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Polarization operator of phonons in quadratic approximation

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Abstract. Using the method of the retarded Green function the polarization operator of phonons has been calculated with the simultaneous account for the linear and quadratic terms in the Hamilton operator of exciton-phonon interaction. It is shown that at high temperatures and concentrations of excitons the quadratic term may play as important role as linear one.

Keywords: polarization operator, Green function, decoupling.

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1. Introduction

The influence of phonons on various processes in solids [1] in particular on the excitonic ones is studied for a long time [2]. Theoretically it will be carried out more often using Green functions (GFs) as a mathematical tool. Though the various calculation methods of GFs for quasiparticles interacting with phonons are well developed and widely presented in the literature, study of concrete systems frequently requires additional researches. Such necessity arises, in particular, when the Hamiltonian of system is complex, and GF it is necessary to be found in higher than in a first-order approximation, or sometimes in any order of a perturbation theory (PT).

Except for a usual broadening [3], the phonons become apparent to such phenomena as splitting of exciton lines in some materials [4], hierarchy of electronic density [5], coupling with another phonons in superconductors [6, 7], electron correlation [8], etc. The interpretation of these effects is more often impossible within the framework of linear approach on the operators of exciton-phonon interaction.

The importance of the account of square-law interaction was specified earlier in the works [9-14]. In [9, 10] basing on bilinear interaction with phonons the most common estimations of the spectral characteristics were only made. Tkach [13] was the first who accentuated that in the case of weak coupling, when calculating GF, it is impossible to be restricted to the first order of PT, because the contributions from the linear and bilinear terms may differ by signs and be comparable with the contributions of the higher orders, instead of exceeding them. In [14] the quadratic term was accounted for the estimation of temperature shift of exciton bands of absorption in the frame of momenta method.

However absence of reliable models, in which such interaction strictly appeared in a Hamiltonian found from the first principles, resulted in the fact that in the theory of excitons for a long time it was not paid necessary attention. There is no reason to neglect this contribution ad hoc.

The purpose of this work was to conduct a careful study about the contribution of bilinear term of exciton-phonon interaction in the polarization operator of phonons.

2. Basic equations

Let's consider an ideal crystal, as system of the periodically placed quantum oscillators, in which during irradiation by light the excitons can be created. Owing to scattering on a phonon subsystem the time of their life is limited. Let's count, that the movement of an exciton in the phonon bath remains coherent and can be described by a Bloch wave. Thus, the exited states of a crystal one can consider as the system of excitons and phonons interacting among themselves. In case, when this interaction is possible to regard as weak, the most important role will be played by few-phonon processes, and the Hamiltonian of such system in the notation of second quantization can be written as follows:

$$H = H_{ex} + H_{ph} + H_{int} \qquad (1)$$

where

$$H_{ex} = \sum_{\mu,\mathbf{k}} E_\mu(\mathbf{k})\, \hat{a}^+_{\mu,\mathbf{k}} \hat{a}_{\mu,\mathbf{k}} \tag{2}$$

is operator of excitons energy in an ideal lattice;

$$H_{ph} = \sum_{\mathbf{q}s} \Omega_s(\mathbf{q}) \left(\hat{b}^+_{\mathbf{q}s} \hat{b}_{\mathbf{q}s} + \frac{1}{2} \right) \tag{3}$$

is operator of phonons energy;

$$\begin{aligned} H_{int} = &\sum_{\mu\mathbf{k},s\mathbf{q}} \varphi_s(\mathbf{q}) \hat{a}_{\mu,\mathbf{k}+\mathbf{q}} \hat{a}_{\mu,\mathbf{k}} \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right) + \\ &+ \sum_{\begin{pmatrix} \mu\mu_1, ss_1, \\ \mathbf{k},\mathbf{q},\mathbf{q}_1 \end{pmatrix}}{}' \Phi_{\mu\mu_1, ss_1}(\mathbf{q},\mathbf{q}_1)\, \hat{a}^+_{\mu,\mathbf{k}+\mathbf{q}+\mathbf{q}_1} \hat{a}_{\mu_1,\mathbf{k}} \times \\ &\times \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right)\left(\hat{b}_{\mathbf{q}_1 s_1} + \hat{b}^+_{-\mathbf{q}_1 s_1}\right), \end{aligned} \tag{4}$$

refers the operator of interaction excitons with phonons, accounting for the first two terms of expanding of their energy interaction into a series in deviation of atoms from an equilibrium state. The prime in the last sum means, that the summation is taken over all sets $s \neq s_1$, and $\mathbf{q} \neq \mathbf{q}_1$. In Eq. (4) we adopt the next notations as well: $E_\mu(\mathbf{k})$ is the energy of an exciton of μ-th zone with a quasi-momentum $\mathbf{k}$; $\varphi_s(\mathbf{q})$ denotes the linear and Φ – quadratic functions of exciton-phonon coupling; $\Omega_s(\mathbf{q})$ is the energy of phonons of s-th branch with a quasi-momentum $\mathbf{q}$; $\hat{a}^+, \hat{a}$ and $\hat{b}^+, \hat{b}$ are, respectively, the operators of creation and annihilation of both the excitons and phonons which obey Bose commutation relations.

