Nonperturbative renormalization of the interaction of quantum dots with the phonon reservoir

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Abstract. The quantum dynamics of a single quantum dot with phonon reservoir is investigated by making use generalized quantum dynamics equation [Gainutdinov R.Kh. 1999 J. Phys. A \textbf{32} 5675]. The self-energy function is calculated nonperturbatively taking into account the renormalization of the vertex function. In this paper, we show that the nonperturbative renormalization of the vertex function significantly affects the nature of the interaction of the quantum dot with the phonon reservoir.

1. Introduction
A practical implementation of a quantum computer should protect the qubit from destructive interaction with the environment, as well as the ability to perform logical operations on the qubit using various gates. Dephasing processes caused by the nondissipative exchange of information between quantum systems and environments are one of the obstacles to the creation of devices for quantum information \cite{1–3}. However, a significant contribution to the qubit-environment interaction comes also from quantum fluctuations in which the environment degrees of freedom manifest themselves in a virtual state. Solving these problems requires not only the development of experimental methods, but also theoretical ones. Some, at first glance, formal problems may require a different approach. Successful development of methods of quantum electrodynamics (QED), such as waveguide QED \cite{4}, cavity QED \cite{5} and circuit QED \cite{6, 7} allows one to describe the quantum dynamics of these systems. However, some problems require a more careful approach. Because of nonlocality of the interaction problems associated with ultraviolet divergences arising in quantum field theory are solved in quantum electrodynamics by renormalization. However, as Richard Feniman said: ”Renormalization theory is simply a way to sweep the difficulties of the divergences of electrodynamics under the rug” \cite{8}. So, it is important to understand that the renormalization procedure is not formal, but has a deep physical meaning. As we show, renormalization theory are important not only for eliminating divergences, but also for the nature of self-energy processes. There are two kind of physical processes that give contribution to the self-energy function. That are the off-shell quantum fluctuation processes keeping the system in the initial state, and decaying processes in the case when the state is unstable. In this paper, we show that the nonperturbative renormalization of...
the vertex function significantly affects the nature of the interaction of the quantum dot with the phonon reservoir. Under this point we consider processes of quantum fluctuations with stationary qubit and phonon reservoir.

2. Method

To describe the processes associated with quantum fluctuations as a nonlocal-in-time interaction we use generalized quantum dynamics (GQD) approach [9] that allows one to solve the problem nonperturbatively. This method is based on the generalized dynamical equation (GDE) that has been derived in [9] as the most general dynamical equation consistent with the current concepts of quantum physics.

In a general case the time evolution of a quantum system is described by the evolution equation

\[ |\Psi(t)\rangle = U(t, t_0) |\Psi(t_0)\rangle, \]

where \( U(t, t_0) \) is the unitary evolution operator,

\[ U^\dagger(t, t_0)U(t, t_0) = U(t, t_0)U^\dagger(t, t_0) = 1, \]

with the group property

\[ U(t, t')U(t', t_0) = U(t, t_0), U(t_0, t_0) = 1. \]

The amplitude \( \langle \psi_2 | U(t, t_0) | \psi_1 \rangle \) can be represented as a sum of contributions from all alternative ways of realization of the corresponding evolution process. Dividing these alternatives into different classes, we can then analyse such a probability amplitude in different ways. For example, subprocesses with definite instants of the beginning and end of the interaction in the system can be considered as such alternatives. In this way the amplitude \( \langle \psi_2 | U(t, t_0) | \psi_1 \rangle \) can be written in the form

\[ \langle \psi_2 | U(t, t_0) | \psi_1 \rangle = \langle \psi_2 | \psi_1 \rangle + \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1 \langle \psi_2 | S(t_2, t_1) | \psi_1 \rangle, \]

