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Study of the Electron-Phonon Interaction on Quantum Dot

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ABSTRACT

In this present paper, we presented about the study of the electron-phonon interaction on quantum dot. First, we consider a one-dimensional (1D) electron system incorporating the electron-electron and electron-phonon interactions using the Luttinger model. We explicitly consider both the electron-optical-phonon interaction and the electron-acoustic-phonon interaction together with the electron-electron interaction.

Keywords : Electron- Phonon Interaction, FTL, Momentum, Quantum Dot

I. INTRODUCTION

Quantum dots (QD's) are ultra-low-dimensional structures with quantum confinement in all the spatial directions. Consequently, extensive investigations have been carried out on QD's during the last three decades using the parabolic confinement potential (PCP) model. A huge amount of literature [1-15] has indeed piled up on this subject. However, we have also pointed out in Chapter 1 that more recent experiments have suggested that the confining potential in a QD to be anharmonic and in this context, the Gaussian confinement potential (GCP) model has turned out to be a particularly useful model [16-21]. We shall refer to a QD with GCP as a Gaussian QD (GQD) and that with PCP as a parabolic QD (PQD). Because of the realistic nature of the Gaussian potential, a good number of investigations have been reported in recent years on GQD's [22-26]. Of course, one can also use power law anharmonic potentials, but these potentials suffer from divergence syndrome at large distances, while the Gaussian potential is by construction bound to give convergent results. One may, however, argue that in a QD the spatial coordinates never extend to a very large value to lead to any divergence problem, nevertheless, it is always appealing to work with a prescription that is mathematically sound and works in all limits. The interaction of an electron with longitudinal optical (LO) phonons is known to play an important role on the electronic properties of semiconductor QD's [27-30] since the electron-phonon interaction energy scale is comparable to the other energies scales in such QD's. Many works have predicted the polaronic effects in polar semiconductor QD's [31-34].

II. MATERIALS AND METHODS

The Hamiltonian of an electron moving in a GQD and interacting with the LO phonons of frequency ω_0 is given by

$$H' = \frac{p'^2}{2m^*} + V'(p') + h\omega_0 \sum_{q'} b_{q'}^+ b_{q'} + \sum_{q'} \left(\xi_{q'}' e^{-iq'.p} b_{q'}^+ + h.c\right) \quad (1)$$

where all the vectors are two-dimensional (2D). In Eqn. (4.1), the first term is the electron kinetic energy with p' as the momentum operator the electron and m* its effective mass, the second term is the confinement potential which we take as

$$V'(p') = -V_0' e^{-p'^2/2R'^2} \quad (2)$$

where p' is the position vector of the electron, V_0' the depth and the range of the potential, the third term is the phonon Hamiltonian, $b_{q'}^+ (b_{q'})$ being the creation (annihilation) operator of a phonon of wave vector q' with dispersionless frequency ω_0 and the fourth term is the electron-phonon interaction with $\xi_{q'}'$ as the electron-phonon interaction coefficient. We shall work in the Feynman units [30] in which the energy is scaled by the phonon energy $h\omega_0$, length by the weak-coupling polaron radius, $r_0 = (h/m^*\omega_0)^{1/2}$ and the wave vector by $q_0 = 1/r_0$. This is equivalent to putting $h = m^* = \omega_0 = 1$. In these units, the dimensionless Hamiltonian reads as:

$$H = \frac{H'}{h\omega_0} = \frac{p^2}{2} - V_0 e^{-p^2/2R^2} + \sum_q b_q^+ b_q + \sum_q \left(\xi_q e^{-iq.p} b_q^+ + h.c\right) \quad (3)$$

where

where everything is dimensionless, $p = \frac{p'}{r_0}, q = \frac{q'}{q_0}, p = \frac{p'}{hq_0}, V_0 = \frac{V_0'}{h\omega_0}, R = \frac{R'}{r_0}$, and $\xi_q = \frac{\xi_{q'}'}{h\omega_0} = (\sqrt{2}\pi\alpha/vq)^{1/2}$, where v is the dimensionless volume in two-dimensions and is the dimensionless electron-phonon coupling constant.

