# Renormalized spectrum of a quasiparticle interacting with three-mode phonons in Davydov's model with damping at cryogenic temperature


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## Motivation for the research

The rapid development of nanophysics has significantly actualized the theory of the interaction of systems of multi-band (multi-level) quasiparticles with multi-mode phonons. Such problems are important, in particular, for understanding of the physical processes occurring in nanoheterostructures, which are the basic structural elements of quantum cascade lasers and infrared detectors.

## Theory and analysis of results

We study the influence of dissipative mechanisms (taken into account by phenomenological decay) on the formation of properties of coefficient of the electromagnetic field absorption by localized quasiparticles interacting with one- and two-mode polarization phonons at T = 0K in Davydov's model of the system.

From Kubo's theory [1, 2, 4] about the response of an isotropic system to external action it is known that the absorption coefficient of the electromagnetic field ($\chi(\tilde{\omega})$) is related with the Fourier image of the retarded Green's function $(G(\tilde{\omega}))$ of quasiparticle by the expression

$$\chi(\tilde{\omega}) = \frac{4\pi\hbar\omega_f^2 d^2}{v\omega v_g} \mathrm{I}(\tilde{\omega}); \qquad \mathrm{I}(\tilde{\omega}) = -\mathrm{Im}\, G(\tilde{\omega}); \quad (\tilde{\omega} = \omega + i\eta),\ \eta \to +0. \qquad (1)$$

Here $\mathrm{I}(\tilde{\omega})$ is a function of the shape of the electromagnetic field absorption band, $d = er$ is a dipole moment, $v$ is a unit cell volume, $\omega_f$ is a frequency of dipole transition, $\omega$ is an electromagnetic field frequency, $v_g$ is a group velocity.

Further, studying only the shape of the field absorption band, we consider a system consisting of a localized quasiparticle (exciton, impurity, etc.) interacting with non-dispersive three-mode polarization phonons at T = 0K. The Hamiltonian of this system (excluding dissipative processes) in the representation of occupation numbers over all variables can be written as

$$\hat{\mathrm{H}} = \sum_{\vec{k}} E_0 \hat{A}^+_{\vec{k}} \hat{A}_{\vec{k}} + \sum_{\lambda=1}^{3} \sum_{\vec{q}} \Omega_\lambda \left(\hat{B}^+_{\lambda\vec{q}} \hat{B}_{\lambda\vec{q}} + 1/2\right) + \sum_{\vec{k}\lambda\vec{q}} \varphi_\lambda(\vec{q})\, \hat{A}^+_{\vec{k}} \hat{A}_{\vec{k}} \left(\hat{B}_{\lambda\vec{q}} + \hat{B}^+_{\lambda-\vec{q}}\right). \qquad (2)$$

Here $E_0$ is an energy of uncoupling quasiparticle, $\Omega_\lambda$ is an energy of $\lambda$- th phonon mode, $\varphi_\lambda(\vec{q})$ is a quasiparticle binding function with $\lambda$ -th phonon mode. Quasiparticle $(\hat{A}^+_{\vec{k}}, \hat{A}_{\vec{k}})$ and phonon $(\hat{B}^+_{\lambda\vec{q}}, \hat{B}_{\lambda\vec{q}})$ operators of second quantization satisfy Bose commutative relationships. In Davydov's model for the system under research, it is fulfilled the condition $\hat{n}^2 = \hat{n} = \sum_{\vec{k}} \hat{A}^+_{\vec{k}} \hat{A}_{\vec{k}}$ , which means that the eigenvalues of both of these operators ($\hat{n}$ i $\hat{n}^2$) can be either 1 or 0 , interpreted as a condition of presence (1) or absence (0) of "pure" quasiparticle state.

To calculate the Fourier image of the retarded Green's function without a decay, the Hamiltonian (4) is first diagonalized by the transition from the operators $\hat{A}_{\vec{k}}, \hat{B}_{\lambda\vec{q}}$ to new ones $\hat{a}_{\vec{k}}, \hat{b}_{\lambda\vec{q}}$ using a unitary operator [3]. As a result, the Hamiltonian (2) in the new operators gets a diagonal form

$$\hat{\mathrm{H}} = \sum_{\vec{k}} \mathscr{E} \hat{a}^+_{\vec{k}} \hat{a}_{\vec{k}} + \sum_{\lambda\vec{q}} \Omega_\lambda (\hat{b}^+_{\lambda\vec{q}} \hat{b}_{\lambda\vec{q}} + 1/2); \ \left(\mathscr{E} = E_0 - \sum_{\lambda\vec{q}} \Omega_\lambda^{-1} |\varphi_\lambda(\vec{q})|^2\right), \qquad (3)$$

Where $\mathscr{E}$ is an energy of new elementary excitations.