where \( \langle \psi_2 | S(t_2, t_1) | \psi_1 \rangle \) is the probability amplitude that if at time \( t_1 \) the system was in the state \( \psi_1 \), then the interaction in the system will begin at time \( t_1 \) and will end at time \( t_2 \), and at this time the system will be in the state \( \psi_2 \) Note that in general \( S(t_2, t_1) \) may be only an operator-valued generalized function of \( t_1 \) and \( t_2 \), since only \( U(t, t_0) = 1 + \int_{t_0}^{t} dt_2 \int_{t_0}^{t_2} dt_1 S(t_2, t_1) \) must be an operator on the Hilbert space. Nevertheless, it is convenient to call \( S(t_2, t_1) \) an ”operator”, using this word in the generalized sense. In the case of an isolated system the operator \( S(t_2, t_1) \) can be represented in the form

\[ S(t_2, t_1) = \exp(iH_0t_2)\tilde{T}(t_2 - t_1)\exp(-iH_0t_1), \]

with \( H_0 \) being the free Hamiltonian.

As has been shown in [9], for the evolution operator \( U(t, t_0) \) given by equation (4) to be unitary for any times \( t_0 \) and \( t \), the operator \( S(t_2, t_1) \) must satisfy the following equation:

\[ (t_2 - t_1)S(t_2, t_1) = \int_{t_1}^{t_2} dt_4 \int_{t_1}^{t_4} dt_4 (t_4 - t_3)S(t_2, t_4)\tilde{S}(t_3, t_1). \]

This equation allows one to obtain the operators \( \tilde{S}(t_2, t_1) \) for any \( t_1 \) and \( t_2 \), if the operators \( \tilde{S}(t_2', t_1') \) corresponding to infinitesimal duration times \( \tau = t_2' - t_1' \) of interaction are known. It is
natural to assume that most of the contribution to the evolution operator in the limit \( t_2 \to t_1 \) comes from the processes associated with the fundamental interaction in the system under study. Denoting this contribution by \( H_{\text{int}}(t_2, t_1) \), we can write
\[
\hat{S}(t_2, t_1) \xrightarrow{t_2 \to t_1} H_{\text{int}}(t_2, t_1) + o(\epsilon), \tag{7}
\]
where \( \tau = t_2 - t_1 \). The parameter \( \epsilon \) is determined by demanding that \( H_{\text{int}}(t_2, t_1) \) must be so close to the solution of equation (6) in the limit \( t_2 \to t_1 \) that this equation has a unique solution having the behavior (7) near the point \( t_2 = t_1 \). Being a generalization of the interaction Hamiltonian, operator \( H_{\text{int}}(t_2, t_1) \) is called the generalized interaction operator. One of the energy representations of GDE (6) takes the form
\[
\frac{dT(z)}{dz} = -T(z)G_0(z)^2T(z), \tag{8}
\]
where
\[
T(z) = i \int_0^\infty d\tau \exp(i(z - H_0)\tau)\hat{S}(t_2, t_1)\exp(-i(z - H_0)\tau). \tag{9}
\]
Being equivalent to the Schrödinger equation in the case when the interaction in a quantum system is instantaneous, GDE allows one to extend dynamics to the case of nonlocal-in-time interactions. This equation provides a new insight into many problems in atomic physics \([10–13]\), nuclear physics \([9, 14–16]\) and quantum optics \([17, 18]\). The method allows one to take into account from the very beginning that the contribution to the Green operator \( G(z) \), which comes from the processes associated with the self-interaction of particles, 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 \( G_0^{(v)}(z) \), which describes the evolution of the system when particles propagate freely or interact with vacuum, and, hence, has the structure
\[
\langle m'|G_0^{(v)}(z)|m \rangle = \frac{\langle m'|m \rangle}{z - E_m - C_m(z)} \tag{10}
\]
with \( |m \rangle \) being the eigenvectors of the free Hamiltonian \( (H_0|m \rangle = E_m|m \rangle) \). Other contributions are described by the operator \( G^{(I)}(z) = G_0^{(v)}(z)M(z)G_0^{(v)}(z) \)
\[
G(z) = G_0^{(v)}(z) + G^{(I)}(z) = G_0^{(v)}(z) + G_0^{(v)}(z)M(z)G_0^{(v)}(z), \tag{11}
\]
where the operator \( M(z) \) describes the processes in which some particles interact each with other. The equations for \( C(z) \) and \( M(z) \) are derived from GDE. The equation for the function \( C_m(z) \) referred to as the self-energy function reads
\[
\frac{dC_m(z)}{dz} = -\langle m|M(z)\left(G_0^{(v)}(z)\right)^2M(z)|m \rangle, \langle m | m \rangle = 1, \tag{12}
\]
and the conditions
\[
z - E_m^{(0)} - C_m(z) = 0 \tag{13}
\]
determines the physical masses of particles. In the case when we deal with an atom and \( |m \rangle \) describes an atomic state, equation (13) determines the self-energy correction (the Lamb shift) to the energy \( E_m \) of the state \( |m \rangle \). An approximative solution of this equation is \( E_m \approx E_m^{(0)} + C_m^{(0)}(E_m^{(0)}) \equiv E_m^{(0)} + \Delta E_m - \frac{i}{2}\Gamma_m \), with \( \Delta E_m \) and \( \Gamma_m \) being the Lamb shift and
the natural width of the energy level of the state $|m\rangle$ respectively. For this approximation to be valid the variation of $C_m(z)$ in the energy interval between $E_m^{(0)}$ and $E_m$ must be negligible. This is the case for atoms in free space. In fact, at leading order in $\alpha$ the equation for $C_m(z)$ is reduced to the equation