The mean value of occupation numbers of phonon states due to their interaction with excitons are changed. The magnitude of this change is possible to be calculated by various methods [15]. At final temperatures it is convenient to take an advantage of retarded Green functions technique, which permits analytical continuation in complex plane. As it has been shown by Bogoljubov and Tjablikov [16], such functions satisfy to an infinite chain of the coupled equations, which should be solved self-consistently. The search for the solution of such set of equations is usually reduced to search for the conditions for which it is possible to break a chain, and thus to get the finite set of equations.

The technique of deriving GF on an example of calculation of phonon Green function for systems Hamiltonian of which contains simultaneously the linear and square-law terms on the operators of exciton-phonon interaction we shall demonstrate below.

Let's write down the equation of movement for operators $\hat{a}_{\mu,\mathbf{k}}, \hat{a}^+_{\mu,\mathbf{k}}, \hat{b}_{\mathbf{q}s}, \hat{b}^+_{-\mathbf{q}s}$.

In accordance with the Heisenberg representation, the change in time of the any operator $\hat{F}$ is determined by the equation:

$$i\hbar \frac{d\hat{F}}{dt} = \left[\hat{F}, \hat{H}\right], \tag{5}$$

where $\hat{H}$ is the Hamilton operator of the system.

Proceeding from this and using the Hamiltonian (1) it is easy to obtain

$$\begin{cases} i\hbar \dfrac{d}{dt} \hat{a}_{\mu,\mathbf{k}} = E_{\mu,\mathbf{k}} \hat{a}_{\mu,\mathbf{k}} + \\ + \sum_{\mu_1, s\mathbf{q}} \varphi_{\mu\mu_1}(s\mathbf{q}) \hat{a}_{\mu_1,\mathbf{k}-\mathbf{q}} \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right) + \\ + \sum'_{\begin{pmatrix} \mu_1, ss_1, \\ \mathbf{q},\mathbf{q}_1 \end{pmatrix}} \Phi_{\mu\mu_1}(s\mathbf{q}, s_1\mathbf{q}_1) \hat{a}_{\mu_1,\mathbf{k}-\mathbf{q}-\mathbf{q}_1} \times \\ \qquad \times \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right)\left(\hat{b}_{\mathbf{q}_1 s_1} + \hat{b}^+_{-\mathbf{q}_1 s_1}\right); \\ \hbar \dfrac{d}{dt} \hat{a}^+_{\mu,\mathbf{k}} = -E_{\mu,\mathbf{k}} \hat{a}^+_{\mu,\mathbf{k}} - \\ - \sum_{\mu_1, s\mathbf{q}} \varphi_{\mu\mu_1}(s\mathbf{q}) \hat{a}^+_{\mu_1,\mathbf{k}+\mathbf{q}} \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right) + \\ + \sum'_{\begin{pmatrix} \mu_1, ss_1, \\ \mathbf{q},\mathbf{q}_1 \end{pmatrix}} \Phi_{\mu\mu_1}(s\mathbf{q}, s_1\mathbf{q}_1) \hat{a}^+_{\mu_1,\mathbf{k}+\mathbf{q}+\mathbf{q}_1} \times \\ \qquad \times \left(\hat{b}_{\mathbf{q}s} + \hat{b}^+_{-\mathbf{q}s}\right)\left(\hat{b}_{\mathbf{q}_1 s_1} + \hat{b}^+_{-\mathbf{q}_1 s_1}\right), \end{cases} \tag{6}$$

where the functions φ and Φ satisfy next conditions

$$\begin{aligned} &\varphi_{\mu\mu_1}(\mathbf{q}s) = \varphi^+_{\mu\mu_1}(-\mathbf{q}s), \\ &\Phi_{\mu\mu_1}(\mathbf{q}s, \mathbf{q}_1 s_1) = \Phi^+_{\mu\mu_1}(-\mathbf{q}s, -\mathbf{q}_1 s_1), \end{aligned} \tag{7}$$

which follow from a hermicity of the operator of exciton-phonon interaction.