To make progress, we consider the Gaussian potential as a parabolic potential plus a perturbation. It is reasonable to make such an assumption since the deviation of the Gaussian potential from the parabolic potential would be very small for small values of r. So we rewrite the Hamiltonian Eqn.(4.3) as

$$H = H_0 + H_1 + H_2 \quad (4)$$

where

$$H_0 = \frac{p^2}{2} + \left[\frac{1}{2}\omega_h^2 p^2 - V_0\right] + \sum_q b_q^+ b_q \quad (5)$$

$$H_1 = -\lambda\left[\frac{1}{2}\omega_h^2 p^2 + V_0\left(e^{-p^2/2R^2} - 1\right)\right] \quad (6)$$

$$H_2 = \sum_q \left(\xi_q e^{-iq.p} b_q^+ + h.c\right) \quad (7)$$

where $\lambda = 0$ for PQD, $\lambda = 1$ for GQD, $\omega_h^2 = V_0^2/R^2$, and H_1 and H_2 are the perturbations. We include the contribution from within the mean-field approximation (MFA) as:

$$H_1 = \lambda\left[\frac{V_0}{<p^2>} - \frac{1}{2}\omega_h^2 - V_0\frac{<e^{-p^2/2R^2}>}{<p^2>}\right]p^2 \quad (8)$$

where the expectation values are calculated with respect to the GS wave function (Ψ_{GS}) of the space part of the unperturbed harmonic oscillator Hamiltonian with frequency ω_h i.e., $\Psi_{GS} = (\omega h/\pi)^{1/2} \exp\left(-\frac{\omega_h p^2}{2}\right)$. With this Ψ_{GS} we obtain,

$$< p^2 >= \frac{1}{\omega_h} \quad (9)$$

and

$< e^{-p^2/2R^2} >= 2\omega_h R^2(1+2\omega_h R^2)^{-1}$ (10)

The Total Hamiltonian then reads

$H = \frac{p^2}{2} + \frac{1}{2}w^2p^2 - V_0 + \sum_q b_q^+ b_q + \sum_q \left(\xi_q e^{-iq.p} b_q^+ + h.c\right)$ (11)

with the

$\omega = \left[(1-\lambda)\omega_h^2 + 2\lambda V_0 \omega_h \{1 - 2\omega_h R^2(1+2\omega_h R^2)^{-1}\right]^{½}$ (12)

which is actually $\frac{\omega'}{\omega_0}$where ω' is the effective confinement frequency in actual units. The effective unperturbed energy (in Feynman units) is thus given by:

$E^0_{j_1,j_2} = (j_1 + j_2 + 1)w - V_0$ (13)

and we write the total energy corresponding to H as $E_n=E_n/hw_0$, where E_n is the energy in actual units and is the energy in Feynman units. We shall study the effect of H_2 using the perturbation theory and calculate the correction ΔE_n to the effective unperturbed electronic energy. Because of the presence of degeneracy in our problem, we need to use a degenerate perturbation theory and we shall employ the IWBPT [31-34]. The advantage with IWBPT is that it gives the correct pinning behaviour for weak electron-phonon interaction. The second-order correction to the unperturbed energy due to the electron-phonon interaction is given by

$\Delta E_n = -\sum_j \sum_{\vec{q}} \frac{\left|\langle \varphi_j^0(\rho)\left|\xi_q e^{-iq.\rho}\right|\varphi_n^0(\rho)\rangle\right|^2}{E_j^0 - E_n^0 - \Delta_n + 1}$ (14)

with $\Delta_n = \Delta E_n - \Delta E_0^{RSPT}$where ΔE_0^{RSPT} is the Rayleigh–Schr dinger perturbation theory (RSPT) correction to the GS for the electron-phonon interaction and $\varphi_j^0(\vec{r})$is the wave function of a harmonic oscillator with frequency ω. Since ΔE_n is present on the right-hand side, we need to calculate the energy self-consistently. Eqn. (14) with $\Delta_n = 0$ gives the RSPT result which works well for the GS when ω <<1 . In Eqn. (14), if we put $\Delta_n = \Delta E_n$, that will be the case for Wigner-Brillouin Perturbation theory (WBPT) which can actually take care of the splitting of the degenerate energy levels. Eqn. (14) with $\Delta_n = \Delta E_n - \Delta E_0^{RSPT}$ is the case for IWBPT which gives the correct pinning effect.

