lambda'}B^{\dagger}_{k\lambda}\right] = \delta_{k'k}\delta_{\lambda'\lambda}.$$

Substituting expression (9) into Hamiltonian (8) and performing diagonalization, we have

$$\hat{\mathcal{H}}_{k\lambda} = \hbar\omega_k\left(B^{\dagger}_{k\lambda}B_{k\lambda} + \frac{1}{2}\right) - \frac{2\left(\Lambda_{k\lambda}\right)^2}{\hbar\omega_k}. \tag{10}$$

For this, the function $u_k\lambda$ must be purely real:

$$u_{k\lambda} = \frac{\Lambda_{k\lambda}}{\hbar\omega_k}. \tag{11}$$

It is known that such a linear transformation of creation/annihilation operators (11) is carried out by a unitary transformation operator $\hat{U} = e^{\hat{D}}$ (where $\hat{D} = \hat{D}^{\dagger}$ — is a Hermitian operator):

$$B = e^{-\hat{D}}\hat{b}e^{\hat{D}} = \hat{b} + \frac{\Lambda_{k\lambda}}{\hbar\omega_k}, \tag{12}$$

where indices $(k\lambda)$ for operators $\hat{b}^{\dagger}$ and $\hat{b}$ are omitted for now. Since states with different $(k\lambda)$ are independent, orthogonal, we can, without loss of generality, omit these indices to avoid cumbersome notation. We seek the operator $\hat{D}$ in the form

$$\hat{D} = \alpha(\hat{b}^{\dagger} - \hat{b}),$$

with real function

$$\alpha = \frac{\Lambda_{k\lambda}}{\hbar\omega_k}.$$

The unitary transformation operator in general has the form

$$\hat{U}(\alpha) = e^{\left(\alpha\hat{b}^{\dagger} - \alpha\hat{b}\right)}.$$

It transforms the "old" vacuum function $\left|n_{k\lambda}\right\rangle = \left|0\right\rangle$ into the corresponding "new" vacuum:

$$\left|\nu_{k\lambda} = 0\right\rangle = \left|\alpha\right\rangle = \hat{U}(\alpha)\left|n_{k\lambda} = 0\right\rangle = e^{(\alpha^{*}\hat{b}^{\dagger} - \alpha\hat{b})}\left|n_{k\lambda} = 0\right\rangle. \tag{13}$$

Taking into account the Baker-Campbell-Hausdorff equality, we obtain

$$e^{\alpha^{*}\hat{b}^{\dagger} - \alpha\hat{b}}\left|n_{k\lambda} = 0\right\rangle = e^{-|\alpha|^2/2}e^{\alpha^{*}\hat{b}^{\dagger}}e^{-\alpha\hat{b}}\left|n_{k\lambda} = 0\right\rangle = e^{-|\alpha|^2/2}\sum_{\nu=0}^{\infty}\frac{(\alpha^{*})^{\nu}}{\sqrt{\nu!}}\left|\nu\right\rangle = \left|\alpha\right\rangle_{k\lambda}. \tag{14}$$

We also assumed that $\hat{b}\left|n = 0\right\rangle \equiv 0$. The obtained superposition of oscillator states with different

numbers of phonons in a given mode represents a coherent state, similar to Glauber photon states. The concept of coherent states was introduced by Schrödinger in 1926. They are eigenstates of the obtained Hamiltonian (13) and correspond to energy taking into account interaction with the electronic subsystem:

$$\varepsilon_{k\lambda} = \hbar\omega_k\left(\alpha_{k\lambda} + \frac{1}{2}\right) - \frac{2\left(\Lambda_{k\lambda}\right)^2}{\hbar\omega_k}. \tag{15}$$

The following expressions are valid for them (see [29] for details):

$$\begin{aligned} \hat{b}\left|\alpha\right\rangle_{k\lambda} &= \alpha_{k\lambda}\left|\alpha\right\rangle_{k\lambda}, \\ \alpha_{k\lambda} &= \frac{\Lambda_{k\lambda}}{\hbar\omega_k}, \end{aligned} \tag{16}$$

which correspond to the eigenvalue of energy (15), where the average number of phonons in the coherent state corresponding to the given mode equals

$$\begin{aligned} \left\langle n\right\rangle_{k\lambda} &= \left\langle\alpha\right|\hat{b}^\dagger\hat{b}\left|\alpha\right\rangle_{k\lambda} = \left|\alpha\right|^2_{k\lambda}, \\ \left|\alpha\right\rangle_{k\lambda} &= e^{-\langle n\rangle_{k\lambda}/2}\sum_{n=0}^{\infty}\left|n\right\rangle_{k\lambda}\frac{\sqrt{\left\langle n\right\rangle_{k\lambda}}^n}{\sqrt{n!}}, \end{aligned} \tag{17}$$

and the distribution function for the number of phonons in the given mode corresponds to the Poisson distribution (see Appendix)

$$W_{k\lambda}(n) = e^{-\langle n\rangle_{k\lambda}}\frac{\left\langle n\right\rangle^n_{k\lambda}}{n!}. \tag{18}$$

Taking into account (16), (17), and that the interaction constant itself for the given mode $\Lambda_{k\lambda}$ is still a complex function of frequency (7), the obtained coherent states have a specific character and depend on the frequency of the propagating oscillation mode. Here

$$\left\langle n\right\rangle_{k\lambda} = \left|\alpha\right|^2_{k\lambda} \propto \frac{1}{\omega_k^3}.$$

4. EXACT SOLUTION OF THE TIME-DEPENDENT PROBLEM OF PHONON INTERACTION WITH ELECTRONIC SUBSYSTEM. ENERGY FLOW

Let's consider the situation when the optomechanical interaction between optically pumped excitons and propagating acoustic waves contains an explicit time dependence due to polariton generation of excitons under laser pulse impact on the nanostructure. Then

$$\Lambda_{k\lambda}(t) = e\Xi(t)e_{k\lambda}\mathrm{k}\sqrt{\frac{1}{2m\hbar\omega_k N}}\left\langle\eta_f(t)\right|\hat{c}_f^\dagger\hat{c}_i\left|\eta_i(t)\right\rangle. \tag{19}$$

The Hamiltonian of such a system will be rewritten accordingly as

$$\hat{H}_{k\lambda}(t) = \hbar\omega_k\left(\hat{b}^\dagger_{k\lambda}\hat{b}_{k\lambda} + \frac{1}{2}\right) - \Lambda_{k\lambda}(t)\left\{\hat{b}^\dagger_{k\lambda} + \hat{b}_{k\lambda}\right\}.$$

We consider the solution for each oscillation mode independently. In this case, we need to solve the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi_{k\lambda}(t)}{\partial t} = \hat{H}_{k\lambda}(t)\Psi_{k\lambda}(t). \tag{20}$$

As in [30], we will seek the general form of the solution as

$$\begin{aligned} &\Psi_{k\lambda}(t) = \\ &= C_{k\lambda}(t)e^{\alpha_{k\lambda}(t)b^\dagger_{k\lambda}}e^{\beta_{k\lambda}(t)b_{k\lambda}}e^{\gamma_{k\lambda}(t)b^\dagger_{k\lambda}b_{k\lambda}}\Psi_{k\lambda}(-\infty), \end{aligned} \tag{21}$$

where $\Psi_{k\lambda}(-\infty)$ — is the wave vector of the system in the initial state before the electronic perturbation affects it, $\alpha(t)$, $\beta(t)$, $\gamma(t)$ — are the sought-after time functions. Substituting (21) into (20) and taking into account the following commutation relations [30]:

$$\begin{aligned} &[e^{\beta_{k\lambda}\hat{b}_{k\lambda}}, \hat{b}^\dagger_{k\lambda}] = \beta_{k\lambda}e^{\beta_{k\lambda}\hat{b}_{k\lambda}}, \Rightarrow \\ &\quad\Rightarrow e^{\beta_{k\lambda}\hat{b}_{k\lambda}}\hat{b}^\dagger_{k\lambda} = (\hat{b}^\dagger_{k\lambda} + \beta_{k\lambda})e^{\beta_{k\lambda}\hat{b}_{k\lambda}}, \\ &[e^{\alpha_{k\lambda}b^\dagger_{k\lambda}}, \hat{b}_{k\lambda}] = -\alpha_{k\lambda}e^{\alpha_{k\lambda}\hat{b}^\dagger_{k\lambda}}, \Rightarrow \\ &\quad\Rightarrow e^{\alpha_{k\lambda}\hat{b}^\dagger_{k\lambda}}\hat{b}_{k\lambda} = (\hat{b}_{k\lambda} - \alpha_{k\lambda})e^{\alpha_{k\lambda}\hat{b}^\dagger_{k\lambda}}, \end{aligned} \tag{22}$$

we arrive at the equation (for each mode k,λ)

$$\begin{aligned} i\hbar&\left\{\frac{\dot{C}(t)}{C(t)} + \dot{\alpha}(t)\hat{b}^\dagger + \dot{\beta}(t)(\hat{b} - \alpha(t)) + \right. \\ &\left. + (\hat{b}^\dagger + \beta)(\hat{b} - \alpha(t))\dot{\gamma}(t)\right\}\Psi_{k\lambda}(t) = \\ &= \left\{\hbar\omega(\hat{b}^\dagger\hat{b} + \tfrac{1}{2}) - \Lambda(t)(\hat{b}^\dagger + \hat{b})\right\}\Psi_{k\lambda}(t). \end{aligned} \tag{23}$$