The equation of movement for the operators $\hat{b}, \hat{b}^+$ look like:

$$\begin{cases} i\hbar \dfrac{d}{dt} \hat{b}_{\mathbf{q}s} = \Omega_s(\mathbf{q}) \hat{b}_{\mathbf{q}s} + \sum_{\mu\mu_1, \mathbf{k}} \varphi_{\mu\mu_1}(-s\mathbf{q}) \hat{a}^+_{\mu,\mathbf{k}-\mathbf{q}} \hat{a}_{\mu_1,\mathbf{k}} + \\ + 2 \sum'_{\begin{pmatrix} \mu\mu_1, \\ s_1\mathbf{k} \end{pmatrix}} \Phi_{\mu\mu_1}(s, -\mathbf{q}, s_1, -\mathbf{q}_1) \hat{a}^+_{\mu,\mathbf{k}-\mathbf{q}-\mathbf{q}_1} \hat{a}_{\mu_1,\mathbf{k}} \times \\ \times \left(\hat{b}_{-\mathbf{q}_1 s_1} + \hat{b}^+_{\mathbf{q}_1 s_1}\right), \\ i\hbar \dfrac{d}{dt} \hat{b}^+_{\mathbf{q}s} = -\Omega_s(\mathbf{q}) \hat{b}^+_{\mathbf{q}s} - \sum_{\mu\mu_1, \mathbf{k}} \varphi_{\mu\mu_1}(s\mathbf{q}) \hat{a}^+_{\mu,\mathbf{k}+\mathbf{q}} \hat{a}_{\mu_1,\mathbf{k}} - \\ - \sum'_{\begin{pmatrix} \mu\mu_1, \\ s_1\mathbf{k}' \end{pmatrix}} \Phi_{\mu\mu_1}(s\mathbf{q}, s_1\mathbf{q}_1) \hat{a}^+_{\mu,\mathbf{k}+\mathbf{q}+\mathbf{q}_1} \hat{a}_{\mu_1,\mathbf{k}} \left(\hat{b}_{\mathbf{q}_1 s_1} + \hat{b}^+_{-\mathbf{q}_1 s_1}\right) \end{cases} \tag{8}$$

where

$$\Omega_s(\mathbf{q}) = \Omega_s(-\mathbf{q}). \tag{9}$$

The retarded Green function of phonons is given by

$$\mathcal{D}_r(s\mathbf{q}, t) = -i\hbar\Theta(t) << [\hat{b}_{\mathbf{q}s}(t), \hat{b}^+_{\mathbf{q}s}(0)] >>. \tag{10}$$

The angular brackets symbolize an average over the phonon distribution in energy. Let's derive the equation of movement for $\mathcal{D}_r$. Making use of Eq. (8), as well as relationship

$$\frac{\partial}{\partial t}\Theta(t) = \delta(t) \tag{11}$$

we find

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\mathcal{D}_r(s\mathbf{q},t) &= \delta(t) + \Omega_s(\mathbf{q})\mathcal{D}_r(s\mathbf{q},t) + \\ &+ \sum_{\mu\mu_1\mathbf{k}}\varphi_{\mu\mu_1\mathbf{k}}(-\mathbf{q}s)G_1(\mathbf{k}-\mathbf{q},\mathbf{k};s\mathbf{q}\,|\,t) + \\ &+ 2\sum_{\begin{pmatrix}\mu\mu_1\mathbf{k}\\ s_1\mathbf{q}_1\end{pmatrix}}{}^{'}\Phi_{\mu\mu_1}(-\mathbf{q}s,-\mathbf{q}_1s_1)\big[G_2(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k},\mathbf{q}_1s_1;\mathbf{q}s\,|\,t) + \\ &+ G_3(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k},-\mathbf{q}_1s_1;\mathbf{q}s\,|\,t)\big]. \end{aligned} \tag{12}$$

The right-hand part of Eq. (12) includes Green functions of the higher order than that of the initial function, namely

$$\begin{cases} G_1(\ldots) = -i\hbar\Theta(t) << [\hat{a}^+_{\mathbf{k}-\mathbf{q}}(t)\hat{a}_{\mathbf{k}}(t), b^+_{\mathbf{q}s}(0)] >>, \\ G_2(\ldots) = -i\hbar\Theta(t) << [\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}(t)\hat{a}_{\mathbf{k}}(t)\hat{b}^+_{\mathbf{q}_1s_1}(t), b^+_{\mathbf{q}s}(0)] >>, \\ G_3(\ldots) = -i\hbar\Theta(t) << [\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}(t)\hat{a}_{\mathbf{k}}(t)\hat{b}_{-\mathbf{q}_1s_1}(t), b^+_{\mathbf{q}s}(0)] >>. \end{cases} \tag{13}$$

Regarding the overlap of separate zones as weak, further we shall omit the summation over symbols μ and μ_1. For the sake of brevity we shall eliminate also argument t in the operators located more to the left of a point. Let us differentiate the expression (13) with respect to time, accounting for the Eqs. (6), (8). Because some cumbersome, we bring below only the equation of movement for one of functions (13), namely for G_2 function.

