Nonperturbative effects in self-energy functions of quantum dots coupled to an acoustic phonon reservoir

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Abstract. The problem of description of the strong interaction of a quantum dot (QD) with an acoustic phonon reservoir is discussed. It is shown that the generalized dynamical equation of motion derived in [Gainutdinov R. Kh. 1989 J. Phys. A: Math. Gen. 22 269] as the most general equation of motion consistent with the current concepts of quantum physics and provides an effective way to solve the problem of the QD in the excitonic regime with the phonon reservoir beyond the perturbation theory. A nonperturbative solution for the exciton self-energy function was found. At temperatures, more than 10 K these self-energy functions differ profoundly from that obtained in the second-Born approximation.

1. Introduction
Semiconductor quantum dots have unique optoelectronic properties [1], which make them attractive as candidates for many applications such as new types of single-photon sources [2–4], quantum repeaters [4–9] and computation building blocks of quantum computers [10–14]. Although, semiconductor quantum dots are embedded in a surrounding solid and, in general, the interaction is very strong and gives rise to the dephasing, which presents a serious challenge for practical realization of quantum computers. Also, the strong interaction of the quantum dot expresses itself in quantum fluctuations by being reversible processes in which reservoir degrees of freedom demonstrate themselves in virtual intermediate states. In each act of fluctuation, the system could go to other state and come back to the initial state. Quantum fluctuations are described by the self-energy function. The real part of this function determines the self-energy of the QD states known as the polaron shift, and it is especially important that the energy dependence of the self-energy functions have a significant effect on the emission spectra of a strongly coupled QD-cavity systems. These energy functions are exhibited their non-Markovian character of the dynamics of QDs coupled to a reservoir. In other words, in this case, nonlocality in time of the effective interaction in the system manifests itself explicitly, because an effective interaction in reduced systems is, in general, nonlocal both in space and in time.

A straightforward and effective way to describe nonlocal in time interactions is provided by a generalized dynamic equation (GDE) derived by Gainutdinov [15] as the most general equation of motion, consistent with the current concepts of quantum physics. This equation turned out an important tool for solving many problems in nuclear physics [16–18], quantum
optics [19] and atomic physics [20]. In this work, we show that GDE provides an effective way to solve the problem of the exciton-phonon interaction beyond the perturbation theory, and the nonperturbative solution for the self-energy function of the QD in the exciton regime differ profoundly from that obtained in the second-Born approximation.

2. Method
In the energy representation, Gainutdinov equation takes form [21–25]:

$$\frac{dT(z)}{dz} = -T(z)(G_0(z))^2T(z),$$

(1)

where $G_0(z) = (z - H_0)^{-1}$ with $H_0$ being the free Hamiltonian, and $T(z)$ is defined as

$$T(z) = i \int_0^\infty d\tau \exp(i(z - H_0)t_2)\tilde{S}(t_2, t_1)\exp(-i(z - H_0)t_1),$$

(2)

with $\tilde{S}(t_2, t_1)$ being the contribution to the evolution operator from the processes, in which the interaction in the system begins at time $t_1$ and ends in time $t_2$, extends quantum dynamics to the case where dynamics of a system is governed by nonlocal in time interaction. Peculiarities of interaction in quantum systems are contained in the boundary condition for Eq. 2. In particular, this fact is very important in solving various problems of many-particle physics. Operator $T(z)$ determines the Green operator

$$G(z) = G_0(z) + G_0(z)T(z)G_0(z).$$

(3)

The contribution to the Green operator $G(z)$, which comes from he processes associated with the self-interaction of the system, has the same structure as the free Green operator $G_0(z)$. For this reason it is natural to replace $G_0(z)$ by the operator $\hat{G}_0(z)$, which describes the evolution of the system in the case where the interaction in the system is reduced to the self-interaction and hence has the structure

$$\hat{G}_0(z) = (z - H_0 - C(z))^{-1},$$

(4)

where the operator $C(z)$ has the same eigenvectors as $H_0(C(z)|n) = C_n(z)|n\rangle, H_0|n\rangle = E_n|n\rangle$. Correspondingly, the operator $T(z)$ is the operator describing the whole interaction in the system except the self-interaction. These operators are related as follows

$$G(z) = G_0(z) + G_0(z)T(z)G_0(z) = \hat{G}_0(z) + \hat{G}_0(z)M(z)\hat{G}_0(z).$$