Arranging the coefficients for combinations of creation/annihilation operators in the given mode, we get

$$i\hbar\left\{\left(\frac{\dot{C}_{k\lambda}(t)}{C_{k\lambda}(t)}-\dot{\beta}_{k\lambda}(t)\alpha_{k\lambda}(t)-\beta_{k\lambda}\alpha_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t)\right)+\right.$$
$$+(\dot{\alpha}_{k\lambda}(t)-\alpha_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t))\hat{b}^{\dagger}_{k\lambda}+$$
$$\left.+(\dot{\beta}_{k\lambda}(t)+\dot{\beta}_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t))\hat{b}_{k\lambda}+\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda}\dot{\gamma}_{k\lambda}(t)\right\}\Psi_{k\lambda}(t)=$$
$$=\left\{\hbar\omega_k(\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda}+\frac{1}{2})-\Lambda_{k\lambda}(t)(\hat{b}^{\dagger}_{k\lambda}+\hat{b}_{k\lambda})\right\}\Psi_{k\lambda}(t). \tag{24}$$

Equating the coefficients for corresponding combinations of creation/annihilation operators in the given mode on the left and right, we arrive at a system of equations for determining the sought functions $\alpha(t)$, $\beta(t)$, $\gamma(t)$, which is general for various initial conditions:

1) for coefficients at operator $\hat{b}^{\dagger}_{k\lambda}\hat{b}_{k\lambda}$, we have the equation

$$i\hbar\dot{\gamma}_{k\lambda}(t)=\hbar\omega_k;$$

2) for coefficients at operator $\hat{b}_{k\lambda}$, we have the equation

$$i\hbar\left(\dot{\beta}_{k\lambda}(t)+\beta_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t)\right)=-\Lambda_{k\lambda}(t);$$

3) for coefficients at operator $\hat{b}^{\dagger}_{k\lambda}$, we have the equation

$$i\hbar\left(\dot{\alpha}_{k\lambda}(t)-\alpha_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t)\right)=-\Lambda_{k\lambda};$$

4) for free terms we have the equation

$$i\hbar\left(\frac{\dot{C}_{k\lambda}(t)}{C_{k\lambda}(t)}-\dot{\beta}_{k\lambda}(t)\alpha_{k\lambda}(t)-\beta_{k\lambda}\alpha_{k\lambda}(t)\dot{\gamma}_{k\lambda}(t)\right)=\frac{\hbar\omega_k}{2}.$$

Thus, we arrive at a system of equations that determines the general form of the solution to the time-dependent problem:

$$\begin{aligned}
&\dot{\gamma}_{k\lambda}(t)=-i\omega_k,\\
&\dot{\beta}_{k\lambda}(t)-i\omega_{k\lambda}\beta_{k\lambda}(t)=\frac{i\Lambda_{k\lambda}(t)}{\hbar},\\
&\dot{\alpha}_{k\lambda}(t)+i\omega_k\alpha_{k\lambda}(t)=\frac{i\Lambda_{k\lambda}(t)}{\hbar},\\
&\frac{\dot{C}_{k\lambda}(t)}{C_{k\lambda}(t)}-\alpha_{k\lambda}(t)(\dot{\beta}_{k\lambda}(t)-\beta_{k\lambda}(t)i\omega_k)=-\frac{i}{2}\omega_k.
\end{aligned} \tag{25}$$

From here, we obtain the general form of solutions for the desired coefficients that completely define the wave function (wave vector) at any moment in time:

$$\begin{aligned}
C_{k\lambda}(t)&=\exp\left(-i\frac{\omega t}{2}\right)\exp\left\{-\frac{1}{\hbar^2}\int_{-\infty}^{t}dt'\times\right.\\
&\left.\times\left(\Lambda_{k\lambda}(t')e^{-i\omega t'}\int_{-\infty}^{t'}dt''\left(\Lambda_{k\lambda}(t'')e^{i\omega t''}\right)\right)\right\},\\
\alpha_{k\lambda}(t)&=\frac{ie^{-i\omega_k t}}{\hbar}\int_{-\infty}^{t}\Lambda_{k\lambda}(t')e^{i\omega_k t'}dt',\\
\beta_{k\lambda}(t)&=\frac{ie^{i\omega_k t}}{\hbar}\int_{-\infty}^{t}\Lambda_{k\lambda}(t')e^{-i\omega_k t'}t'dt',\\
\gamma_{k\lambda}(t)&=-i\omega_k t.
\end{aligned} \tag{26}$$

Next, we consider a possible solution to the problem that corresponds to experiments of type [18], where coherent superposition of electronic states is obtained as a result of ultrashort laser pulse impact on the electronic system. Before the laser field impact, the system was initially in a vacuum state for all modes $\Psi_{k\lambda}(-\infty)=|0\rangle_{k\lambda}$. Initial conditions can be taken in the form

$$\begin{aligned}
\alpha_{k\lambda}(-\infty)&=0,\\
\beta_{k\lambda}(-\infty)&=0,\\
C_{k\lambda}(-\infty)&=1.
\end{aligned} \tag{27}$$

Let us consider, for example, the evolution of a phonon "wave packet" appearance of which is due to interaction with an electronic wave packet generated by the exciton component of the polariton, and described by the matrix element in (19) $\left\langle\eta_f(t)\left|\hat{c}^{\dagger}_f\hat{c}_i\right|\eta_i(t)\right\rangle$, which is a temporal signal $\Lambda(t)$ of "electron-phonon interaction" in the form of function

$$\Lambda_{k\lambda}(t)=\Lambda_{k\lambda_0}e^{-\frac{|t|}{\tau}}, \tag{28}$$

Then, using the obtained general expressions (28) for coefficients $C_{k\lambda}(t)$, $\alpha_{k\lambda}(t)$, $\beta_{k\lambda}(t)$, $\gamma_{k\lambda}(t)$, we get explicit time dependencies:

$$\begin{aligned}
\alpha_{\omega}(t)&=\frac{ie^{-i\omega t}}{\hbar}\int_{-\infty}^{t}\Lambda_0e^{-|t'|/\tau}e^{i\omega t'}dt''=\\
&=\frac{ie^{-i\omega t}}{\hbar}\Lambda_0\left\{\frac{2\tau}{1+(\tau\omega)^2}-\frac{\tau e^{-t/\tau}e^{i\omega t}}{1-i\tau\omega}\right\}\underset{t\to\infty}{\to}\\
&\underset{t\to\infty}{\to}\frac{ie^{-i\omega t}}{\hbar}\Lambda_0\frac{2\tau}{1+(\tau\omega)^2},
\end{aligned}$$

$$\beta_\omega(t) = \frac{ie^{i\omega t}}{\hbar}\Lambda_0\int\limits_{-\infty}^{t} e^{-|t'|/\tau}e^{-i\omega t'}dt' = \frac{ie^{i\omega t}}{\hbar}\Lambda_0\frac{2\tau}{1+(\tau\omega)^2}, \gamma(t) = -i\omega t, \quad (29)$$

$$C_\omega(t) = e^{-i\omega t/2}\exp\left\{-\frac{1}{\hbar^2}\int\limits_{-\infty}^{t}dt'\times\right.$$

$$\left.\times\left\{\Lambda_0 e^{-|t'|/\tau}e^{-i\omega t'}\int\limits_{-\infty}^{t'}dt''(\Lambda_0 e^{-|t''|/\tau}e^{i\omega t''})\right\}\right\}\underset{t\to\infty}{\to}$$

$$\underset{t\to\infty}{\to} e^{-i\omega t/2}\exp\left\{-\frac{\Lambda_0^2}{2\hbar^2}\left|\frac{2/\tau}{(1/\tau)^2+\omega^2}\right|^2\right\}. \quad (30)$$

Taking into account the initial conditions (27), (28), the wave function can be written as

$$\Psi_{k\lambda}(t) = C_{k\lambda}(t)e^{\alpha(t)b^\dagger}e^{\beta(t)b}e^{\gamma(t)b^\dagger b}\left|0\right\rangle =$$

$$= C_{k\lambda}(t)\sum_{\nu=0}^{\infty}\frac{\alpha_{k\lambda}^{\nu}(t)}{\nu!}b_{k\lambda}^{\dagger\nu}\left|0\right\rangle = C_{k\lambda}(t)\sum_{\nu=0}^{\infty}\frac{\alpha_{k\lambda}^{\nu}(t)}{\sqrt{\nu!}}\left|\nu\right\rangle,$$

$$e^{\beta_{k\lambda}(t)b_{k\lambda}}e^{\gamma_{k\lambda}(t)b_{k\lambda}^\dagger b_{k\lambda}}\left|0\right\rangle = \quad (31)$$

$$= e^{\beta(t)b}\sum_{\nu=0}^{\infty}\frac{\gamma_{k\lambda}^{\nu}(t)}{\nu!}\hat{n}_{k\lambda}^{\nu}\left|0\right\rangle = e^{\beta_{k\lambda}(t)b_{k\lambda}}\cdot\hat{1}\left|0\right\rangle = \left|0\right\rangle.$$

