Tunneling-induced self-energy shift of energy levels of a quantum dot

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Abstract.

The self-interaction of a quantum dot tunnel with Coulomb interaction coupled to two noninteracting leads is investigated. The self-energy function describing this interaction is added to a bare energy of a dot state. In the standard way of determining the self-interaction (tunneling-induced) corrections to bare energies of emitters (atoms, quantum dots, etc) the variations of the self-energy functions with energy are ignored, and these corrections are considered to be equal to the values of the self-energy functions for bare energies of states. We show that actually in the case of quantum dots the variations of the self-energy functions in the energy interval between the bare and true energies can be strong, and this can have a significant effect on the values of the tunneling-induced shifts of energy levels of quantum dots.

1. Introduction

Semiconductor quantum dots are nanometer-sized three-dimensional structures which confine electrons in all three directions. This confinement gives rise to a discrete energy spectrum [1]. Quantum dots have offered unique opportunities to investigate quantum optical effects in solid state systems such as quantum interference [2], Rabi oscillations [3–7], photon anti-bunching [8], etc. The remarkable feature of quantum dots is that the interaction of electromagnetic field with them can differ profoundly from that with ordinary atoms. This fact manifests itself in the recently observed [9] Mollow triplet from self-assembled quantum dots. The observed resonance fluorescence spectrum showed a dramatical disagreement with the predictions of quantum optics [10]. This disagreement can originate from the fact that in the standard theory of the resonance fluorescence from a two-level atom the nondecay transitions caused by the self-interaction processes are not taken into account. In the case of quantum dots the role of the virtual photons in the self-interaction of ordinary atoms can be played, for example, by electrons that leave the quantum dot and then come back. Such a self-interaction can be much more significant than the interaction of an atom with its own radiation field. In this paper we investigate the effect of such a self-interaction on the tunneling-induced shift of energy levels of a quantum dot.

2. Methods

In our investigation we use the method [11] that allows one to solve the problem nonperturbatively. This method is based on the generalized dynamical equation (GDE) that
has been derived in [11] as the most general dynamical equation consistent with the current concepts of quantum physics. 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 [12–15], nuclear physics [16–19] and quantum optics [20, 21]. The method allows one to take into account from the every 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

\[
\langle m | G_0^{(v)}(z) | m \rangle = \langle m | m \rangle (z - E_m - C_m(z))^{-1},
\]

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 \( G^{(I)}(z) = G_0^{(v)}(z)M(z)G_0^{(v)}(z) \):

\[
G(z) = G_0^{(v)}(z) + G^{(I)}(z) \equiv G_0^{(v)}(z) + G_0^{(v)}(z)M(z)G_0^{(v)}(z),
\]

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

\[
\frac{dC_m(z)}{dz} = - \langle m | M(z) \left( G_0^{(v)}(z) \right)^2 M(z) | m \rangle, \langle m | m \rangle = 1,
\]

and the condition

\[
z - E_m^{(0)} - C_m(z) = 0
\]

determines the physical masses of particles. In the case when we deal with an atom and \(|m\rangle\) describes an atomic state, equation (3) 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

\[
E_m \approx E_m^{(0)} + C_m^{(0)}(E_m^{(0)}) \approx E_m^{(0)} + \Delta E_m^L - \frac{1}{2} \Gamma_m, \quad \text{with} \quad \Delta E_m^L \text{ and } \Gamma_m \text{ being the Lamb shift and the natural width of the energy level of the state } |m\rangle \text{ respectively.}
\]

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 [22, 23]

\[
\frac{dC_m^{(0)}(z)}{dz} = - \langle m | H_I \left( G_0^{(v)}(z) \right)^2 H_I |m\rangle, \langle m | m \rangle = 1,
\]

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 parameterized 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. The self-energy functions of the quantum dot states