The terms within the angular brackets are Green functions of the higher order for which, in turn, it is necessary to write the equations of movement, etc. There are no basic difficulties in this sense, but in connection with fast growth of number of the operators and their mixing the record of the equation already at the third stage of differentiation becomes difficult for intelligent perception. However, using the commutation relations, it is always possible to reduce the GF with the mixed phonon operators to the function, in which all operators with «+» like b_s^+ will be placed more to the left hand side of the allocated operators b_s, and on the contrary. According to the terminology offered in [18], first function is named as left-hand side ordered, and the second one — as right-hand side ordered GFs. Thus, it is possible to express the derivative of the function of any order (certain type) with respect to time, through the appropriate functions of the lower orders (the same, or that and another types). For functions of the higher order, it results in the infinite chain (or set of the equation), accurate solution of which cannot be done analytically. For its approximate solution, it is necessary somehow to get the restricted set of the equations. It is achieved just by decoupling a GF of the high or-der on a GFs of the lower orders. The correctness of such procedure realization which, clearly, to the certain extent is arbitrary [19-21], may be attained by meeting the demands of the Wick theorem for correlation functions in the limit of vanishing coupling when interactions in system $(\varphi,\Phi \to 0)$ tend to zero. To such demands just satisfies a method of decoupling symmetric over all operators proposed by Lubchenko, Nitsovich and Tkach [18].

To get the equation for determination of $\mathcal{D}_r(s\mathbf{q},t)$ we execute procedure of pairing of the operators under the average sign,basing on the Wick theorem for the quantum averages and making use the mentioned «symmetrical» method. Let's show it on an example of the function included in the equation for G_2

$$\begin{aligned} i\hbar\frac{\partial G_2}{\partial t} &= \delta(t)\hbar << \left[\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\hat{a}_{\mathbf{k}}\hat{b}^+_{\mathbf{q}_1s_1}, \hat{b}^+_{\mathbf{q}s}(0)\right] >> + \left[E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \Omega_{s_1}(\mathbf{q}_1)\right]G_2 - \\ &- i\hbar\Theta(t)\Bigg\{-\sum_{s_2\mathbf{q}_2}\varphi_{s_2}(\mathbf{q}_2) << \left[(\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1+\mathbf{q}_2}\hat{a}_{\mathbf{k}} - \hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\hat{a}_{\mathbf{k}-\mathbf{q}_2})(\hat{b}_{\mathbf{q}_2s_2} + \hat{b}^+_{-\mathbf{q}_2s_2})\hat{b}^+{}_{\mathbf{q}_1s_1}, \hat{b}^+_{\mathbf{q}s}(0)\right] >> - \\ &- \sum_{(s_2\mathbf{q}_2,s_3\mathbf{q}_3)}{}^{'}\Phi_{s_2,s_3,}(\mathbf{q}_2,\mathbf{q}_3) << \left[(\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3}\hat{a}_{\mathbf{k}} - \hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\hat{a}_{\mathbf{q}-\mathbf{q}_2-\mathbf{q}_3})\times\right. \\ &\left.\times(\hat{b}_{\mathbf{q}_2s_2} + \hat{b}^+_{-\mathbf{q}_2s_2})(\hat{b}_{\mathbf{q}_3s_3} + \hat{b}^+_{-\mathbf{q}_3s_3})\hat{b}^+_{-\mathbf{q}_1s1}, \hat{b}^+_{\mathbf{q}s}(0)\right] - \sum_{\mathbf{k}_1}\varphi_{s1}(\mathbf{q}_1) << \left[\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k}_1+\mathbf{q}_1}\hat{a}_{\mathbf{k}_1}, \hat{b}^+_{\mathbf{q}s}(0)\right] >> - \\ &- 2\sum_{(s_2\mathbf{q}_2,\mathbf{k})}{}^{'}\Phi_{s_1,s_2}(\mathbf{q}_1,\mathbf{q}_2) << \left[\hat{a}^+_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k}_1+\mathbf{q}_1+\mathbf{q}_2}\hat{a}_{\mathbf{k}_1}, (\hat{b}_{\mathbf{q}_2s_2} + \hat{b}^+_{-\mathbf{q}_2s_2})\hat{b}^+_{\mathbf{q}s}(0)\right] >> \Bigg\}. \end{aligned} \tag{14}$$