It is easy to show that the wave vector normalization condition with the obtained coefficient values (29), (30) is fully satisfied

$$\left\langle\Psi_{k\lambda}(t)\right|\left|\Psi_{k\lambda}(t)\right\rangle = \left|C_{k\lambda}(t)\right|^2\sum_{\nu=0}^{\infty}\frac{\left|\alpha_{k\lambda}(t)\right|^{2\nu}}{\nu!} =$$

$$= \left|C_{k\lambda}(t)\right|^2 e^{\left|\alpha_{k\lambda}(t)\right|^2} = 1,$$

$$\left|C_{k\lambda}(t)\right|^2 = e^{-\left|\alpha_{k\lambda}(t)\right|^2}, \Rightarrow \left|C_{k\lambda}(t)\right| = e^{-\left|\alpha_{k\lambda}(t)\right|^2/2} =$$

$$= \exp\left\{-\frac{\Lambda_0^2}{2\hbar^2}\left|\frac{2\tau}{1+(\omega_k\tau)^2}\right|^2\right\}, \quad (32)$$

$$\left|\alpha_{k\lambda}(t)\right|^2 = \left(2\frac{\Lambda_0\tau}{\hbar}\right)^2\left\{\frac{1}{\left(1+(\tau\omega_k)^2\right)^2} - \right.$$

$$-\frac{e^{-t/\tau}}{\left(1+(\tau\omega_k)^2\right)^{3/2}}\cos\left(\omega_k t+\operatorname{arctg}(\omega_k\tau)\right)+$$

$$\left.+\frac{e^{-2t/\tau}}{4\left(1+(\tau\omega_k)^2\right)}\right\}\underset{t\to\infty}{\to}\left(\frac{2\tau\Lambda_0}{\hbar}\right)^2\frac{1}{\left(1+(\tau\omega_k)^2\right)^2}. \quad (33)$$

Then the thermal energy flux carried by phonons in coherent states is defined as:

$$\left\langle j\right\rangle_{k\lambda} = \hbar\omega_k c_s\left\langle\Psi_{k\lambda}(t)\right|\hat{n}_{k\lambda}\left|\Psi_{k\lambda}(t)\right\rangle =$$

$$= \hbar\omega c_s\left|C_{k\lambda}(t)\right|^2\sum_{\nu=0}^{\infty}\nu\frac{\left|\alpha_{k\lambda}(t)\right|^{2\nu}}{\nu!} =$$

$$= \hbar\omega c_s\left|\alpha_{k\lambda}(t)\right|^2\left|C_{k\lambda}(t)\right|^2 e^{\left|\alpha_{k\lambda}(t)\right|^2}, \quad (34)$$

where c_s is the speed of sound in the crystal (phase velocity for the given mode):

$$c_s = \frac{\omega_k}{k}.$$

Considering the normalization condition (32), the spectral density of thermal energy flux will be equal to

$$\left\langle j\right\rangle_\omega = \frac{d\varepsilon}{d\omega} = \hbar\omega c_s\frac{g_s\omega^2}{(2\pi)^3 c_s^3}\frac{2\pi}{3}\left|\alpha_\omega(t)\right|^2 =$$

$$= \hbar\omega\frac{\omega^2}{(2\pi)^2 c_s^2}\left(\frac{2\Lambda_0\tau}{\hbar}\right)^2\left\{\frac{1}{\left(1+(\tau\omega)^2\right)^2} - \right.$$

$$\left.\frac{e^{-t/\tau}\cos\left(\omega t+\operatorname{arctg}(\omega\tau)\right)}{\left(1+(\omega\tau)^2\right)^{3/2}}+\frac{e^{-2t/\tau}}{4\left(1+(\tau\omega)^2\right)}\right\}\underset{t\to\infty}{\to}$$

$$\underset{t\to\infty}{\to}\frac{\hbar\omega^3}{c_s^2}\left(\frac{2\tau\Lambda_0}{2\pi\hbar}\right)^2\frac{1}{\left(1+(\tau\omega)^2\right)^2}. \quad (35)$$

For the time interval $T = 2\pi / \omega \ll t < \tau$ the flux density will have the form

$$\langle j \rangle_\omega = \hbar\omega \frac{\omega^2}{(2\pi)^2 c_s^2} \left(\frac{2\Lambda_0 \tau}{\hbar} \right)^2 \times$$

$$\times \left\{ \frac{1}{\left(1 + (\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1 + (\tau\omega)^2\right)} \right\}. \quad (36)$$

For the interval $\tau < t \to \infty$ we have

$$\langle j \rangle_\omega = \frac{d\varepsilon}{d\omega} = \hbar\omega \frac{g_s \omega^2}{(2\pi)^3 c_s^2} \frac{2\pi}{3} \left|\alpha_\omega(t)\right|^2 \underset{t\to\infty}{\to}$$

$$\underset{t\to\infty}{\to} \frac{\hbar\omega^3}{c_s^2} \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{1}{\left(1 + (\tau\omega)^2\right)^2}. \quad (37)$$

Then the total quantum-mechanical energy flux carried by coherent phonons, without considering the thermal factor, is determined as the integral

$$J = \int_{-\infty}^{\infty} \langle j \rangle_\omega \, d\omega = \int_{-\varpi_D}^{\varpi_D} \frac{\left|\alpha(t)\right|^2}{4\pi^2 c_s^2} \hbar\omega\omega^2 d\omega =$$

$$= \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{2\hbar}{c_s^2} \left\{ \int_0^{\varpi_D} \frac{\omega^3}{\left(1 + (\tau\omega)^2\right)^2} d\omega + \right.$$

$$\left. + \frac{e^{-2t/\tau}}{4} \int_0^{\varpi_D} \frac{\omega^3}{\left(1 + (\tau\omega)^2\right)} d\omega \right\} =$$

$$= \left(\frac{\Lambda_0}{\varpi} \right)^2 \frac{2}{\hbar c_s^2} \left\{ \left(1 - \frac{e^{-2t/\tau}}{2} \right) \ln\left(1 + (\tau\omega_D)^2\right) + \right.$$

$$\left. + \frac{1}{\left(1 + (\tau\omega_D)^2\right)} - 1 + \frac{e^{-2t/\tau}}{2} (\tau\omega_D)^2 \right\}, \quad (38)$$

Taking into account the expression for sound velocity,

$$c_s = \frac{\omega_D}{2\pi} \sqrt[3]{\left(\frac{4\pi}{3n} \right)}, \quad (39)$$

the complete expression for the energy flux will have the form

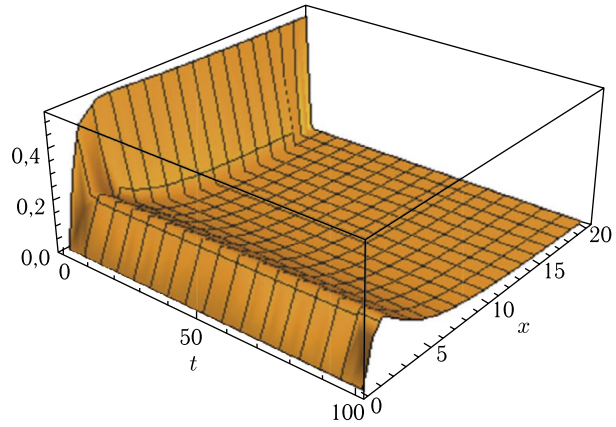

Fig. 1. Total energy flux as a function of time $t = t / \tau$ and inverse decay time $x = \omega_D \tau$. At $x \sim 2$ maximum flux is observed and there is no flux decay over time

$$J = 3nc_s \frac{\Lambda_0}{(\tau\omega_D)^2} \times$$

$$\times \frac{\Lambda_0}{\hbar\omega_D} \left\{ \left(1 - \frac{e^{-2t/\tau}}{2} \right) \ln\left(1 + (\tau\omega_D)^2\right) + \right.$$

$$\left. + \frac{1}{\left(1 + (\tau\omega_D)^2\right)} - 1 + \frac{e^{-2t/\tau}}{2} (\tau\omega_D)^2 \right\}. \quad (40)$$

The indicated dependence of the total energy flux on the combination of internal crystal characteristics, such as the Debye frequency ω_D and coherence time τ, are shown in Fig. 1. It is clearly visible that at certain ratios of these parameters, specifically $x = \tau\omega_D \sim 2$, the magnitude of the total energy flux does not decay with time. Taking into account those indicated in work [1] for boron arsenide (BAs) Debye frequencies of acoustic phonons $\omega_D \sim 12.8$ THz and characteristic coherence times $\tau \sim 10^{-13}$ s, we see that they fit into the specified estimate, which can be associated with the establishment of superthermal conductivity regime [1,24-27,31,32]. In paper [32], the dynamics of coherent optical phonons in tellurium after intense femtosecond laser pulse exposure is studied. The main mechanism of anomalous thermal phenomena in the material, up to "nontemperature" phase transition, is considered to be the so-called DECP (Displacive Excitation of Coherent Phonons). It is shown that the time required for a carrier to diffuse over one absorption length (50 nm) is about 600 fs $= 6 \cdot 10^{-13}$ s, characteristic frequencies at which resonant thermal conductivity

effects are observed are 3-3.6 THz. Our estimate of the parameter $x = \tau\omega$ for this system is $x = \tau\omega = 1.8 - 2.16$, which corresponds to the nondecaying energy flux shown in Fig. 1.

Moreover, to avoid using reference values of the speed of sound in crystals or Debye frequency obtained for macroscopic materials when evaluating the behavior of nanoscale objects, one can use the microscopic value of the Debye frequency as the maximum possible frequency of harmonic excitation propagation, corresponding to the minimum wavelength equal to two lattice constants a of the specific nanocrystal:

$$\omega_{max} = \frac{2\pi}{\lambda_{min}}\sqrt{\frac{\gamma}{m}}a = \pi\sqrt{\frac{\gamma}{m}},$$

in our case, the interaction constant instead of γ will be Ξ.

