



## THE SHIFT OF ENERGY LEVELS OF A QUANTUM DOT IN SINGLE ELECTRON TRANSISTOR

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*Abstract.* The shift of Energy levels of a quantum dot in single electron transistor model is investigated. The self-energy function which related to shift of Energy levels, describing this interaction is added to a bare energy of a dot state. In the standard way of determining the self-interaction corrections to bare energies of quantum dots, 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.** In recent years interest arose into the study of transport through quantum dots. This interest is driven by two reasons. First, small devices like quantum dots open the possibility for future applications in electronics as transistors, memory cells, sensors etc. Small devices are especially interesting in high frequency applications due to their small capacitances. The second reason for the interest into these systems is a basic physics point of view. Quantum dots are similar to atoms or molecules since a certain number of electrons are confined in a potential. But, in contrast to real atoms, in these artificial systems the number of electrons, the size of the system and the strength of the confinement potential can easily be changed [1].

Single Electron Transistor (SET) has been made with critical dimensions of just a few nanometer using metal, semiconductor, carbon nanotubes or individual molecules [2-12]. A SET consists of a small conducting island (Quantum Dot (Q.D)) coupled to source and drain leads by tunnel junctions and capacitively coupled to one or more gate. Unlike Field Effect transistor, Single electron device based on an intrinsically quantum phenomenon, the tunnel effect. The electrical behaviour of the tunnel junction depends on how effectively barrier transmit the electron wave, which decrease exponentially with the thickness and on the number of electron waves modes that impinge on the barrier, which is given by the area of tunnel junction divided by the square of wave length. Figure (1) shows the schematic of SET [13, 14].

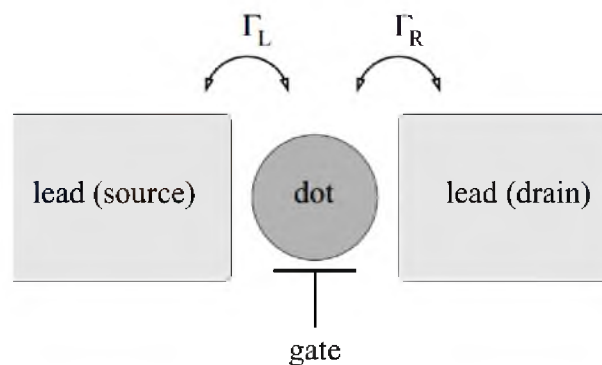


Fig. 1. Model of a quantum dot attached to two leads. We choose the left lead to be the source and the right lead to be the drain. Additionally a gate voltage is applied to the dot. Electrons tunnel from the dot to the leads

and vice versa with the respective tunneling rate,  $\Gamma_L$  to the left lead and  $\Gamma_R$  to the right lead.



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 by using generalized dynamical equation (GDE) we investigate the effect of such a self-interaction on the tunneling-induced shift of energy levels of a quantum dot.

**2. Theory.** In our study we use non-perturbative methods of its description based on the GDE, which in [15] has been derived as a direct consequence of the first principles 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 [16–19], nuclear physics [20–23] and quantum optics [24, 25]. 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  $G_0(z)$ . So 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

$$\langle m' | G_0^{(v)}(z) | m \rangle = \frac{\langle m' | m \rangle}{z - E_m - C_m(z)} \tag{1}$$

With  $|m\rangle$  being the eigenvectors of the free Hamiltonian ( $H_0 |m\rangle = E_0 |m\rangle$ ). 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

$$dC_m(z)/dz = -\langle m | M(z) [G_0^{(v)}(z)]^2 M(z) | m \rangle, \langle m | m \rangle = 1 \tag{2}$$

The condition

$$z - E_m^{(0)} - C_m(z) = 0 \tag{3}$$

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 approximated solution of this equation is

$$E_m \equiv E_m^{(0)} + C_m^{(0)}(E_m^{(0)}) \equiv E_m^{(0)} + \Delta E_m^L - i\Gamma_m/2, \text{ with } \Delta E_m^L \text{ and } \Gamma_m \text{ being the Lamb shift and the}$$

natural width of the energy level of the state  $|m\rangle$  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 [26, 27]

$$dC_m^{(0)}(z)/dz = -\langle m | H_I [G_0^{(v)}(z)]^2 H_I | m \rangle, \langle m | m \rangle = 1 \tag{4}$$

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 cannot be parameterized by a shift and a width, and one has to derive the self-energy function from a non-perturbative solution of the equations for  $C_m(z)$  and  $M(z)$ .