There are several different kinds of quantum dots which differ in both their method of manufacture and their electronic and optical properties. In this work we investigate the self-interaction of a single-level quantum dot with arbitrary strong one-site Coulomb interaction.
tunnel coupled to two noninteracting leads. This model was used in [24] for analyzing tunneling-induced quantum fluctuation in such quantum dots. The Hamiltonian of system consisting of the quantum dot and leads is described by $H = H_{qd} + H_{tun} + H_{lead}$, where $H_{qd}$ is the Hamiltonian of the quantum dot, $H_{tun}$ is the Hamiltonian of tunneling process between the leads and the quantum dot and $H_{lead}$ is the Hamiltonian of the leads. The quantum dot can be described by the single-level Anderson impurity model, $H_{qd} = \sum_{\sigma = \uparrow, \downarrow} z d_{\sigma}^\dagger d_{\sigma} + U n_{\uparrow} n_{\downarrow}$, where the creation (annihilation) operator for an electron with spin $\sigma$ on the dot is given by $d_{\sigma}^\dagger$ and $d_{\sigma}$, $n_{\sigma} = d_{\sigma}^\dagger d_{\sigma}$ is the corresponding number operator. The on-site repulsion $U$ describes the energy cost for double occupation (when we have two electrons in the quantum dot). The Hamiltonian $H_{tun}$ is given by $H_{tun} = \sum_{\alpha,k,\sigma} V_{\alpha} c_{\alpha,k,\sigma}^\dagger d_{\sigma} + H.c.$, where $V_{\alpha}$ is the momentum and spin-independent tunnel matrix element, $c_{\alpha,k,\sigma}^\dagger (c_{\alpha,k,\sigma})$ is the creation (annihilation) operator for electrons with spin $\sigma$ and momentum $k$ in lead $\alpha = l, r$. The Hamiltonian $H_{lead}$ is given by $H_{lead} = \sum_{\alpha,k,\sigma} \varepsilon_{\alpha,k} c_{\alpha,k,\sigma}^\dagger c_{\alpha,k,\sigma}$. The chemical potentials of the two leads differ by the applied bias $\mu_l - \mu_r = -eV$. We assume that the density of states $\rho_{\alpha}$ in the leads is constant for transport and defines the tunnel coupling strength $R_{\alpha}$ as $R_{\alpha} = 2\pi \rho_{\alpha} |V_{\alpha}|^2$, where $V_{\alpha}$ is the tunnel matrix element and $R = R_l + R_r$. We will denote the states of quantum-dot as $|\Psi_0\rangle$ for an empty dot, $|\Psi_\sigma\rangle$ for a singly occupied dot with spin $\sigma = \uparrow, \downarrow$ and $|\Psi_d\rangle$ for a doubly occupied dot. In this model we assume that reservoirs are in equilibrium and we average over the reservoir part of the initial states according to the Fermi distribution

$$f_{\alpha}(E) = \frac{1}{1 + \exp\left(\frac{E - \mu_{\alpha}}{k_B T}\right)}.$$ 

Solving the leading-order equation (4) yields the following expressions for the self-energy functions $C_0(z)$, $C_\sigma(z)$ and $C_d(z)$ of the quantum-dot states $|\Psi_0\rangle$, $|\Psi_\sigma\rangle$ and $|\Psi_d\rangle$ respectively:

$$C_0(z) = 2 \sum_{\alpha} \frac{R_{\alpha}}{2\pi} \int d\omega \frac{f_{\alpha}(\omega)}{z - \varepsilon + \omega}$$ 

$$C_\sigma(z) = \sum_{\alpha} \frac{R_{\alpha}}{2\pi} \int d\omega \left( \frac{1 - f_{\alpha}(\omega)}{z - \omega} + \frac{f_{\alpha}(\omega)}{z - 2\varepsilon - U + \omega} \right)$$ 

$$C_d(z) = 2 \sum_{\alpha} \frac{R_{\alpha}}{2\pi} \int d\omega \frac{1 - f_{\alpha}(\omega)}{z - \varepsilon - \omega}.$$ 