5. COHERENT HEAT FLOW AT FINITE TEMPERATURE

Let us now consider the problem for finite temperatures. Here it is necessary to take into account the entire continuum of modes across the spectrum of allowed frequencies. The spectral density of heat flow at finite temperature should account for the thermal distribution of phonon numbers in a given mode (Planck distribution function)

$$\langle j\rangle_{\omega T} = \left\langle \frac{d\varepsilon}{d\omega}\right\rangle_T =$$

$$= \hbar\omega c_s \frac{g_s\omega^2}{(2\pi)^3 c_s^3}\frac{2\pi}{3}|\alpha(t)|^2\left(\frac{1}{e^{\hbar\omega/T}-1}\right) \approx$$

$$\approx \left(t \gg T = \frac{2\pi}{\omega}\right) \approx \hbar\omega\frac{\omega^2}{(2\pi)^2 c_s^2}\left(\frac{2\Lambda_0\tau}{\hbar}\right)^2 \times$$

$$\times\left\{\frac{1}{\left(1+(\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1+(\tau\omega)^2\right)}\right\}\left(\frac{1}{e^{\hbar\omega/T}-1}\right)\underset{t\to\infty}{\to}$$

$$\underset{t\to\infty}{\to}\frac{\hbar\omega^3}{c_s^2}\left(\frac{2\tau\Lambda_0}{2\pi\hbar}\right)^2\frac{1}{\left(1+(\tau\omega)^2\right)^2}\left(\frac{1}{e^{\hbar\omega/T}-1}\right). \quad (41)$$

The dependencies of the spectral density (41) on frequency are shown in Fig. 2.

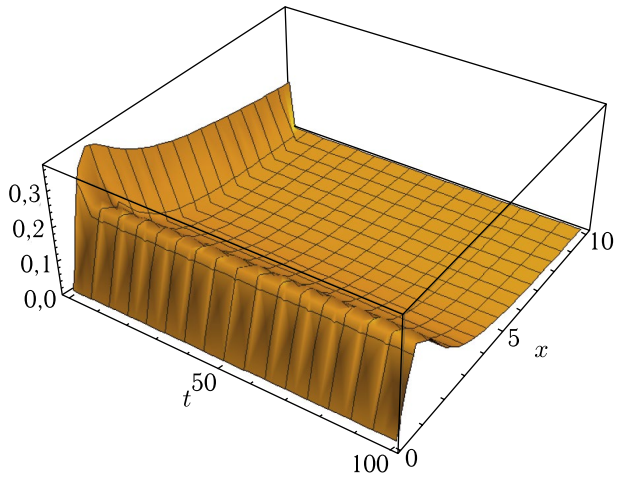

Fig. 2. Spectral density of flow taking into account the equilibrium Planck distribution. Here $t = t/\tau$, $x = \omega\tau$. At a given phonon relaxation time, there is a resonant frequency $\omega^* \sim 3/2\tau$, when the spectral density of flow does not decay with time (superthermal conductivity)

To evaluate the parameters, let's take expression (41) in the form

$$j_\omega = \left(\frac{\hbar}{\tau T}\right)(\omega\tau)T\frac{(\tau\omega)^2}{(2\pi)^2 c_s^2}\left(\frac{2\Lambda_0}{\hbar}\right)^2 \times$$

$$\times\left\{\frac{1}{\left(1+(\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1+(\tau\omega)^2\right)}\right\}\left\{\frac{1}{e^{(\hbar/\tau T)(\tau\omega)}-1}\right\},$$

$$\tau \sim 10^{-13}, \quad \frac{\hbar}{T} \sim 10^{-14} - 10^{-15}, \quad \frac{\hbar}{\tau T} \sim 0.1\text{–}0.01.$$

Let's consider the total flow taking into account temperature in the low-temperature limit, $T \le \Lambda_0$ (here temperature is written in the energy scale $T = k_B T^\circ$). It is necessary to consider the orders of magnitude: coherence time τ is determined by characteristic relaxation times of the electronic system in solid state, i.e. $\tau \sim 10^{-13}$ s. The characteristic parameter included in the Planck distribution function,

$$\frac{\hbar}{k_B T^\circ} = \frac{10^{-27}}{1.4\cdot 10^{-16} T^\circ} = \frac{10^{-11}}{1.4\cdot T^\circ},$$

in the temperature range T° from 300 to 1000 K, varies:

$$\frac{\hbar}{k_B T^\circ} = \frac{10^{-11}}{1.4\cdot T^\circ} \sim 10^{-14}\text{–}10^{-15}\,\text{s}.$$

Then it is necessary to take into account the fact that

$$\tau\omega > \frac{\hbar\omega}{k_B T^{\circ}},$$

i.e., we are dealing with quasi-adiabatic interaction, where the system can be described by the equilibrium Planck distribution function. The condition of small gradient means that the inequality $\tau c_s \ll l$, is satisfied, where l — is the spatial scale of temperature change. In other words, the temperature change itself occurs over relatively long times, $l / c_s \gg \tau$, thus, the integration of spectral flux density over frequency considering temperature can be performed as at constant temperature:

$$J = \int_0^{\varpi_D} \langle j \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) d\omega =$$

$$= \int_0^{\varpi_D} \frac{|\alpha(t)|^2}{4\pi^2 c_s^2} \left(\frac{\hbar\omega}{e^{\hbar\omega/T} - 1} \right) \omega^2 d\omega =$$

$$= \hbar \left(\frac{\Lambda_0 \tau}{\hbar \pi c_s} \right)^2 \int_0^{\varpi_D} \left\{ \frac{1}{\left(1 + (\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1 + (\tau\omega)^2\right)} \right\} \times$$

$$\times \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) \omega^3 d\omega. \qquad (42)$$

5.1. High-temperature limit

In case of phonon relaxation time, $\tau\omega_D > 1$, $\hbar\omega_D / T \sim 1$, we have

$$\mathrm{J}_{HT} = \int_0^{\infty} \frac{\langle j \rangle_\omega}{e^{\hbar\omega/T} - 1} d\omega = \left(\frac{\Lambda_0}{2\pi\hbar} \right)^2 \times$$

$$\times \frac{T}{\tau c_s^2} \left[\pi + \frac{1}{2} e^{-2t/\tau} \left\{ (\tau\omega_D)^2 - \ln\left(1 + (\tau\omega_D)^2\right) \right\} \right] =$$

$$= \frac{3}{2} \frac{n T c_s}{\tau\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D} \right)^2 \times$$

$$\times \left\{ \pi + \frac{e^{-2t/\tau}}{2} \left[(\tau\omega_D)^2 - \ln\left(1 + (\tau\omega_D)^2\right) \right] \right\} \qquad (43)$$

(see Appendix for calculation details). In fact, we arrive at the classical linear temperature dependence that emerges in the high-temperature limit in a macroscopic crystal. However, there is still a contribution directly related to the coherence time τ, which decays exponentially with time, which is quite consistent with the conclusions in works [14, 32, 33] for the high-temperature limit taking into account phonon coherence.

5.2. Low-temperature limit

1. In case of phonon relaxation time, $\tau\omega_D < 1$, $\hbar\omega_D / T \gg 1$, we have

$$J_{LT\tau} \approx \int_0^{\varpi_D} \langle j \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) d\omega =$$

$$= \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{\hbar}{\tau^4 c_s^2} \int_0^{\infty} \left(\frac{1}{e^{\hbar\omega\tau/\tau T} - 1} \right) \frac{(\tau\omega)^3}{\left(1 + (\tau\omega)^2\right)^2} d(\tau\omega) \approx$$

$$\approx \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{\hbar}{\tau^4 c_s^2} \left(\frac{\tau T}{\hbar} \right)^4 \zeta_R(4)\Gamma(4) =$$

$$= \frac{2}{5} n c_s \frac{(\pi T)^4}{(\hbar\omega_D)^3} \left(\tau\omega_D \frac{\Lambda_0}{\hbar\omega_D} \right)^2, \qquad (44)$$

$$\zeta_R(4) = \frac{\pi^4}{90}.$$

Here, expression (39) for sound velocity is taken into account. The result turns out to be the same as for ordinary thermal phonons in the absence of coherence if the coherence factor $(\tau\Lambda_0 / \hbar) \to 1$.