**2. Results and Discussion.** We study the self-interaction of a single-level quantum dot with arbitrary strong one-site Coulomb interaction tunnel coupled to two non-interacting leads. The Hamiltonian of system consisting of quantum dot and leads is described by [28]

$$H = H_{Q.D} + H_{T.P} + H_L \quad (5)$$

Where  $H_{Q.D}$  is the Hamiltonian of quantum dot,  $H_{T.P}$  is the Hamiltonian of tunneling process between leads and quantum dot and the Hamiltonian of leads is  $H_L$ .

The quantum dot can be described by the single-level Anderson impurity model, and  $H_{Q.D}$  equal to

$$H_{Q.D} = \sum_{\sigma=\uparrow,\downarrow} E d_{\sigma}^{\dagger} d_{\sigma} + U n_{\uparrow} n_{\downarrow} \quad (6)$$

Where the creation (annihilation) operator for an electron with spin  $\sigma$  on the dot is given by  $d_{\sigma}^{\dagger}$  and  $d_{\sigma}$ , also  $n_{\sigma} = d_{\sigma}^{\dagger} d_{\sigma}$  is the number operator. The on-site repulsion  $U$  describes the energy cost for double occupation (when we have two electrons in quantum dot) and stems from Coulomb interaction. The Hamiltonian  $H_{T.P}$  is given by

$$H_{T.P} = \sum_{\alpha,k,\sigma} V_{\alpha} C_{\alpha,k,\sigma}^{\dagger} d_{\sigma} + H.C. \quad (7)$$

Where  $V_{\alpha}$  is the momentum and spin-independent tunnel matrix element,  $C_{\alpha,k,\sigma}^{\dagger}$  ( $C_{\alpha,k,\sigma}$ ) is creation (annihilation) operators for electrons with spin  $\sigma$  and momentum  $k$  in lead and  $\alpha=l,r$ . The Hamiltonian  $H_L$  is given by

$$H_L = \sum_{\alpha,k,\sigma} E_{\alpha,k} C_{\alpha,k,\sigma}^{\dagger} C_{\alpha,k,\sigma} \quad (8)$$

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 dots as  $|\Psi_{\sigma}\rangle$  for a singly occupied dot with spin  $\sigma = \uparrow, \downarrow$  and an empty dot  $|\Psi_0\rangle$ . The corresponding energies are  $E_{\sigma}$  and  $E_0$ .

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 [28]

$$f_{\alpha}(\omega) = \left( 1 + \exp\left(\frac{\omega - \mu_{\alpha}}{K_B T}\right) \right)^{-1} \quad (9)$$



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. Solving the leading-order equation (4)

yields the following expressions for the self-energy function  $C_\sigma(z)$  of the quantum-dot state  $|\Psi_\sigma\rangle$

$$C_\sigma(z) = \sum_\alpha \frac{R_\alpha}{2\pi} \int d\omega \left( \frac{1-f_\alpha(\omega)}{z-\omega} + \frac{f_\alpha(\omega)}{z+\omega-2\varepsilon-U} \right) \quad (10)$$

And the self-energy function  $C_0(z)$  of the quantum-dot state  $|\Psi_0\rangle$

$$C_0(z) = 2 \sum_\alpha \frac{R_\alpha}{2\pi} \int d\omega \left( \frac{f_\alpha(\omega)}{z+\omega-\varepsilon} \right) \quad (11)$$