$$-i\hbar\Theta(t)<<\left[\hat{a}^{+}_{\mathbf{k-q-q_1}}\hat{a}_{\mathbf{k-q_2-q_3}}\hat{b}_{\mathbf{q_2}s_2}\hat{b}_{\mathbf{q_3}s_3}\hat{b}^{+}_{\mathbf{q_1}s_1},\hat{b}^{+}_{\mathbf{q}s}(0)\right]>>\approx$$
$$\approx -i\hbar\Theta(t)<<\hat{b}_{\mathbf{q_2}s_2}\hat{b}^{+}_{\mathbf{q_1}s_1}>>\times$$
$$\times<<\left[\hat{a}^{+}_{\mathbf{k-q-q_1}}\hat{a}_{\mathbf{k-q_2-q_3}}\hat{b}_{\mathbf{q_3}s_3},\hat{b}^{+}_{\mathbf{q}s}(0)\right]>>-$$
$$-i\hbar\Theta(t)<<\hat{b}_{\mathbf{q_3}s_3}\hat{b}^{+}_{\mathbf{q_1}s_1}>>\times$$
$$\times<<\left[\hat{a}^{+}_{\mathbf{k-q-q_1}}\hat{a}_{\mathbf{k-q_2-q_3}}\hat{b}_{\mathbf{q_2}s_2},\hat{b}^{+}_{\mathbf{q}s}(0)\right]>>=$$
$$=\left(1+\bar{\nu}_{\mathbf{q_1}s_1}\right)\delta_{s_1,s_2}\delta_{\mathbf{q_1q_2}}G_3(\mathbf{k-q-q_1},\mathbf{k-q_2-q_3},s_3\mathbf{q_3};s\mathbf{q})+$$
$$+\left(1+\bar{\nu}_{\mathbf{q_1}s_1}\right)\delta_{s_1,s_3}\delta_{\mathbf{q_1q_3}}G_3(\mathbf{k-q-q_1},\mathbf{k-q_2-q_3},s_2\mathbf{q_2};s\mathbf{q}), \quad (15)$$

where

$$\bar{\nu}_{qs}=<<\hat{b}^{+}_{\mathbf{q}s}\hat{b}_{\mathbf{q}s}>>\equiv-\frac{1}{\pi}\int_{-\infty}^{\infty}\partial\omega\frac{\Im\mathscr{D}(s,\omega)}{e^{\frac{\omega}{k_BT}}-1} \quad (16)$$

is the mean number of phonons in the $s\mathbf{q}$ state. Proceeding from the proof executed in [17], according to which a statistical average for product of odd number of the phonon operators is infinitesimal quantity, we have neglected contributions from terms containing the following averages:

$$<<\hat{b}_{\mathbf{q_1}s_1}>>,\quad <<\hat{b}^{+}_{\mathbf{q_1}s_1}>>,\quad <<\hat{b}_{\mathbf{q_1}s_1}\hat{b}_{\mathbf{q_2}s_2}\hat{b}_{\mathbf{q_3}s_3}>>,$$
$$<<\hat{b}^{+}_{\mathbf{q_1}s_1}\hat{b}^{+}_{\mathbf{q_2}s_2}\hat{b}^{+}_{\mathbf{q_3}s_3}>>,..., \quad (17)$$

Upon performing the similar decoupling with respect to all averages included in Eq.(14), we have obtained the following equation of movement for G_2 Green function:

$$i\hbar\frac{\partial G_2(s_1\mathbf{q_1})}{\partial t}=\left(E_{\mathbf{k}}-E_{\mathbf{k-q-q_1}}-\Omega_{s_1}(\mathbf{q_1})\right)G_2(s_1\mathbf{q_1})+$$
$$+\varphi_{s_1}(\mathbf{q_1})\left[(\bar{\nu}_{\mathbf{q_1}s_1}-\bar{n}_{\mathbf{k}})G_1(\mathbf{k-q-q_1},\mathbf{k-q_1};\mathbf{q}s)-\right.$$
$$-(1+\bar{\nu}_{\mathbf{q_1}s_1}+\bar{n}_{\mathbf{k-q-q_1}})G_1(\mathbf{k-q},\mathbf{k};\mathbf{q}s)-$$
$$-\delta_{\mathbf{q_1},0}\bar{N}G_1(\mathbf{k-q-q_1},\mathbf{k};\mathbf{q}s)-n_{\mathbf{k}}\delta_{s,s_1}\delta_{\mathbf{q},\mathbf{q_1}}\times$$
$$\left.\times\sum_{\mathbf{k_1}}G_1(\mathbf{k+q_1},\mathbf{k_1};\mathbf{q}s)\right]+2(\bar{\nu}_{\mathbf{q_1}s_1}-\bar{n}_{\mathbf{k}})\times$$
$$\times\sum_{s_2\mathbf{q_2}}{}'\Phi_{s_1,s_2}(-\mathbf{q_1},-\mathbf{q_2})\left[G_3(\mathbf{k-q-q_1},\mathbf{k-q_1+q_2},-\mathbf{q_2}s_2;\mathbf{q}s)+\right.$$
$$\left.+G_2(\mathbf{k-q-q_1},\mathbf{k-q_1+q_2},\mathbf{q_2}s_2;\mathbf{q}s)\right]-$$
$$-2(1+\bar{\nu}_{\mathbf{q_1}s_1}+\bar{n}_{\mathbf{k-q-q_1}})\times$$
$$\times\sum_{s_2\mathbf{q_2}}{}'\Phi_{s_1,s_2}(\mathbf{q_1},-\mathbf{q_2})\left[G_3(\mathbf{k-q-q_2},\mathbf{k},-\mathbf{q_2}s_2;\mathbf{q}s)+\right.$$
$$\left.+G_2(\mathbf{k-q-q_2},\mathbf{k},\mathbf{q_2}s_2;\mathbf{q}s)\right]-$$
$$-2\bar{n}_{\mathbf{k}}\sum_{s_2\mathbf{q_2},\mathbf{k_1}}{}'\Phi_{s_1,s_2}(-\mathbf{q_1},-\mathbf{q_2})\delta_{s,s_1}\delta_{\mathbf{q},-\mathbf{q_1}}\times$$
$$\times\left[G_3(\mathbf{k+q_1-q_2},\mathbf{k_1},-\mathbf{q_2}s_2;\mathbf{q}s)+\right.$$
$$\left.+G_2(\mathbf{k_1+q_1-q_2},\mathbf{k_1},\mathbf{q_2}s_2;\mathbf{q}s)\right] \quad (18)$$