$$\frac{dC_m^{(0)}(z)}{dz} = -\langle m|H_I(G_0^{(\nu)}(z))^2 H_I|m\rangle, \langle m | m \rangle = 1$$

with $H_I$ being the interaction Hamiltonian. By solving this equation with an appropriate boundary condition we arrive at the ordinary expressions for the self-energy shifts and widths of energy levels. However, in the case of quantum dots the variation of the self-energy function in the relevant vicinity of the point $z = E_m^{(0)}$ can be very significant and, as a result, the above approximation is invalid. In this case the self-interaction function can not be parametrized by a shift and a width, and one has to derive the self-energy function from a nonperturbative solution of the equations for $C_m(z)$ and $M(z)$.

3. Exciton-reservoir interaction

Let us consider quantum dot strongly coupled with the resonator field and acoustic phonon reservoir. To describe the processes of quantum fluctuation of quasiparticles between quantum dot levels dressed by the resonator field and boson’s mode we use boundary conditions $M_m^{(0)}(z) = H_I$. The IBM Hamiltonian describing phonons and exciton-phonon coupling reads [19,20]

$$H_I = \sum_q \omega_q b_q^\dagger b_q + \sum_q g_q^2(b_q + b_q^\dagger) |x\rangle \langle x|,$$

where $|x\rangle$ is the vector of the excitonic state, $q$ denote the different phonon modes with energy $\omega_q$, the creation ($b_q^\dagger$) and annihilation ($b_q$) operators of phonons with momentum $q$ and frequency $\omega_q$ obey the usual commutation relations for bosons, and $g_q^2$ is the deformation potential coupling, which depends on the material parameters of the host semiconductor and the exciton wave function. So, the equation (14) can be written as

$$\frac{dC_{x,\mu}(z)}{dz} = -\sum_{\nu} \sum_{\mu} \frac{\langle x, \mu| H_I |x, \mu, \nu\rangle \langle x, \mu, \nu| H_I |x, \mu\rangle}{(z - E_x - C_x(z))^2}. \tag{16}$$

Here we take the average over reservoir degrees of freedom

$$C_x(z) = \sum_q \left\{ \frac{|g(q)|^2(1 + n(q))}{z - E_x - \omega(q)} + \frac{|g(q)|^2 n(q)}{z - E_x + \omega(q)} \right\}. \tag{17}$$