(5)

By making use of this representation, equation of motion (1) can be represented in the form of two equations, for $M(z)$ and $C(z)$. The equation for $C_n(z)$, that is of central importance for the problem under study, reads

$$\frac{d\langle n|C(z)|n\rangle}{dz} = -\sum_m \frac{\langle n|M(z)|m\rangle\langle m|M(z)|n\rangle}{(z - E_m - C_m(z))^2}. $$

(6)

3. The exciton self-energy in a nonperturbative regime
At temperatures higher than 10 K the interaction of a QD with its surroundings becomes strong, and, as a consequence, the perturbation theory becomes inapplicable. The surroundings practically consist of an infinite number of degrees of freedom, which act together as a whole identity referred to as reservoir. The remarkable feature of equation of motion (1) is that its form does not depend on the peculiarities of the interaction. This makes it possible to find formal solutions for various physical problems, which also do not depend on the peculiarities
of interaction. The equation for the self-energy function of a quantum dot in excitonic regime coupled to phonon reservoir takes the form

\[
\frac{dC_{X\mu}(z)}{dz} = -\sum_{\mu'} \frac{\langle x; \mu | M(z) | x; \mu' \rangle \langle x; \mu' | M(z) | x; \mu \rangle}{(z - E_X - E_{\mu'} - C_{X\mu}(z))^2},
\]

(7)

with |\mu\rangle being the eigenstates of the Hamiltonian \(H_R\) of the reservoir with eigenenergy \(E_{\mu}\). Since the reservoir is practically consists of an infinite number of degrees of freedom the change in the energy of the state of the QD in the excitonic regime |X, \mu\rangle caused by reservoir-QD interaction is extremely small compared to the energy of these states. For this reason, it is convenient to set \(E_{\mu}\) to be the zero energy point. The zero point for \(\mu\) is changed correspondingly \(\mu' = z - E_{X\mu} \rightarrow z\). The reservoir-QD interaction creates and destroys particles in the reservoir. We will restrict ourselves to the case where only one phonon is created and destroyed in the interaction process. In this way we can derive the equation

\[
\frac{dC_{X\mu}(z)}{dz} = \sum_q \frac{\langle x; \mu | M(z) | x; \mu' + q \rangle \langle x; \mu' + q | M(z) | x; \mu \rangle}{(z - E_X - \omega(q) - C_{X\mu}(z - \omega(q)))^2} + \]

(8)

\[+ \frac{\langle x; \mu | M(z) | x; \mu' - q \rangle \langle x; \mu' - q | M(z) | x; \mu \rangle}{(z - E_X + \omega(q) - C_{X\mu}(z + \omega(q)))^2}.
\]

The boundary condition for this equation is

\[C_{X\mu} \rightarrow 0.\]

(9)

The corresponding boundary condition for the interaction operator \(M(z)\) reads

\[M(z) \rightarrow H_{qx},\]

(10)

where \(H_{qx}\) is the exciton-phonon interaction Hamiltonian. In the independent boson model (IBM) \(H_{qx}\) takes the form

\[H_{qx} = \sum_q g_q^x (b_q + b_q^+) ,\]

(11)

where |x\rangle and |\mu\rangle are states of a QD exciton and an eigenstate of the reservoir respectively, \(q\) denotes the different phonon modes with energy \(\omega q\) the creation \((b_q^+)\) and annihilation \((b_q)\) operators of phonons with momentum \(q\) and frequency \(\omega q\) obey the usual commutation relations for bosons, and \(g_q^x\) is the deformation potential coupling which depends on the material parameters of the host semiconductor and the exciton wave function. In a first approximation, one can set \(M(z)\) to be equal to \(H_{qx}\). In this way, we obtain the equation

\[\frac{dC(z)}{dz} = -\sum_q \frac{\langle x; \mu | H_{qx} | x; \mu' + 1q \rangle \langle x; \mu' + 1q | H_{qx} | x; \mu \rangle}{(z - E_X - \omega(q) - C_{X\mu}(z - \omega(q)))^2} + \]