2. In the case of large coherence time, $\omega_D \tau > 1$, $\hbar\omega_D / T \gg 1$, we have

$$J_{LT\mathrm{T}} = \int_0^{\omega_D} \langle j \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) d\omega =$$

$$= \hbar \left(\frac{\Lambda_0 \tau}{\hbar \pi c_s} \right)^2 \int_0^{\infty} \left\{ \frac{1}{\left(1 + (\tau\omega)^2\right)^2} + \right.$$

$$\left. + \frac{e^{-2t/\tau}}{4\left(1 + (\tau\omega)^2\right)} \right\} \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) \omega^3 d\omega =$$

$$= J_{LTI} + J_{LTII}(t). \qquad (45)$$

Here, the stationary J_{LTI} and temporal $J_{LTII}(t)$ parts of the heat flux in the low-temperature limit have the form

$$J_{LTI} = \left(\frac{\tau\Lambda_0}{\pi\hbar c_s}\right)^2 \frac{\hbar}{2\tau^4}\left(\frac{\tau T}{\hbar}\right)^2 \zeta_R(2),$$

$$J_{LTII}(t) \approx \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{4\tau^4 c_s^2} e^{-2t/\tau} \times$$

$$\times \int_0^\infty \left(\frac{1}{e^{\hbar(\tau\omega)/\tau T} - 1}\right) \frac{(\tau\omega)^3}{(\tau\omega)^2} d(\tau\omega) = \quad (46)$$

$$= \left(\frac{\Lambda_0}{2\pi\hbar^2} T\right)^2 \frac{\hbar}{c_s^2} e^{-2t/\tau} \zeta_R(2)\Gamma(2),$$

$$\zeta_R(2) = \frac{\pi^2}{6}.$$

The total flux, taking into account time dependence, then has the form

$$J_{LTT} = \frac{\pi^2}{2} \frac{n c_s T^2}{\hbar\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2 \left\{1 + \frac{e^{-2t/\tau}}{2}\right\}. \quad (47)$$

Let's consider the corresponding contributions to internal energy and heat capacity. For this, we calculate the quantum-mechanical average energy value for one mode with frequency ω:

$$\langle u \rangle = \hbar\omega \langle \Psi(t) | \hat{n} | \Psi(t) \rangle =$$

$$= \hbar\omega |\alpha(t)|^2 |C(t)|^2 e^{|\alpha(t)|^2} =$$

$$= \hbar\omega |\alpha(t)|^2,$$

$$\langle u \rangle_\omega = \frac{d\varepsilon}{d\omega} = 4\pi\hbar\omega \frac{g_s \omega^2}{(2\pi)^3 c_s^3} |\alpha(t)|^2 = \quad (48)$$

$$= \hbar\omega \frac{3\omega^2}{2\pi^2 c_s^3} \left(\frac{2\Lambda_0\tau}{\hbar}\right)^2 \left\{\frac{1}{\left(1 + (\tau\omega)^2\right)^2} - \right.$$

$$\left. - \frac{e^{-t/\tau}\cos\left(\omega t + \operatorname{arctg}(\omega\tau)\right)}{\left(1 + (\tau\omega)^2\right)^{3/2}} + \frac{e^{-2t/\tau}}{4(1 + (\tau\omega)^2)}\right\} \underset{t\to\infty}{\to}$$

$$\underset{t\to\infty}{\to} \frac{6\hbar\omega^3}{c_s^3} \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{1}{\left(1 + (\tau\omega)^2\right)^2}.$$

The specific internal energy (no temperature considered) per unit volume equals

$$U = \int_0^{\omega_D} \langle u \rangle_\omega \, d\omega =$$

$$= 18 \frac{\Lambda_0^2}{\hbar\omega_D (\tau\omega_D)^2} n \left\{\left(1 - \frac{e^{-2t/\tau}}{2}\right) \ln\left(1 + (\tau\omega_D)^2\right) + \right.$$

$$\left. + \frac{1}{\left(1 + (\tau\omega_D)^2\right)} - 1 + \frac{e^{-2t/\tau}}{2} (\tau\omega_D)^2 \right\}. \quad (49)$$

Taking into account finite temperature, we have an expression for internal energy in the form

$$U(T) = \int_0^{\varpi_D} \langle u \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1}\right) d\omega =$$

$$= 6 \int_0^{\varpi_D} \frac{|\alpha(t)|^2}{4\pi^2 c_s^3} \left(\frac{\hbar\omega}{e^{\hbar\omega/T} - 1}\right) \omega^2 d\omega =$$

$$= 6 \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{c_s^3} \int_0^\infty \left(\frac{1}{e^{\hbar\omega/T} - 1}\right) \times$$

$$\times \left\{\frac{1}{\left(1 + (\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1 + (\tau\omega)^2\right)}\right\} \omega^3 d\omega. \quad (50)$$

5.3. High-temperature limit

In the case of large coherence time (phonon relaxation time), $\tau\omega_D > 1$, $\hbar\omega_D / T \sim 1$, we have

$$\frac{U_{HT}(T)}{V} = \int_0^{\varpi_D} \langle u \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1}\right) d\omega =$$

$$= 3nT \frac{3}{\tau\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2 \times$$

$$\times \left\{\pi + \frac{e^{-2t/\tau}}{2} \left[(\tau\omega_D)^2 - \ln\left(1 + (\tau\omega_D)^2\right)\right]\right\}. \quad (51)$$

$$C_V = 3N \frac{3}{\tau\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2 \times$$

$$\times \left\{\pi + \frac{e^{-2t/\tau}}{2} \left[(\tau\omega_D)^2 - \ln\left(1 + (\tau\omega_D)^2\right)\right]\right\}.$$

It is clearly seen that the heat capacity in the high-temperature limit does not depend on temperature, as in the case of "free" phonons in the same limit,

while maintaining a specific contribution due to the interaction constant with the electronic subsystem, and the characteristic coherence time parameter.

5.4. Low-temperature limit

1. In the case of small coherence time, $\tau\omega_D < 1$, $\hbar\omega_D / T \gg 1$, we have

$$\frac{U_{LT\tau}}{V} \approx \int_0^{\varpi_D} \langle u \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) d\omega = 6 \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{\hbar}{\tau^4 c_s^3} \times$$
$$\times \int_0^{\infty} \left(\frac{1}{e^{\hbar\omega\tau/\tau T} - 1} \right) \frac{(\tau\omega)^3}{\left(1 + (\tau\omega)^2\right)^2} d(\tau\omega) \approx$$
$$\approx \left(\frac{\tau\Lambda_0}{\pi\hbar} \right)^2 \frac{6\hbar}{\tau^4 c_s^3} \left(\frac{\tau T}{\hbar} \right)^4 \zeta_R(4)\Gamma(4) = \quad (52)$$
$$= \frac{12}{5} n \frac{(\pi T)^4}{(\hbar\omega_D)^3} \left(\tau\omega_D \frac{\Lambda_0}{\hbar\omega_D} \right)^2,$$
$$C_V = \frac{12}{5} N \pi^4 \frac{T^3}{(\hbar\omega_D)^3} \frac{4}{\pi} \left(\tau \frac{\Lambda_0}{\hbar} \right)^2.$$

Here, expression (39) for sound velocity is taken into account. For comparison, let's present the expression for crystal heat capacity in the phonon model at low-temperature limit:

$$C_V = \frac{4}{5} \pi^4 g_s N \frac{T^3}{(\hbar\omega_D)^3} = \frac{12}{5} \pi^4 N \frac{T^3}{(\hbar\omega_D)^3}.$$

Hence, it follows that the characteristic temperature dependence ($\sim T^3$ Debye's law) is preserved, but additional factors appear, including dependence on excitation pulse duration τ (coherence time) and polariton-phonon interaction constant. Being a measurable quantity, heat capacity will allow to "see" the presence of phonon coherence.

2. In the case of a long coherence time, $\omega_D \tau > 1$, $\hbar\omega_D / T \gg 1$, we have

$$U_{LT\mathrm{T}} = \int_0^{\omega_D} \langle u \rangle_\omega \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) d\omega = 6 \frac{\hbar}{c_s} \left(\frac{\Lambda_0 \tau}{\hbar\pi c_s} \right)^2 \times$$
$$\times \int_0^{\infty} \left\{ \frac{1}{\left(1 + (\tau\omega)^2\right)^2} + \frac{e^{-2t/\tau}}{4\left(1 + (\tau\omega)^2\right)} \right\} \times \quad (53)$$
$$\times \left(\frac{1}{e^{\hbar\omega/T} - 1} \right) \omega^3 d\omega =$$
$$= \frac{18 n T^2}{\hbar\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D} \right)^2 \zeta_R(2) \left\{ 1 + \frac{e^{-2t/\tau}}{2} \right\} =$$
$$= 3\pi^2 n \frac{T^2}{\hbar\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D} \right)^2 \left\{ 1 + \frac{e^{-2t/\tau}}{2} \right\},$$
$$C_V = 6\pi^2 N \frac{T}{\hbar\omega_D} \left(\frac{\Lambda_0}{\hbar\omega_D} \right)^2 \left\{ 1 + \frac{e^{-2t/\tau}}{2} \right\}.$$

In the case of a long pulse duration (coherence time), coherent phonon states give special distinctive features to the temperature dependence, namely, the lattice heat capacity acquires an uncharacteristic linear dependence on temperature, similar to the contribution to the heat capacity of free electrons in metal – degenerate electron gas:

$$C_V = \frac{N}{2} \pi^2 \left(\frac{T}{\varepsilon_F} \right).$$

6. Results and conclusions

In conclusion, it should be noted that the considered model of coherent phonon formation in a three-dimensional crystal, where polaritonic generation of the medium by a laser pulse is preliminarily assumed, is abstract in nature and not tied to a specific experiment. A fixed fact in the analytical calculation was the dimensionality of the system (crystal) – 3D, i.e., both electrons and phonons can freely propagate along three orthogonal axes. Expression (35) for the spectral flux "silently" implies a recalculation from

$$d^3k \to \frac{g_s \omega^2}{(2\pi)^3 c_s^3} \frac{2\pi}{3} d\omega.$$

Consideration of systems with reduced dimensionality (quasi-two-dimensional or quasi-onedimensional crystal) will naturally lead to changes in expressions for both spectral flux density and expressions for total fluxes, as it is associated with changes in the density of microstates per energy interval. A more detailed examination of how changes in system dimensionality affect the nature of coherent phonon state formation is certainly an independent problem.