Now at T = 0K the two-time retarded Green's function

$$G(\vec{k}, t) = -i\theta(t) \left\langle 0 \left| [\hat{A}^+_{\vec{k}}(t), \hat{A}_{\vec{k}}(0)] \right| 0 \right\rangle, \qquad (4)$$

taking into account the Hamiltonian (3), the relationship between old and new operators and using Weyl operator identity [1,2], the exact expression is obtained

$$G(\vec{k}, t) = -i\theta(t) \exp\left\{-\frac{i\mathscr{E}t}{\hbar} + \sum_{\lambda=1}^{2} \alpha_\lambda \left\{\exp\left(-\frac{i\Omega_\lambda t}{\hbar}\right) - 1\right\}\right\}; \ \alpha_\lambda = \Omega_\lambda^{-2} \sum_{\vec{q}} |\varphi_\lambda(\vec{q})|^2, \qquad (5)$$

where $\alpha_\lambda$ is a dimensionless parameter characterizing the binding energy of a quasiparticle with $\lambda$ -th mode of phonons.

The integration of expression (5) is performed exactly. Introducing phenomenological decay by replacing a small value ( $\gamma > 0$ ) by a finite value ( $\eta \to +0$) a representation of the Fourier image of the retarded Green's function is obtained, which is convenient for physical analysis, from which the shape function is obtained in the form

$$\begin{aligned} I_3(\alpha_1; \alpha_2; \alpha_3; \xi) = \gamma e^{-\alpha} \Bigg\{ & \frac{1}{\xi^2 + \gamma^2} + \sum_{\lambda=1}^{3} \sum_{n_\lambda=1}^{\infty} \frac{\alpha_\lambda^{n_\lambda}}{n_\lambda! [(\xi - n_\lambda P_\lambda)^2 + \gamma^2]} + \\ & \sum_{n_1, n_2=1}^{\infty} \frac{\alpha_1^{n_1} \alpha_2^{n_2}}{n_1! n_2! [(\xi - n_1 - n_2 P_2)^2 + \gamma^2]} + \sum_{n_1, n_3=1}^{\infty} \frac{\alpha_1^{n_1} \alpha_3^{n_3}}{n_1! n_3! [(\xi - n_1 - n_3 P_3)^2 + \gamma^2]} + \\ & + \sum_{n_2, n_3=1}^{\infty} \frac{\alpha_2^{n_2} \alpha_3^{n_3}}{n_2! n_3! [(\xi - n_2 P_2 - n_3 P_3)^2 + \gamma^2]} + \\ & + \sum_{n_1, n_2, n_3=1}^{\infty} \frac{\alpha_1^{n_1} \alpha_2^{n_2} \alpha_3^{n_3}}{n_1! n_2! n_3! [(\xi - n_1 - n_2 P_2 - n_3 P_3)^2 + \gamma^2]} \Bigg\}. \end{aligned} \qquad (6)$$

Here are some convenient denominated variables and parameters

$$I(\xi) = \Omega_1 \mathrm{I}(\omega); \quad \gamma = \frac{\Gamma}{\Omega_1}; \ \alpha = \sum_{\lambda=1}^{3} \alpha_\lambda; \quad P_\lambda = \frac{\Omega_\lambda}{\Omega_1}; \quad (\lambda = 1,2,3) \qquad (7)$$

Similar to the case of the two-mode phonons [3], as well as for the three-mode ones, the calculation and analysis of the properties of the shape functions $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ is performed for the example of the system with typical parameters indicated in Figure 1. Frequency domain ($\xi$), in which the main and satellite peaks are well identified without "merging" with the background, the same as in the two-mode system [3].

Figure 1 shows that the peaks of phonon satellites of all modes are best manifested at small decay values ( $\gamma$) , and with its increase, they quickly disappear either in the general background or in peaks of degenerate states.