Let us assume that the variations of these self-energy functions with $z$ are weak. In this case $\Delta E_{0}^{(ap)} = C_0(E_0)$, $\Delta E_{\sigma}^{(ap)} = C_\sigma(E_\sigma)$ and $\Delta E_{d}^{(ap)} = C_d(E_d)$ can be considered as the approximative energy shifts of the corresponding energy levels of the quantum dot. The imaginary parts of these shifts $\text{Im}E_{0}^{(ap)}$, $\text{Im}E_{\sigma}^{(ap)}$ and $\text{Im}E_{d}^{(ap)}$ describe dissipative phenomena. Note that the expressions for the energy shifts that follow from equations (5)-(7), are just the same that have been derived in Ref. [24] in second order in the tunnel matrix element $V_{n' n}$. However, as it follows from the results of our calculations the variations with $z$ of the self-energy functions of the quantum-dot states are strong, and one has to solve equation (3) exactly. Figure 1 where the results of calculations of the self-energy correction

$$\delta\varepsilon = \Delta E_\sigma - \Delta E_0$$ 

are depicted, shows that the energy shifts obtained in this way can differ dramatically from their approximative values. In our calculations we have used the fact that the part that is independent of the Fermi distribution function of $C_\sigma(z)$ given by equation (6) can be included
Figure 1. Results of calculation of the real part of the corrections $\delta \varepsilon$ defined by equation (9) (solid line) and equation (10) (dashed line) for the parameters $U = 30 R, \mu = 300 R$ at the zero temperature and in the assumption that the left lead is the same as the right lead.

into the correction to the energy of empty level. In this way from equations (5), (6) and (8) we get

$$
\delta \varepsilon = \sum_{\alpha} R_{\alpha} \frac{1}{2\pi} \int d\omega \left( -f_{\alpha}(\omega) \frac{z_{\alpha} - \omega}{z_{\sigma} - \omega} + f_{\alpha}(\omega) \frac{z_{\alpha} - 2\varepsilon - U + \omega}{z_{0} - \varepsilon + \omega} - 2 f_{\alpha}(\omega) \frac{z_{0} - \varepsilon + \omega}{z_{0} - \varepsilon + \omega} \right),
$$

(9)

where $z_{0}$ and $z_{\sigma}$ are the solutions of equation (3) both for empty and for single occupation energy levels. If we do not take into account the variation of the self-energy function, and put in equations (5) and (6) $z = 0$ and $z = \varepsilon$ respectively we arrive at the expression derived in [24]:

$$
\delta \varepsilon^{\text{(ap)}} = - \sum_{\alpha} R_{\alpha} \frac{1}{2\pi} \int d\omega \left( f_{\alpha}(\omega) \frac{1}{\omega - \varepsilon} + f_{\alpha}(\omega) \frac{1}{\varepsilon + U - \omega} \right).
$$

(10)

4. Conclusions

Starting with equation (4) we have derived expressions (5), (6) and (7) for the self-energy functions of the quantum-dot states. Setting $z = E_{0}, z = E_{\sigma}$ and $z = E_{d}$ in equation (5), equation (6) and equation (7) respectively we arrive at the expressions for the energy shifts in quantum dots derived in Ref. [24]. This is the manifestation of the fact that in the standard way of solving the problem the energy shift is assumed to be equal to the value of the real part of the corresponding self-energy function at the bare energy. The above approximative solution of equation (2) gives rise just to the same result. If the variations of the self-energy functions $C_{0}(z), C_{\sigma}(z)$ and $C_{d}(z)$ were weak enough, then in solving equation (2) one could restrict oneself to this approximative solution. However, as it follows from the results of calculation, this is not the case, and equation (3) must be solved exactly. Figure 1 shows that the self-interaction energy shifts obtained by solving equation (3) exactly differ dramatically from the approximative shifts $\text{Re} C_{m}(E_{m})$.

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