As for the considered three-dimensional model of coherent phonon formation, despite the abstract formulation, it has its independent experimental confirmation. Thus, pulsed excitation and phase-sensitive detection of coherent phonons and phonon-polaritons provide detailed understanding of the dynamic properties of matter. Experiments [33], based on optical pumping methods with femtosecond time resolution, allow simultaneous determination of the amplitude and phase of coherent lattice motion. Frequencies in the terahertz range and dephasing times in the picosecond range are obtained with high accuracy, particularly in semiconductors and semiconductor heterostructures, where coherent phonon mode and free carriers are excited simultaneously, providing important information about carrier-phonon interaction far from equilibrium.

The article [33] presents an overview of recent achievements in this field of condensed matter physics. The excitation of coherent LO phonons is achieved through the field screening mechanism. Two consecutive pump pulses affect the sample. Their intensity and time delay are adjusted so that the second pulse provides driving force for coherent amplitude equivalent to the amplitude preserved from the first pulse. Additionally, the initial surface field is regulated through a transparent Schottky contact to avoid complete screening of the surface field with the first pulse already. By carefully adjusting the pulse separation, the driving force is either in phase or in antiphase with the initially generated coherent mode.

Thus, complete destruction or resonant enhancement of coherent LO phonons is observed. This method allows generating coherent LO phonons during a clearly defined time interval shorter than the inherent LO phonon dephasing time

Similar experiments are conducted in Sb, where the A mode is manipulated in a similar way. In mixed BiSb crystals, oscillations Bi–Bi, Bi–Sb and Sb–Sb can be enhanced and suppressed using sequences of femtosecond pulses. It is important to note that in all mentioned experiments, there is a common pattern discovered in our work, namely the effect of LO phonon enhancement with undamped thermal conductivity occurs in various materials when meeting the criterion $x = \tau\omega^* \sim 2$, where τ — is coherence time ω^* — frequency at which the spectral energy density reaches its maximum.

In the mentioned work $\tau = 0.25$ Ps $= 0.25 \cdot 10^{-12}$ s, $\omega^* = 8.8$ THz $= 8.8 \cdot 10^{12}$ Hz, $\tau\omega^* = 2.2$.

For bulk GaAs GaAs $\tau = 0.25$ Ps, $\omega^* \sim 9$ THz, $x = \tau\omega^* = 2.25$.

For GaAs/$A_{l0.3}Ga_{0.7}As$-superlattice $\tau = 0.2$ Ps, $\omega^* = 8.5$ THz, $x = \tau\omega^* = 1.7$.

For isotropic crystal Te $\omega^* = 3.5$ THz, $\tau = 0.6$ Ps, $x = \tau\omega^* = 2.1$,

For anisotropic crystal Te $\omega^* = 4.2$ THz, $\tau = 0.5$ Ps, $x = \tau\omega^* = 2.1$.

In the terahertz emission experiment for crystal InP a broad peak is observed at $\omega^* = 1$ THz, $\tau = 2$ Ps, $x = \tau\omega^* = 2$.

In the study of coherent phonon dynamics in a Te single crystal excited by amplified CPM laser pulses with photon energy of 2 eV, the following values were obtained: $\omega^* = 3.6$ THz, $\tau = 0.75$ Ps, $x = \tau\omega^* = 2.7$.

For HTSC material ($YBa_2Cu_3O_{7-x}$ — thin film) for the Ba mode in plane CuO_2 the following values were obtained: $\omega^* = 3.6$ THz, $\tau = 0.7$ Ps, $x = \tau\omega^* = 2.52$, and for mode Cu (2) in plane CuO_2 we have $\omega^* = 4.2$ THz, $\tau = 0.7$ Ps, $x = \tau\omega^* = 2.8$.

Generalized results are presented in the table.

Comparing all three models of heat flow description, one can notice similarities in the nature of time dependence, namely exponential decay in the classical model and the coherent phonon model in the high-temperature limit. However, in the case of coherent contributions, this decay occurs faster due to the coefficient 2 in the exponent of time. Meanwhile, the temperature dependence in the high-temperature limit is identical in all three models, specifically linear with temperature.

In the case of low-temperature limit, the classical consideration has no meaning, especially when dealing with nanocrystals or thin films and quantum wires. The phonon model is applicable for these quantum limits; moreover, it effectively describes cases of sufficiently strong electron-phonon interaction caused by the polariton generation mechanism, but in this case, a system of "coupled" nonlinear equations connecting electronic and vibrational components is solved simultaneously. This solution is not reflected in the table, see [5] for details. The table shows results for thermal properties of free phonons. As for the

Table. Expressions for energy flow magnitude in different models

Temperature/ Model	Coherent states	Thermal phonons	Classical model
Low temperature limit $\hbar\omega_D / T \gg 1$	$\tau\omega_D < 1$, $J_{LT\tau} = \frac{2}{5} nc_s \frac{(\pi T)^4}{(\hbar\omega_D)^3} (\tau\omega_D)^2 \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2$. $\omega_D\tau > 1$, $J_{LTT} = 3nc_s \frac{T^2}{\hbar\omega_D} \zeta_R(2) \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2 \left\{1 + \frac{e^{-2t/\tau}}{2}\right\}$	$J_{LT} = \frac{\pi^4}{10} c_s n \frac{T^4}{(\hbar\omega_D)^3}$	–
High temperature limit $\hbar\omega_D / T \sim 1$	$J_{HT} = \frac{3}{2\tau\omega_D} nTc_s \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2 \times \left\{\pi + \frac{e^{-2t/\tau}}{2}\left[(\tau\omega_D)^2 - \ln(1 + (\tau\omega_D)^2)\right]\right\}$	$J = \frac{c_s nT}{2}$	$J(x,t) \propto 2\kappa T \frac{x}{l} e^{-t/\tau}$

time dependence of the flux in the low-temperature limit, the Gaussian-type time dependence suggested in [14] does not arise in the coherent phonon regime; it maintains an exponential form with a doubled reduction coefficient ($\sim e^{-2t/\tau}$). The coherence itself is reflected in the flux expression as a factor containing the ratio of the polariton-phonon interaction constant and the Debye energy ($\sim (\tau\omega_D)^2 \left(\Lambda_0 / \hbar\omega_D\right)^2$), and in the case of short coherence time as an additional factor $\left(\tau\omega_D\right)^2 < 1$. Meanwhile, the dependence of the flux on coherence time and interaction constant with the electronic subsystem naturally transitions into the expression for the thermal flux of free phonons

$$J_{LT\tau} = \frac{nc_s}{10} \frac{(\pi T)^4}{(\hbar\omega_D)^3} \left\{(2\tau\omega_D)^2 \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2\right\} \rightarrow$$

$$\rightarrow J_{LT} = \frac{nc_s}{10} \frac{(\pi T)^4}{(\hbar\omega_D)^3},$$

if

$$\left\{(2\tau\omega_D)^2 \left(\frac{\Lambda_0}{\hbar\omega_D}\right)^2\right\} \rightarrow 1,$$

i.e., when there is a certain "resonance" of parameters in the system, the coherence time and polariton-phonon interaction constant are related as

$$\left(\frac{2\tau\Lambda_0}{\hbar}\right) \rightarrow 1,$$

which is essentially the uncertainty relation (energy-time)

$$\Lambda_0\tau \geq \left(\frac{\hbar}{2}\right),$$

minimized asymptotically precisely as a result of the coherence of the vibrational system state. The proof of the statement about the minimization of the "position-momentum" uncertainty relation by coherent states can be found in the book [29].

APPENDIX A. PROPERTIES OF SCHRÖDINGER STATES

1. Linear transformation of creation/annihilation operators (11) is carried out by the unitary transformation operator

$$\hat{U} = e^{\hat{D}},$$

where $\hat{D}$ must be a Hermitian operator, $\hat{D} = \hat{D}^\dagger$. We have

$$B = e^{-\hat{D}} \hat{b} e^{\hat{D}} = \hat{b} + \frac{\Lambda_{k\lambda}}{\hbar\omega_k}.$$

Expansion for the operator exponential

$$B = \hat{b} + \frac{\Lambda_{k\lambda}}{\hbar\omega_k} = e^{-\hat{D}} \hat{b} e^{\hat{D}} =$$

$$= \hat{b} + \left[\hat{b}\hat{D}\right] + \left[\hat{b}\left[\hat{b}\hat{D}\right]\right] + \left[\hat{b}\left[\hat{b}\left[\hat{b}\hat{D}\right]\right]\right] + \ldots$$

Operator $\hat{D}$ has the form

$$\hat{D} = c(\hat{b}^\dagger - \hat{b}),$$

where

$$c = -\frac{\Lambda_{k\lambda}}{\hbar\omega_k},$$

which represents a special case of the unitary transformation operator

$$\hat{U}(\alpha) = e^{\left(\alpha^*\hat{b}^\dagger - \alpha\hat{b}\right)}$$

with a real function

$$\alpha = -\frac{\Lambda_{k\lambda}}{\hbar\omega_k}.$$

It transforms the "old" vacuum function $\left|n_{k\lambda}\right\rangle = \left|0\right\rangle$ into the corresponding "new" vacuum, corresponding to the state

$$\left|\nu_{k\lambda} = 0\right\rangle = \left|\alpha\right\rangle = \hat{U}(\alpha)\left|n_{k\lambda} = 0\right\rangle = e^{\left(\alpha^*\hat{b}^\dagger - \alpha\hat{b}\right)}\left|n_{k\lambda} = 0\right\rangle.$$