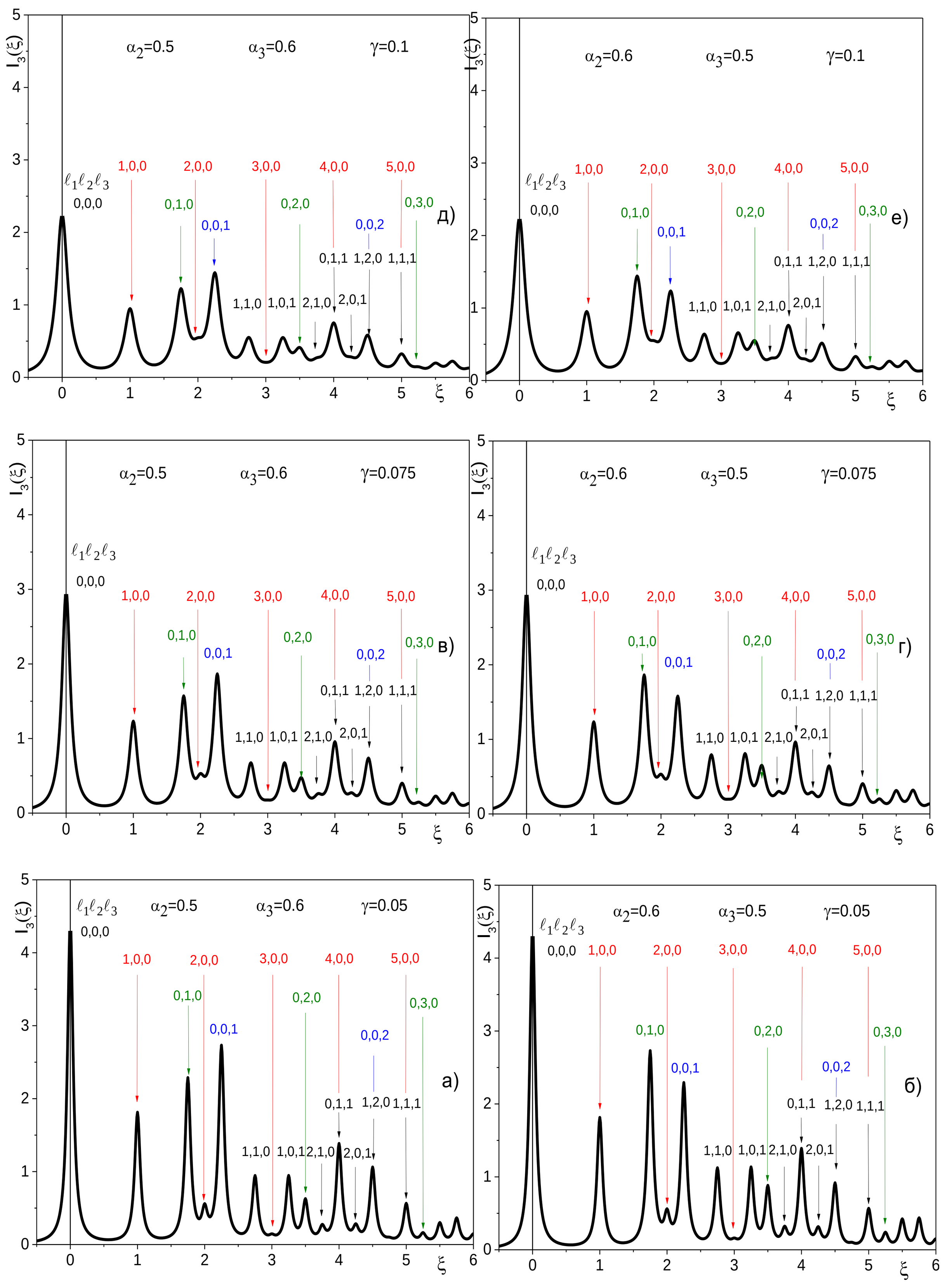


Figure 1. Evolution of the function $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ at fixed values P1=1; P2=1.75; P3=2.25; and different sizes $\alpha_2, \alpha_3, \gamma$ , indicated in the panels of the figure.

The properties of the lower part of the spectrum are best displayed on the example of panels (a, b) of Figure 1 at the smallest decay ($\gamma = 0.05$ ).

So, functions $I_3(\xi)$ in Figures 1a and 1b differ from each other (like the other two pairs) only by the replacement of values ($\alpha_2 \longleftrightarrow \alpha_3$) with the same other parameters.

For clarity and understanding of the analysis of the properties of the functions $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ according to the Figs. 1 a, b, Table 1 shows the calculated values of the coordinates ( $\xi_{\ell_1, \ell_2, \ell_3}$ ) and height ( $h_{\ell_1, \ell_2, \ell_3}$) of function peaks $I_3(\xi)$ depending on the phonon modes ($\lambda = 1, 2, 3$) and numbers of the ground and satellite states $(\ell_1, \ell_2, \ell_3)$.

Table 1.