In our calculations we have used the fact that the part that is independent of the Fermi distribution function of  $C_\sigma(z)$  can be included into the correction to the energy of empty level. Taking into account this fact and using equation (1), self-energy function  $C_\sigma(z)$  will be

$$C_\sigma(z) = \sum_\alpha \frac{R_\alpha}{2\pi} \int_0^\infty d\omega \left[ \frac{1}{(1+\exp(\beta(\omega-\mu)))(\omega-z)} + \frac{1}{(1+\exp(\beta(\omega-\mu)))(\omega-(2\varepsilon+U-z))} \right] \quad (12)$$

Let us assume that the variations of these self-energy functions with  $z$  are weak. In this case the trivial shift of energy level of Q.D  $\delta E^{(ap)}$  can be considered as the approximated energy shifts of the corresponding energy levels of the quantum dot

$$\delta E^{(ap)} = C_\sigma(z = E_\sigma = \varepsilon) - C_0(z = E_0 = 0) \quad (13)$$

And the non-trivial shift of energy level of Q.D which describe fully shift of energy level of Q.D is

$$\delta E^{(ap)} = C_\sigma(z = E_\sigma = \varepsilon) - C_0(z = E_0 = 0) = \sum_\alpha \frac{R_\alpha}{2\pi} \left( \ln \left| \frac{\varepsilon}{\varepsilon+U} \right| + \ln \left| \frac{\varepsilon+U-\mu}{\varepsilon-\mu} \right| \right) \quad (14)$$

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 (2) where the results of calculations of the self-energy correction  $\delta\varepsilon = C_\sigma(z) - C_0(z)$  are depicted shows that the energy shifts obtained in this way can differ dramatically from their approximated values.

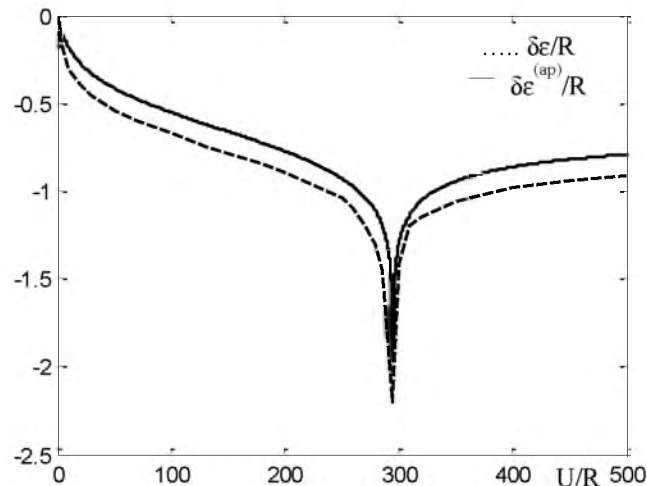


Fig. 2. Calculation results of the trivial (solid line) and non-trivial (dashed line) energy shifts of level of Q.D for the parameters  $\varepsilon = 5R$ ,  $\mu = 300R$  and for different values of the  $U$  at the zero temperature and in the assumption that the left lead is the same as the right lead.

**Conclusion.** In this paper by using equation (4) we have derived equations (10) and (11) for the self-energy functions of the quantum-dot states in SET. By putting  $z=E_{\sigma}$  and  $z=E_0$  in equation (10) and equation (11) respectively we arrive at the expressions for the energy shifts in quantum dots derived in [28]. 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 corresponding self-energy function at the bare energy. The above approximated solution of equation (2) gives rise just to the same result. If the variations of the self-energy functions  $C_0(z)$  and  $C_{\sigma}(z)$  were weak enough, then in solving equation (2) one could restrict oneself to this approximated solution. However, as it follows from the results of calculation, this is not the case, and equation (3) must be solved exactly. Figure (2) shows that the self-interaction energy shifts obtained by solving equation (3) exactly differ dramatically from the approximated shifts.

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