The equation for functions G_1 and G_3 can be found similarly.

Replacing now in Eq. (18) the difference of quasi-momenta $\mathbf{k-q-q_1}$ by $\mathbf{k-q}$ as well as $\mathbf{k}$ in equations for both the G_1 and G_3 by $\rightarrow\mathbf{k+q_1}$ we can easily find the equation of movement for the rest Green functions $G_{2'}(\mathbf{k-q},\mathbf{k+q_1},\mathbf{q_1}s_1;\mathbf{q}s)$ and $G_{3'}(\mathbf{k-q},\mathbf{k+q_1},-\mathbf{q_1}s_1;\mathbf{q}s)$. Hence, we get the closed set of five linear differential equations.

If one take into account that the Fourier transformation for Green functions and for the delta-function has a form:

$$\mathscr{D}_r(s\mathbf{q},t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathscr{D}_r(s\mathbf{q},q_0)e^{-iq_0t}dq_0, \quad (19)$$

$$G_i(s\mathbf{q},t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}G_i(s\mathbf{q},q_0)e^{-iq_0t}dq_0, \quad (20)$$

$$\delta(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}e^{-iq_0t}dq_0, \quad (21)$$

than one can be passed to the set of equations for determination of Fourier-images. Owing to dependence on quasi-momenta this set still remains rather difficult and cannot be exactly solved. But, after procedure of decoupling, which itself is the certain approximation, there is no necessity in it. To solve this set of equations, it is more meaningful to keep only that accuracy, which does not exceed accuracy of the decoupling procedure.

Natural way for the solution is the iterative method, and the criterion of reasonable number of iterations (at the chosen order of the splitted GFs) can be provided with exact equality [18]: $G^{(s_1,-s_2)}_{2[1\,1]}G^{(-s_2,s_1)}_{2[1\,1]}=G(k)\delta_{s_1,-s_2}$, which follows from commutation relations for the phonon operators. In the case of excess of justified number of iterations this relation is carried out not so strictly, but accurate within the terms of higher orders in a coupling function. For the solution of the mentioned set of five equations there are enough of two iterations.

We arrange Green function $\mathscr{D}_r(s\mathbf{q})$ in expressions for G_3, $G_{3'}$ and in the first iteration we shall neglect by the terms with summation over $s_2\mathbf{q_2}$. Then the Fourier-component for it can be obtained from the equation:

$$q_0\mathscr{D}_r(s\mathbf{q})=1+\Omega_{s\mathbf{q}}\mathscr{D}_r(s\mathbf{q})+\sum_{\mathbf{k}}\varphi_s(-\mathbf{q})G_1(\mathbf{k-q},\mathbf{k};\mathbf{q}s)+$$
$$+2\sum_{s_1\mathbf{q_1},\mathbf{k}}{}'\Phi_{s,s_1}(-\mathbf{q},-\mathbf{q_1})[G_2(\mathbf{k-q-q_1},\mathbf{k},\mathbf{q_1}s_1;\mathbf{q}s)+$$
$$+G_3(\mathbf{k-q-q_1},\mathbf{k},-\mathbf{q_1}s_1;\mathbf{q}s)]. \quad (22)$$