Dependencies of coordinates ( $\xi_{\ell_1, \ell_2, \ell_3}$ ) and heights ( $h_{\ell_1, \ell_2, \ell_3}$ ) of function peaks ( $I_3(\xi)$) at ( $\gamma = 0.05$) fixed values P1=1; P2=1.75; P3=2.25; $\alpha_1 = 0.4$ and different values $\alpha_2, \alpha_3, \gamma$ indicated in the panels of Figure 1.

| $\ell_1, \ell_2, \ell_3$ | | 000 | 100 | 200 | 300 | 400 | 500 |
|---|---|---|---|---|---|---|---|
| $h_{\ell_1, \ell_2, \ell_3}$ | а | 4.471 | 1.813 | 0.56 | 0.146 | 1.385 | 0.565 |
| | б | 4.471 | 1.8150 | 0.562 | 0.161 | 1.39 | 0.569 |
| $\xi_{\ell_1, \ell_2, \ell_3}$ | а, б | 0 | 1 | 2 | 3 | 4 | 5 |
| $\ell_1, \ell_2, \ell_3$ | | 010 | 020 | 030 | 001 | 002 | 111 |
| $h_{\ell_1, \ell_2, \ell_3}$ | а | 2.28 | 0.629 | 0.164 | 2.733 | 1.062 | 0.565 |
| | б | 2.731 | 0.883 | 0.241 | 2.293 | 0.918 | 0.569 |
| $\xi_{\ell_1, \ell_2, \ell_3}$ | а, б | 1.75 | 3.5 | 5.25 | 2.25 | 4.5 | 5 |
| $\ell_1, \ell_2, \ell_3$ | | 110 | 101 | 210 | 201 | 011 | 120 |
| $h_{\ell_1, \ell_2, \ell_3}$ | а | 0.946 | 0.947 | 0.277 | 0.285 | 1.385 | 1.062 |
| | б | 1.124 | 1.136 | 0.324 | 0.317 | 1.39 | 0.918 |
| $\xi_{\ell_1, \ell_2, \ell_3}$ | а, б | 2.75 | 3.25 | 3.75 | 4.25 | 4 | 4.5 |

Figures 1 a, b and Table 1 show the following properties of the shape function $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ . Its shape is determined by the superposition of three groups (respectively to the number of modes) of an infinite number of renormalized peaks. The peaks of the function in Figure 1 and their parameters in Table 1 are indicated by colored groups of numbers ( $\ell_1 \ell_2 \ell_3$ ) , to distinguish the mixed and unmixed states, which form the corresponding peaks.

The first peak corresponds to the ground (phononless) state of the system (000). Next, we highlight three groups of an infinite number of peaks, which are formed by unmixed single-mode satellite states of each individual mode, marked with the following colors: ( $\ell_1 00$ ) – red, ( $0 \ell_2 0$) – green, ($00 \ell_3$ ) – blue. All the remaining peaks are formed by mixed two-mode ($\ell_1 \ell_2 0$), ( $\ell_1 0 \ell_3$ ), ( $0 \ell_2 \ell_3$) and mixed three-mode ( $\ell_1, \ell_2, \ell_3$ ) satellite states and are marked in black. Satellite peaks are formed by two types of states: a) non-degenerate (untoned in Table 1), b) degenerate (toned in Table 1).

The peaks of the function $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ are formed by the non-degenerate states of each individual mode ( $\lambda$ ), with an increase in the number of $\ell_\lambda$ only rapidly decrease, and the peaks formed by the degenerate states change differently, since their values are formed by the components of states from three modes, the heights of which depend both on the values of $\alpha_\lambda$ , as well as on the values $\Omega_\lambda$ . Generally, with increasing energies ( $\xi$ ), the average peak intensity decreases. This is due to the decreasing effects on the function $I_3(\alpha_1, \alpha_2, \alpha_3; \xi)$ of multiphonon processes due to the interaction of a quasiparticle with phonons of all modes.

## Conclusions

1. On the basis of the Frohlich-type Hamiltonian, which describes a localized quasiparticle interacting with three-mode dispersionless phonons in the Davydov's model with decay at T=0K, an analytical Fourier calculation of the image of the retarded Green's function was performed. It made possible to obtain and analyze the frequency dependence of its imaginary part, which characterizes the shape function of the absorption band and its spectral parameters.
2. It is shown that the three-mode system has a complex structure of the absorption band shape-function, which is a superposition of Lorentzian peaks corresponding to the three groups of unmixed phonon modes and peaks of all possible combinations of their satellite states.

## References


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