2. State expansion $\left|\alpha\right\rangle$ over a complete set of oscillator phonon states $\left|n\right\rangle$ (in a similar description of photons, they are called Fock states) has the form

$$\left|\alpha\right\rangle = \sum_{n=0}^{\infty}\left|n\right\rangle\left\langle n \mid \alpha\right\rangle,$$

$$\alpha\left\langle n \mid \alpha\right\rangle = \left\langle n\right|\hat{b}\left|\alpha\right\rangle = \left\langle n\right|\hat{b}\left|n+1\right\rangle\left\langle n+1 \mid \alpha\right\rangle = \sqrt{n+1}\left\langle n+1 \mid \alpha\right\rangle,$$

$$\left\langle n+1 \mid \alpha\right\rangle = \frac{\alpha}{\sqrt{n+1}}\left\langle n \mid \alpha\right\rangle.$$

From this follows

$$\left\langle n \mid \alpha\right\rangle = \frac{\alpha^n}{\sqrt{n!}}\left\langle 0 \mid \alpha\right\rangle.$$

Thus,

$$\left|\alpha\right\rangle = \sum_{n=0}^{\infty}\left|n\right\rangle\left\langle n \mid \alpha\right\rangle = \left\langle 0 \mid \alpha\right\rangle\sum_{n=0}^{\infty}\left|n\right\rangle\frac{\alpha^n}{\sqrt{n!}}.$$

The "zero" expansion coefficient $\left\langle 0 \mid \alpha\right\rangle$ is determined from the normalization condition $\left|\alpha\right\rangle$:

$$\left\langle \alpha \mid \alpha\right\rangle = \sum_{n'=0}^{\infty}\left\langle \alpha \mid n'\right\rangle\left\langle n'\right|\sum_{n=0}^{\infty}\left|n\right\rangle\left\langle n \mid \alpha\right\rangle = \left|\left\langle 0 \mid \alpha\right\rangle\right|^2\sum_{\substack{n=0\\n'=0}}^{\infty}\frac{\alpha^{*n'}}{\sqrt{n'!}}\left\langle n' \mid n\right\rangle\frac{\alpha^n}{\sqrt{n!}} = \left|\left\langle 0 \mid \alpha\right\rangle\right|^2\sum_{n=0}^{\infty}\frac{\left|\alpha\right|^{2n}}{n!} = \left|\left\langle 0 \mid \alpha\right\rangle\right|^2 e^{\left|\alpha\right|^2} = 1,$$

$$\left|\left\langle 0 \mid \alpha\right\rangle\right| = e^{-\left|\alpha\right|^2/2}.$$

The average number of phonons in a coherent state equals

$$\left\langle n\right\rangle = \left\langle \alpha\right|\hat{b}^\dagger\hat{b}\left|\alpha\right\rangle = e^{-\left|\alpha\right|^2}\sum_{\substack{n=0\\n'=0}}^{\infty}\frac{\alpha^{*n'}}{\sqrt{n'!}}\left\langle n'\right|\hat{b}^\dagger\hat{b}\left|n\right\rangle\frac{\alpha^n}{\sqrt{n!}} =$$

$$= e^{-\left|\alpha\right|^2}\sum_{n=0}^{\infty}n\frac{\left|\alpha\right|^{2n}}{n!} = \left|\alpha\right|^2 e^{-\left|\alpha\right|^2}\sum_{n=1}^{\infty}\frac{\left|\alpha\right|^{2(n-1)}}{(n-1)!} \equiv$$

$$\equiv \left|\alpha\right|^2 e^{-\left|\alpha\right|^2}\sum_{k=1}^{\infty}\frac{\left|\alpha\right|^{2k}}{k!} = \left|\alpha\right|^2 e^{-\left|\alpha\right|^2} e^{\left|\alpha\right|^2} = \left|\alpha\right|^2.$$

The coherent state has the form

$$\left|\alpha\right\rangle = e^{-\left\langle n\right\rangle/2}\sum_{n=0}^{\infty}\left|n\right\rangle\frac{\sqrt{\left\langle n\right\rangle}^n}{\sqrt{n!}}.$$

Consequently, the probability of finding the number of phonons equal to n in a given coherent state with an average number of phonons $\left\langle n\right\rangle$ follows the Poisson distribution:

$$W_n = e^{-\left\langle n\right\rangle}\frac{\left\langle n\right\rangle^n}{n!}.$$

3. The unitary operator

$$\hat{D}\left(\alpha\right) = e^{-\frac{\left\langle n\right\rangle}{2}}e^{\alpha^*\hat{b}^\dagger}e^{-\alpha\hat{b}}, \quad \alpha^* = \alpha,$$

has the following properties:

1) $\hat{D}(\alpha)\hat{D}^\dagger(\alpha) = \hat{D}^\dagger(\alpha)\hat{D}(\alpha) = 1,$

2) $\hat{D}^\dagger(\alpha) = \hat{D}(-\alpha),$

3) $\hat{D}(\beta)\hat{D}(\alpha) = e^{-\frac{\beta\alpha^* - \beta^*\alpha}{2}}\hat{D}(\beta+\alpha), \Rightarrow$

$$\Rightarrow \hat{D}(\beta)\hat{D}(\alpha) = e^{-\beta\alpha^* - \beta^*\alpha}\hat{D}(\alpha)\hat{D}(\beta),$$

$$\left[\hat{b}\hat{D}\left(\alpha\right)\right] = \alpha\hat{D}(\alpha),$$

$$\left[\hat{b}^\dagger\hat{D}(\alpha)\right] = \alpha^*\hat{D}(\alpha),$$

$$\hat{D}^\dagger(\alpha)\hat{b}\hat{D}(\alpha) = \hat{b} + \alpha,$$

$$\hat{D}^\dagger(\alpha)\hat{b}^\dagger\hat{D}(\alpha) = \hat{b}^\dagger + \alpha^*.$$

4. Let's consider the property of completeness and non-orthogonality. It is known that coherent states $\left|\alpha\right\rangle$ and $\left|\beta\right\rangle$, differing in the average number

of phonons in a given mode $\langle N\rangle \neq \langle K\rangle$, are non-orthogonal states:

$$\langle \alpha \mid \beta\rangle = e^{-\frac{\langle N\rangle+\langle K\rangle}{2}} \sum_{\substack{n=0\\ n'=0}}^{\infty} \frac{\sqrt{\langle N\rangle}^{n'}}{\sqrt{n'!}} \langle n' \mid n\rangle \frac{\sqrt{\langle K\rangle}^{n}}{\sqrt{n!}} =$$

$$= \exp\left(-\frac{\left(\sqrt{\langle K\rangle}-\sqrt{\langle N\rangle}\right)^2}{2}\right),$$

$$\left|\langle \alpha \mid \beta\rangle\right|^2 = \exp\left(-\left(\sqrt{\langle K\rangle}-\sqrt{\langle N\rangle}\right)^2\right).$$

Meanwhile, they possess the property of completeness, which allows expanding any state vector in a series over these states:

$$\int |\alpha\rangle\langle\alpha| d^2\alpha = \int \sum_{\substack{n=0\\ n'=0}}^{\infty} \frac{\alpha^n \alpha^{*n'}}{\sqrt{n!}\sqrt{n'!}} |n\rangle\langle n'| e^{-|\alpha|^2} d^2\alpha =$$

$$= \pi \sum_{n=0}^{\infty} \frac{|n\rangle\langle n|}{n!} \Gamma(n+1) = \pi \sum_{n=0}^{\infty} |n\rangle\langle n|.$$

Thus, the completeness property can be written as

$$\frac{1}{\pi}\int |\alpha\rangle\langle\alpha| d^2\alpha = \sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{1}.$$

5. In work [29], it is shown in detail that coherent states minimize the uncertainty relation. In the coordinate representation, where

$$\hat{b}^{\dagger} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{Q} + \frac{\hat{P}}{i\omega m}\right), \hat{b} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{Q} - \frac{\hat{P}}{i\omega m}\right), \Rightarrow$$

$$\Rightarrow \hat{b}^{\dagger} - \hat{b} = -\sqrt{\frac{2\hbar}{m\omega}}\frac{\partial}{\partial Q},$$

the indicated coherent state, taking into account the described unitary transformation, corresponds to the so-called oscillator with a displaced center:

$$\Psi_{\alpha}(Q) = e^{\alpha\left(\hat{b}^{\dagger}-\hat{b}\right)}\psi_0(Q) =$$

$$= e^{-\sqrt{\frac{2\hbar}{m\omega}}\alpha\frac{\partial}{\partial Q}}\psi_0(Q) = \psi_0\left(Q - \sqrt{\frac{2\hbar}{m\omega}}\alpha\right),$$

$$\Psi_{\alpha}(Q) = \psi_0\left(Q + \sqrt{\frac{2\hbar}{m\omega}}\frac{\Lambda}{\hbar\omega}\right).$$