To perform the summation in Eqn. (4.14), we use the following relation

$\frac{1}{E_j^0 - E_n^0 - \Delta_n + 1} = \int_0^\infty e^{-(E_j^0 - E_n^0 - \Delta_n + 1)t} dt$ (15)

After simplifications, Eqn. (4.14) yields the energy corrections to the GS and the first two ES's as

$-\frac{\Delta E_{GS}}{16\gamma} = B\left(\frac{1}{\omega}, \frac{1}{2}\right)$ (16)

$-\frac{\Delta E_{1ES}}{4\gamma} = B\left(\frac{1-\Delta_1}{\omega} - 1\frac{1}{2}\right) + 3B\left(\frac{1-\Delta_1}{\omega}, \frac{1}{2}\right)$ (17)

$-\frac{\Delta E_{2ES}}{\gamma} = 5B\left(\frac{1-\Delta_2}{\omega} - 2\frac{1}{2}\right) + 6B\left(\frac{1-\Delta_2}{\omega}, 1\frac{1}{2}\right) + 13B\left(\frac{1-\Delta_2}{\omega}, \frac{1}{2}\right)$ (18)

where $\gamma = \left[\alpha\sqrt{\pi}/32\sqrt{\omega}\right]$ and $B(x,y)$ is the beta function. In general, for an -dimensional case the expressions are as follows:

$-\frac{\Delta E_{GS}^{ND}}{8\beta} = B\left(\frac{1}{\omega}, \frac{1}{2}\right)$ (19)

$-\frac{\Delta E_{1ES}^{ND}}{4\beta} = B\left(\frac{1-\Delta_1}{\omega} - 1\frac{1}{2}\right) + (2N-1)B\left(\frac{1-\Delta_1}{\omega}, \frac{1}{2}\right)$ (20)

$$-\frac{\Delta E_{1ES}^{ND}}{\beta} = (2N^2 - 4N + 5)B\left(\frac{1-\Delta_2}{\omega} - 2, \frac{1}{2}\right) + (4N-1)B\left(\frac{1-\Delta_2}{\omega} 1, \frac{1}{2}\right)$$

$+(2N^2 + 4N - 3)B\left(\frac{1-\Delta_2}{\omega}, \frac{1}{2}\right)$ (21)

Where,

$$\beta = -\frac{\alpha}{32\sqrt{\omega}}\left[\frac{I\left(\frac{N-1}{2}\right)}{I\left(\frac{N+1}{2}\right)}\right] \quad (22)$$

In the present problem, the region of interest is: $1-\Delta_n \cong n\omega$ and we consider the term which makes the maximum contribution to the energy in this region for each state (n=1, 2,…) and we obtain,

$$\Delta E_{1ES} = -\frac{\alpha\sqrt{\pi}}{8}\frac{\sqrt{\omega}}{1-\Delta_1-\omega} \quad (23)$$

$$\Delta E_{1ES} = -\frac{5\alpha\sqrt{\pi}}{32}\frac{\sqrt{\omega}}{1-\Delta_2-2\omega} \quad (24)$$

To see the pinning of the energy levels E_{1ES} and E_{2ES} to $[E_0^0 + 1$ phonon state], we have to consider the large limit. In this limiting case, a self-consistent calculation leads us to the following results:

$$E_{1ES} = \frac{N}{2}\omega + 1 + \Delta E_{GS} - \frac{\alpha\sqrt{\pi}\sqrt{\omega}}{8(\omega-1-\Delta E_{GS})} \quad (25)$$

$$E_{2ES} = \frac{N}{2}\omega + 1 + \Delta E_{GS} - \frac{5\alpha\sqrt{\pi}\sqrt{\omega}}{32(2\omega-1-\Delta E_{GS})} \quad (26)$$