Thus, the closed set of equations finally takes the form:

$$\begin{cases} q_0 G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) = (E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}})\, G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) + \sum_{s_1\mathbf{q}_1} \varphi_{s_1}(-q_1)\, [G_2(\mathbf{k}-\mathbf{q},\mathbf{k}+\mathbf{q}_1;\mathbf{q}_1 s_1;\mathbf{q}s) - \\ G_2(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k},\mathbf{q}_1 s_1;\mathbf{q}s) + G_3(\mathbf{k}-\mathbf{q},\mathbf{k}+\mathbf{q}_1;-\mathbf{q}_1 s_1;\mathbf{q}s) - G_3(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k},-\mathbf{q}_1 s_1;\mathbf{q}s)]; \\ \left(q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} + \Omega_{s_1}(\mathbf{q}_1)\right) G_2 = -\varphi_{s_1}(\mathbf{q}_1)\Big[\bar{n}_{\mathbf{k}}\delta_{ss_1}\delta_{-\mathbf{q}\mathbf{q}_1}\sum_{\mathbf{k}_1} G_1(\mathbf{k}_1+\mathbf{q}_1,\mathbf{k}_1;\mathbf{q}s) - \left(1+\bar{\nu}_{\mathbf{q}_1 s_1} + \bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}\right)\times \\ \times G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) + (\bar{\nu}_{\mathbf{q}_1 s_1} - \bar{n}_{\mathbf{k}})\, G_1(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k}-\mathbf{q}_1;\mathbf{q}s) - \delta_{-\mathbf{q}_1,0}\bar{N} G_1(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k};\mathbf{q}s)\Big]; \\ \left(q_0 - E_{\mathbf{k}+\mathbf{q}_1} + E_{\mathbf{k}-\mathbf{q}} + \Omega_{s_1}(\mathbf{q}_1)\right) G_{2'} = -\varphi_{s_1}(\mathbf{q}_1)\Big[\bar{n}_{\mathbf{k}+\mathbf{q}_1}\delta_{ss_1}\delta_{-\mathbf{q},\mathbf{q}_1}\sum_{\mathbf{k}_1} G_1(\mathbf{k}_1+\mathbf{q}_1,\mathbf{k}_1;\mathbf{q}s) + \left(\bar{\nu}_{\mathbf{q}_1 s_1} - \bar{n}_{\mathbf{k}+\mathbf{q}_1}\right)\times \\ \times G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) - (1+\bar{\nu}_{\mathbf{q}_1 s_1} + \bar{n}_{\mathbf{k}-\mathbf{q}})\, G_1(\mathbf{k}-\mathbf{q}+\mathbf{q}_1,\mathbf{k}+\mathbf{q}_1;\mathbf{q}s) - \delta_{\mathbf{q}_1,0}\bar{N} G_1(\mathbf{k}-\mathbf{q},\mathbf{k}+\mathbf{q}_1;\mathbf{q}s)\Big]; \\ \left(q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \Omega_{s_1}(\mathbf{q}_1)\right) G_3 = \bar{n}_{\mathbf{k}}\delta_{s,s_1}\delta_{\mathbf{q},-\mathbf{q}_1}(q_0 - \Omega_s(\mathbf{q}))\mathcal{D}_r(\mathbf{q}s) + \varphi_s(\mathbf{q}_1)\Big[\left(1+\bar{\nu}_{\mathbf{q}_1 s_1} + \bar{n}_{\mathbf{k}}\right)\times \\ G_1(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k}-\mathbf{q}_1;\mathbf{q}s) - (\bar{\nu}_{\mathbf{q}_1 s_1} - \bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1})\, G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) + \delta_{\mathbf{q}_1,0}\bar{N} G_1(\mathbf{k}-\mathbf{q}-\mathbf{q}_1,\mathbf{k};\mathbf{q}s)\Big]; \\ \left(q_0 - E_{\mathbf{k}+\mathbf{q}_1} + E_{\mathbf{k}-\mathbf{q}} - \Omega_{s_1}(\mathbf{q}_1)\right) G_{3'} = \bar{n}_{\mathbf{k}+\mathbf{q}_1}\delta_{ss_1}\delta_{\mathbf{q},-\mathbf{q}_1}(q_0 - \Omega_s(\mathbf{q}))\mathcal{D}_r(\mathbf{q}s) + \varphi_s(\mathbf{q}_1)\times \\ \times\Big[\left(1+\bar{\nu}_{\mathbf{q}_1 s_1} + \bar{n}_{\mathbf{k}+\mathbf{q}_1}\right) G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) - \left(\bar{\nu}_{\mathbf{q}_1 s_1} - \bar{n}_{\mathbf{k}-\mathbf{q}_1}\right) G_1(\mathbf{k}-\mathbf{q}+\mathbf{q}_1,\mathbf{k}+\mathbf{q}_1;\mathbf{q}s) + \delta_{\mathbf{q}_1,0}\bar{N} G_1(\mathbf{k}-\mathbf{q},\mathbf{k}+\mathbf{q}_1;\mathbf{q}s)\Big]. \end{cases} \quad (23)$$

where the symbol q_0 in the right-hand part of functions G, for shortness, is omitted; $\bar{N} = \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}}$ there is a complete number of excitons in a zone. The last set of four equations (23) allow us easily to find expressions for functions G_2, G_2', G_3 and G_3'. So, substituting them into the first equation of the set (23) and neglecting the terms of the order of $|\varphi_s(\mathbf{q})|^2$, we obtain the following equation for function $G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s)$

$$G_1(\mathbf{k}-\mathbf{q},\mathbf{k};\mathbf{q}s) = \frac{\varphi_s(\mathbf{q})\mathcal{D}_r(\mathbf{q}s)\left(\bar{n}_{\mathbf{k}-\mathbf{q}} - \bar{n}_{\mathbf{k}}\right)}{q_0 - E_{\mathbf{k}} - E_{\mathbf{k}-\mathbf{q}}}. \quad (24)$$