In the case of low temperatures the self-energy function in the denominator of equation (16) cannot be neglected. Substituting $C_x(E)$ represented in the form

$$C_x(E) = (E - E_x) \chi_l + \tilde{C}_x(E), \tag{18}$$

($E_x$ is assumed to include the self-energy shift $C_x(E_x)$) with

$$\chi_l = \frac{dC_{n,off}(z)}{dz} \tag{19}$$

into equation (18), and neglecting $\tilde{C}_x(E)$ that is small for the relevant energies we get

$$C_x^{(2)}(E) = \sum_q \left\{ \frac{|g(q)|^2 Z_l^2(1 + n(q))}{(E - E_x - \omega(q) + i0) Z_2^2} + \frac{|g(q)|^2 Z_l^2 n(q)}{(E - E_x + \omega(q) - i0) Z_2^2} \right\}. \tag{20}$$
where
\[ Z_2 = (1 - \chi_1)^{\frac{1}{2}}. \] (21)

The factor \( Z_2 \) can be regarded as a constant renormalizing the exciton propagator. Appearance of the factor \( Z_1 \) manifests the fact that the renormalization of the exciton propagator must be accompanied by a renormalization of the exciton-phonon coupling. An additional factor \( Z_2 \) appears because of the renormalization of the propagators associated with external lines. Since as usual \( Z_1 = Z_2 \), these constants in equation (20) compensate each other and we come back to equation (17), in which the parameter \( Z_2 \) does not manifest itself. However, there are physical situations where this parameter and hence the self-energy function \( C_x(E) \) come into play. This, for example, takes place in the case when the quantum dot is strongly coupled to a resonator. In this case emitted spectrum depends on the exciton self-energy function [20].

4. Renormalization of the exciton-reservoir interaction

Let us now determine the parameter \( Z_1 \) renormalizing the exciton-phonon coupling. The part of the interaction operator \( M_{qr}(z) \) described by ladder diagrams that are formed by successively substituting terms \( H_{qr} \tilde{G}_0(z) H_{qr} \tilde{G}_0(z) \ldots \tilde{H}_{qr} \) into equation (9)

\[ \frac{dM_{L2}^{L2}(z)}{dz} = -H_{qr} \tilde{G}_0(z) \left( 1 - \frac{dC_x(z)}{dz} \right) \tilde{G}_0(z) H_{qr}, \] (22)

\[ M_{qr}^{L2}(z) = H_{qr} \tilde{G}_0(z) H_{qr}, \] (23)

\[ \frac{dM_{L3}^{L3}(z)}{dz} = -H_{qr} \tilde{G}_0(z) \left( 1 - \frac{dC_x(z)}{dz} \right) \tilde{G}_0(z) H_{qr} \tilde{G}_0(z) H_{qr} - \]

\[ -H_{qr} \tilde{G}_0(z) H_{qr} \tilde{G}_0(z) H_{qr} \tilde{G}_0(z) \left( 1 - \frac{dC_x(z)}{dz} \right) \tilde{G}_0(z) H_{qr}, \] (24)

\[ M_{qr}^{L3}(z) = H_{qr} \tilde{G}_0(z) H_{qr} \tilde{G}_0(z) H_{qr} = H_{qr} \left( \tilde{G}_0(z) H_{qr} \right)^2, \] (25)

\[ M_{qr}^{Ln}(z) = H_{qr} \left( \tilde{G}_0(z) H_{qr} \right)^{n-1}. \] (26)

Note that the interaction operators \( H_{qr} \) in these equations are not connected with each other. Thus the ladder terms can be represented as

\[ M_{qr}^{L}(z) = H_{qr} + \sum_{n=1}^{\infty} H_{qr} \left( \tilde{G}_0(z) H_{qr} \right)^n. \] (27)

Other terms in the solution of the equation (27) contains loops associated with emission and absorption of a quanta in the interaction process. Because we focus on the renormalization of the exciton-phonon coupling we will restrict ourselves to the contributions from processes described by a loop with one interaction Hamiltonian inside it:

\[ \langle x | H_{qr} | x, q \rangle + \langle x | M(E_x + i0) \tilde{G}_0(E_x + i0) H_{qr} \tilde{G}_0(E_x - E_q + i0) M(E_x + i0) | x \rangle. \] (28)