Here, the ground state functions of a harmonic oscillator with frequency ω are denoted as $\psi_0(Q)$, and the coherent state – as

$$\Psi_{\alpha}(Q) = \Psi_{\langle n\rangle}(Q).$$

APPENDIX B.
INTEGRALS

1. Let's consider the high-temperature limit $\hbar\omega / T \sim 1$, $\tau\omega \gg 1$, $\Rightarrow \hbar(\omega\tau) / \tau T \sim 1$. Тогда

$$J = \int_0^{\varpi_D} \langle j\rangle_{\omega}\left(\frac{1}{e^{\hbar\omega/T}-1}\right)d\omega =$$

$$= \hbar\left(\frac{\Lambda_0\tau}{\hbar\pi c_s}\right)^2 \int_0^{\varpi_D}\left\{\frac{1}{\left(1+(\tau\omega)^2\right)^2}\frac{e^{-2t/\tau}}{4\left(1+(\tau\omega)^2\right)}\right\}\times$$

$$\times\left(\frac{1}{e^{\hbar\omega/T}-1}\right)\omega^3 d\omega =$$

$$= I + II(t),$$

$$I = \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{c_s^2}\int_0^{\infty}\left(\frac{1}{e^{\hbar\omega T}-1}\right)\frac{\omega^3}{\left(1+(\tau\omega)^2\right)^2}d\omega =$$

$$= [\tau\omega = x] = \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \times$$

$$\times\frac{\hbar}{\tau^4 c_s^2}\int_0^{\infty}\left(\frac{1}{e^{\hbar x/\tau T}-1}\right)\frac{(x)^3}{\left(1+x^2\right)^2}dx \approx$$

$$\approx \left[x > 1, \frac{\hbar x}{\tau T} < 1\right] \approx$$

$$\approx \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{\tau^4 c_s^2}\frac{T\tau}{\hbar}\int_0^{\infty}\frac{x^2}{\left(1+x^2\right)^2}dx =$$

$$= \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{\tau^4 c_s^2}\frac{T\tau}{\hbar}\left\{-\frac{x}{\left(1+x^2\right)} + \frac{1}{2}x\right\}_0^{\infty} =$$

$$= \frac{\pi}{4}\left(\frac{\Lambda_0}{\pi\hbar}\right)^2 \frac{T}{\tau c_s^2},$$

$$II(t) = \left(\frac{\tau\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{4c_s^2}e^{-2t/\tau}\times$$

$$\times\int_0^{\omega_D}\left(\frac{1}{e^{\hbar\omega/T}-1}\right)\frac{\omega^3}{\left(1+(\tau\omega)^2\right)}d\omega =$$

$$= \left(\frac{\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{4\tau^2 c_s^2} e^{-2t/\tau} \times$$

$$\times \int_0^{\tau\omega_D} \left(\frac{1}{e^{\hbar x/\tau T} - 1}\right) \frac{x^3}{\left(1+x^2\right)} dx \approx$$

$$\approx \left[\tau\omega = x > 1, \frac{\hbar x}{\tau T} < 1\right] \approx \left(\frac{\Lambda_0}{\pi\hbar}\right)^2 \frac{\hbar}{4\tau^2 c_s^2} e^{-2t/\tau} \times$$

$$\times \int_0^{\tau\omega_D} \left(\frac{1}{1 + \frac{\hbar x}{\tau T} - 1}\right) \frac{x^3}{\left(1+x^2\right)} dx =$$

$$= \left(\frac{\Lambda_0}{2\pi\hbar}\right)^2 \frac{T}{2\tau c_s^2} e^{-2t/\tau} \left\{\left(\tau\omega_D\right)^2 - \ln\left(1 + \left(\tau\omega_D\right)^2\right)\right\}.$$

2. Let's examine the internal energy and energy flux of the crystal lattice for free phonons. For comparison, let's present the known expressions for flux density and internal energy for free thermal phonons:

$$J = \frac{2\pi}{3} \frac{g_s c_s}{\left(2\pi c_s\right)^3} \int_0^{\omega_D} \frac{\hbar\omega}{e^{\hbar\omega/T} - 1} \omega^2 d\omega =$$

$$= \frac{2\pi}{3} \frac{g_s c_s}{\left(2\pi\hbar c_s\right)^3} T^4 \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx =$$

$$= \frac{g_s c_s}{2\left(\hbar\omega_D\right)^3} n T^4 \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx,$$

$$\Theta_D = \frac{\hbar\omega_D}{T}.$$

In the low-temperature limit, $\hbar\omega / T = \Theta_D \gg 1$, we have

$$J = c_s n \frac{g_s e_z T^4}{2\left(\hbar\omega_D\right)^3} \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx =$$

$$= c_s n \frac{g_s e_z T^4}{2\left(\hbar\omega_D\right)^3} \int_0^{\infty} \frac{x^3}{e^x - 1} dx =$$

$$= c_s n \frac{g_s e_z T^4}{2\left(\hbar\omega_D\right)^3} T^4 \Gamma(4)\zeta_R(4) = c_s n \frac{\pi^4 T^4}{10\left(\hbar\omega_D\right)^3} e_z,$$

$$U = \frac{3N g_s}{\left(\hbar\omega_D\right)^3} T^4 \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx =$$

$$= \frac{3N g_s}{\left(\hbar\omega_D\right)^3} T^4 \int_0^{\infty} \frac{x^3}{e^x - 1} dx =$$

$$= \frac{3N g_s}{\left(\hbar\omega_D\right)^3} T^4 \Gamma\left(4\right)\zeta_R\left(4\right) = \frac{\pi^4}{5} g_s N \frac{T^4}{\left(\hbar\omega_D\right)^3},$$

$$C_V = \frac{12}{5}\pi^4 N \frac{T^3}{\left(\hbar\omega_D\right)^3}, \quad g_s = 3.$$

Thus, we obtained Debye's law: $C \propto T^3$.

In the high-temperature limit, $\hbar\omega / T = \Theta_D \leq 1$, we have

$$J = c_s n \frac{g_s e_z T^4}{2\left(\hbar\omega_D\right)^3} \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx =$$

$$= c_s n \frac{g_s e_z T^4}{2\left(\hbar\omega_D\right)^3} \int_0^{\Theta_D} \frac{x^3}{1 + x - 1} dx =$$

$$= c_s n \frac{g_s e_z T^4 \Theta_D^3}{6\left(\hbar\omega_D\right)^3} = c_s n \frac{g_s e_z T}{6} = \frac{c_s n T}{2} e_z,$$

$$U = \frac{3N g_s}{\left(\hbar\omega_D\right)^3} T^4 \int_0^{\Theta_D} \frac{x^3}{e^x - 1} dx = N g_s T = 3NT,$$

$$C_V = 3N.$$

Thus, we obtained the Dulong-Petit law.

APPENDIX C

Let's consider the classical heat conduction problem for a semi-infinite medium with boundary conditions of the third kind. For internal energy

$$u = \alpha N k_B T,$$

where $N = nV$ — total number of particles in the system, α — numerical factor (i.e. $u \propto k_B T$), the heat conduction equation takes place

$$\dot{u} - \kappa u'' = f(x,t)$$

with boundary and initial conditions

$$\left.\frac{\partial u}{\partial x}\right|_{x=0} = 0, \quad \left(\frac{\partial u}{\partial x} + hu\right)_{x=l} = 0,$$

$$u(x,0) = \varphi(x) = 0,$$

$$f(x,t) = \frac{\Psi(x,t)}{C_p n} = e^{-\alpha t} f_0 \begin{cases} 1, & x \le x_0, \\ 0, & x > x_0, \end{cases}$$

$$f_0 = \frac{\Psi_0}{C_p n},$$

$$\dot{u} - \kappa u'' = 0, \quad u = X(x)T(t),$$

$$\Rightarrow \frac{\dot{T}(t)}{\kappa T(t)} = \frac{X''(x)}{X(x)} = -\lambda.$$

Here $\kappa = K / C_p n$ — thermal diffusivity coefficient, C_p — dimensionless heat capacity, K [(cm·s)$^{-1}$] — thermal conductivity coefficient, n — concentration. We obtain

$$u(x,t) = \sum_n \frac{2}{\gamma_n} \cos\left(\frac{\gamma_n}{l} x\right) \sin\left(\frac{\gamma_n}{l} x_0\right) \times \frac{1 - \exp\left(-t\left(\kappa\left(\frac{\gamma_n}{l}\right)^2 - \frac{1}{\tau}\right)\right)}{\kappa\left(\frac{\gamma_n}{l}\right)^2 - \frac{1}{\tau}} e^{-\frac{t}{\tau}},$$

where γ_n — solution of the transcendental equation

$$\gamma = \frac{hl}{\gamma} \Rightarrow \gamma_n = b_n l.$$

Heat flux density equals

$$\mathrm{J}(x,t) = -Ke_x \frac{\partial u(x,t)}{\partial x} = e_x \frac{2\kappa\tau}{l} \Psi_0 \sum_n \sin\left(\frac{\gamma_n}{l} x\right) \sin\left(\frac{\gamma_n}{l} x_0\right) \times \frac{1 - \exp\left(-\frac{t}{\tau}\left(\kappa\tau\left(\frac{\gamma_n}{l}\right)^2 - 1\right)\right)}{\kappa\tau\left(\frac{\gamma_n}{l}\right)^2 - 1} e^{-\frac{t}{\tau}}.$$

Taking into account that solutions

$$\gamma_n \to \frac{\pi}{2}(2n+1),$$

energy flux density will equal

$$\mathrm{J}(x,t) \to e_x \frac{2\kappa\tau}{l} \Psi_0 \times \sum_n \sin\left(\frac{\pi}{2}(2n+1)\frac{x}{l}\right) \sin\left(\frac{\pi}{2}(2n+1)\frac{x_0}{l}\right) \times \frac{1 - \exp\left(-\frac{t}{\tau}\left(\kappa\tau\left(\frac{\pi}{2}\frac{(2n+1)}{l}\right)^2 - 1\right)\right)}{\kappa\tau\left(\frac{\pi}{2}\frac{(2n+1)}{l}\right)^2 - 1} e^{-\frac{t}{\tau}}.$$

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