In the second iteration we shall express Green functions $G_2, G_{2'}, G_3, G_{3'}$ through the function (24). Substituting the equations for functions G_2 and G_3 already obtained in this approach, and Eq.(24) in Eq. (22), we can express the $\mathcal{D}_r$ in a Dyson form:

$$\mathcal{D}_r(s\mathbf{q}, s_0 q_0) = \frac{1}{q_0 - \Omega_s(\mathbf{q}) - \Pi(s\mathbf{q}, s_0 q_0)}, \quad (25)$$

where $\Pi(s\mathbf{q}, s_0 q_0)$ is polarization operator of phonons, which is determined by

Analyzing the polarization operator we established, that at $\Phi = 0$ it, as well as was expected, coincides with the appropriate expression obtained by Davydov [22] in the linear on phonon operators approximation.

Conclusions

The additional terms containing square-law on the phonon operators function $\Phi_{s,s_1}(-\mathbf{q},-\mathbf{q}_1)$, bring in the change, which can be rather essential at high temperatures. The important feature of the PO is also that circumstance, that as testifies the deeper analysis, in any order on φ and/or Φ, each term is proportional else to a number of particles in system, or to the mean occupation numbers of appropriate states. Hence, at very small density of quasiparticles, the magnitude of Π becomes small, and look on these reasons the change of a phonon spectrum in the problems touching upon the renormalization of a phonon spectrum can be neglected.

However, at high concentration of excitons, the quadratic coupling function Φ can play comparative with the linear function role in a renormalization of a phonon

$$\Pi(s\mathbf{q}, s_0 q_0) = \sum_{\mathbf{k}} |\varphi_s(\mathbf{q})|^2 \frac{\bar{n}_{\mathbf{k}-\mathbf{q}} - \bar{n}_{\mathbf{k}}}{q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}}} + 2\bar{N}\Phi_{s,s}(\mathbf{q},-\mathbf{q}) + 2\sum_{s_1\mathbf{q}_1,\mathbf{k}}{}' \frac{\varphi_s(\mathbf{q})\varphi_{s_1}(\mathbf{q})\Phi_{s,s_1}(-\mathbf{q},-\mathbf{q}_1)}{q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \Omega_{s_1}(\mathbf{q}_1)} \Big[\left(1+\bar{n}_{\mathbf{k}} + \bar{\nu}_{s_1\mathbf{q}_1}\right)\times$$

$$\times\left(\frac{\bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \bar{n}_{\mathbf{k}-\mathbf{q}_1}}{q_0 - E_{\mathbf{k}+\mathbf{q}_1} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}}\right) + \left(\bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \bar{\nu}_{s_1\mathbf{q}_1}\right)\left(\frac{\bar{n}_{\mathbf{k}-\mathbf{q}} - \bar{n}_{k}}{q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}}}\right)\Big] - 2\sum_{s_1\mathbf{q}_1,\mathbf{k}}{}' \frac{\varphi_s(\mathbf{q})\varphi_{s_1}(\mathbf{q})\Phi_{s,s_1}(-\mathbf{q},-\mathbf{q}_1)}{q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} + \Omega_{s_1}(\mathbf{q}_1)}\times$$

$$\times\left[\left(1+\bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} + \bar{\nu}_{s_1\mathbf{q}_1}\right)\left(\frac{\bar{n}_{\mathbf{k}-\mathbf{q}} - \bar{n}_{\mathbf{k}}}{q_0 - E_{\mathbf{k}} + E_{\mathbf{k}-\mathbf{q}}}\right) + \left(\bar{n}_{\mathbf{k}} - \bar{\nu}_{s_1\mathbf{q}_1}\right)\left(\frac{\bar{n}_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1} - \bar{n}_{\mathbf{k}-\mathbf{q}_1}}{q_0 - E_{\mathbf{k}+\mathbf{q}_1} + E_{\mathbf{k}-\mathbf{q}-\mathbf{q}_1}}\right)\right]. \quad (26)$$

spectrum, because it is proportional to the number of all excitons in system N, whereas the function φ is proportional only to the difference of $\bar{n}_{\mathbf{k-q}} - \bar{n}_{\mathbf{k}}$.

The found above polarization operator of phonons is suited only for weak coupling of excitons with phonons. Having deal with any systems, without restrictions on the coupling force of excitons with phonons, by GF calculation it is worthwhile to use the Matsubara's diagram technique.

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