In the limit \( q \to 0 \) we get this equation

\[ \langle x; \mu | H_{qr} | x; \mu, q \rangle + \langle x; \mu | M(E_x + i0) \tilde{G}_0(E_x + i0) H_{qr} \tilde{G}_0(E_x - E_q + i0) M(E_x + i0) | x \rangle, \] (29)
where the energy of the state $|\mu\rangle$ of the reservoir is chosen to be zero energy point. In the limit $q \to 0$ this equation is reduced to the expression that after averaging over reservoir degrees of freedom takes the form

$$g_x + g_x \sum_{\mu} P_\mu \langle x;\mu | M(E_x + i0) \tilde{G}_0^2(E_x + i0) M(E_x + i0) | x;\mu \rangle =$$

$$= g_x \left( 1 - \frac{dC_x(z)}{dz} \right) \bigg|_{z=E_x} = g_x Z_2^2. \quad (30)$$

Here we have taken into account equations (19,21). From this it follows that $Z_2 = Z_1$. For this reason parameters $Z_1$ and $Z_2$ compensate each other. Thus the vertex $\Gamma_x(q)$ can be represented in the form

$$\Gamma_x(q) = g_x + \Lambda(q) - \Lambda(0), \quad (31)$$

and, as a consequence,

$$\Lambda(q) = \sum_{\mu} \sum_{q} \langle x;\mu | M(E_x + i0) | x;\mu, q_1 \rangle \langle x;\mu, q_2 | H_{ph} | x;\mu, q_2 \rangle \langle x;\mu, q_1 | M(E_x + i0) | x;\mu \rangle \bigg( -E_{q_1} + i0 \bigg) \bigg( -E_{q_1} - E_q + i0 \bigg). \quad (32)$$

This expression can be rewritten as

$$\Lambda(z,q) = \frac{S_{HR}}{\omega_b^2} \int_0^\infty \omega^3(q_1) e^{-\frac{\omega^2(q_1)}{2\omega_b^2}} \times \left( \frac{1 + n(q_1)}{z - E_x - \omega(q_1)} \right) +$$

$$\times \left( \frac{n(q_1)}{(z - E_x + \omega(q_1))(z - E_x + \omega(q_1) + \omega(q))} \right) d\omega(q_1). \quad (33)$$

Then the self-energy is redefined as

$$C_x^{(2)}(z) = \frac{S_{HR}}{\omega_b^2} \int_0^\infty \omega^3(q) e^{-\frac{\omega^2(q)}{2\omega_b^2}} \times \left\{ \frac{1 + n(q)}{z - E_x - \omega(q)} + \frac{n(q)}{z - E_x + \omega(q)} \right\} \times [\Lambda_{ren}(z,q)]^2 d\omega(q), \quad (34)$$

where

$$\Lambda_{ren}(z,q) = \Lambda(z,q) - \Lambda(z,0). \quad (35)$$

Figures (1) and (2) show the dependence of the derivative of self-energy function at $z = E_x$ on the Huang-Rhys [20–22] parameter, which determines the strength of the electron-phonon interaction, and temperature, taking into account the correction from the vertex function.

5. Conclusion

In conclusion, we investigated the self-interaction effect on quantum dynamics and self-energy function of quantum dot interacted with acoustic phonon reservoir. The dependence of the self-interaction processes on energy means that here the non-markovian effects manifest themselves. In other words, the nonlocality in the time of interaction of the qubit with the reservoir is manifested here. It is interesting that the exact derivative of the exciton self-energy function $\chi_1$ appears in the renormalization procedure and from this it follows that $Z_1 = Z_2$. This dimensionless parameter provides us a very important information about the processes of dephasing and decoherence. It is shown that nonperturbative and perturbative calculations differ significantly for realistic Huang-Rhys parameters.
Figure 1. The derivative of the self-energy function $\chi_1 = \frac{dC(z=E_x)}{dz}$ as a function of Huang-Rhys parameter (left) and temperature (right).

Figure 2. The derivative of the self-energy function $\chi_1 = \frac{dC(z=E_x)}{dz}$ by perturbation theory and beyond ones at $S_{HR} = 0.2$ (left) and $S_{HR} = 0.6$ (right).

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