(12)

\[+ \frac{\langle x; \mu | H_{qx} | x; \mu' - 1q \rangle \langle x; \mu' - 1q | H_{qx} | x; \mu \rangle}{(z - E_X + \omega(q) - C_{X\mu}(z + \omega(q)))^2}.
\]

By taking thermal average of both sides of the above equation and taking into account Eq.11 we get
\[
\frac{dC_X(z)}{dz} = -\sum_q \left\{ \frac{|g_q|^2 (1 + n(q))}{(z - E_X - \omega(q) - C_X(z - \omega(q)))^2} + \frac{|g_q|^2 n(q)}{(z - E_X + \omega(q) - C_X(z + \omega(q)))^2} \right\},
\]

(13)

where

\[
C_X(z) = \sum_\mu p_\mu \langle x; \mu | C(z) | x; \mu \rangle
\]

(14)

with \(p_\mu\) being the probability to find the reservoir in the state \(|\mu\rangle\), and \(n(q) = \left[ e^{\omega(q) / k_B T} - 1 \right]^{-1}\) is mean phonon occupation number at bath temperature \(T\). Here we use natural units (\(\hbar = c = k_B = 1\)). When temperatures are low enough, this equation can be solved perturbative. At leading order, one can neglect the self-energy function in the denominators on the right-hand part of the equation, and get the leading-order solution

\[
C_X^{(2)}(z) = \sum_q \left\{ \frac{|g_q|^2 (1 + n(q))}{E - E_X - \omega(q) + \frac{i\hbar}{2}} + \frac{|g_q|^2 n(q)}{E - E_X + \omega(q) + \frac{i\hbar}{2}} \right\},
\]

(15)

where \(\frac{i\hbar}{2}\) is added to the denominators on the right-hand part of this equation to account for the relaxation of states. This expression for the self-energy function is exactly the same that has been derived within independent boson model (IBM) at the second Born approximation level [26,27].

At the same time Eq.15 can be solved beyond the perturbation theory. For this purpose, it is convenient to rewrite the equation in the form

\[
\frac{dC_X(z)}{dz} = \frac{S_{HR}}{\omega_b^2} \int q^3 e^{-\frac{q^2}{2}} \left\{ \frac{1 + n(q)}{(z - \omega(q) + \frac{i\hbar}{2} - C_X(z - \omega(q)))^2} + \frac{n(q)}{(z + \omega(q) + \frac{i\hbar}{2} - C_X(z + \omega(q)))^2} \right\} dq,
\]

(16)

where \(S_{HR}\) is dimensionless Huang-Rhys parameter characterizing the exciton-phonon coupling, and \(\omega_b = s/l\) is a cut-off frequency (\(s\) is the sound velocity and \(l\) is the dot size). In Figs.1,2 we show that the self-energy function derived from the nonperturbative solutions of Eq.16 differ profoundly from that obtained at the second-Born perturbation level.

**Figure 1.** Real (a) and imaginary (b) parts of quantum fluctuation contribution to self-energy function for InAs QDs at \(T = 10 K\), \(\Gamma = 0.077 meV\) and \(S_{HR} = 0.2\). The solid lines represent self-energy function calculated within second-Born approximation, dashed lines represent function calculated beyond the perturbation theory.
Figure 2. Real (a) and imaginary (b) parts of quantum fluctuation contribution to self-energy function for InAs QDs at $T = 40\, K$, $\Gamma = 0.077\, meV$ and $S_{HR} = 0.2$. The solid lines represent self-energy function calculated within second-Born approximation, dashed lines represent function calculated beyond the perturbation theory.

4. Conclusion

In conclusion, we have shown that the generalized dynamical equation provides an effective way to solve the problem of the strong interaction between a single QD and phonon reservoir beyond the perturbation theory. In this way, a nonperturbative solution for exciton self-energy function has been found. The results presented in Figs. 1, 2 show that at temperatures more than 10 K and parameter $S_{HR}$ equal to 0.2 the nonperturbative solution differ profoundly from that obtained in the second-Born approximation [27] to describe the emission from the QD-cavity systems.

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