III.RESULTS AND DISCUSSIONS

Our calculation is valid for any polar semiconductor QD. However, we shall apply our theory to GaAs and InSb QD's for the sake of concreteness. For GaAs, we take $\alpha = 0.07$, $\omega_0 = 5.5 \times 10^{13}/sec$ and $m^* = 0.6 \times 10^{-28} gm$ so that we have $h\omega_0 = 36.25 meV$ and r_0 = 5.63 nm. Thus, for GaAs, V_0 = 0.4 means: $0.4 \times h\omega_0 = 14.6\, meV$ and R = 3 means: 3 × r_0 = 16.9 nm. For InSb, we take $\alpha = 0.02$, $\omega_0 = 3.7 \times 10^{13}/sec$ and $m^* = 0.1279 \times 10^{-28} gm$ so that for InSb we have $h\omega_0 = 24.38\, meV$ and r_0 = 14.93nm. First of all, we notice that the relationship between the effective confinement frequency and the range of the Gaussian potential is not so simple. In Fig 1, we plot ω vs. $\frac{1}{\sqrt{2}}$ for a GaAs QD and interestingly enough, the behaviour is almost linear unless R is extremely large. In this section, we shall always mean the confinement potential to be GCP unless otherwise mentioned.

In Fig 2, we plot the GS and the first two ES energies (E_0, E_1 and E_2) of an electron confined in a GaAs QD as a function of the effective QD size for two values of the depth of the Gaussian potential, V_0. For a particular value of V_0 and the electron-phonon coupling constant α, as R increases, energies decrease monotonically. However, at small values of R, as R increases, the energies decrease very rapidly for all the states and at large values of R, the energies decrease very slowly, ultimately saturating to the bulk limits.

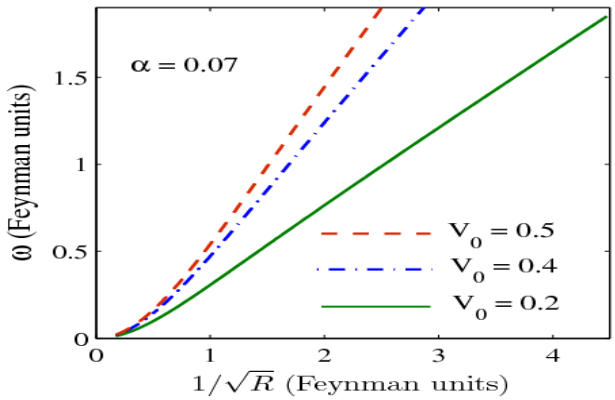

Fig. 1 : ω vs. $\frac{1}{\sqrt{2}}$ for a GaAs QD for three values of V_0.

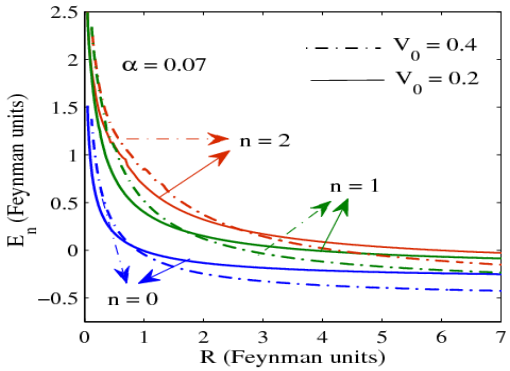

Fig. 2: GS and first two ES energies (E_0, E_1 and E_2) of a GaAs QDas a function of R for two values of V_0.

When the QD size is small, the uncertainty in the momentum is expected to be large and as a result the kinetic energy itself will be large and hence the total energy increases as R decreases. Thus, the polaronic effect is extremely significant for small QD's as has been predicted by a host of investigations. It is also interesting to note that at small energies increase with increasing V_0, while above a certain QD size (which is different for different states), energies decrease with increasing V_0. This behavior can be roughly understood from the results of the finite square potential well problem. If the depth of the potential is and width of the well is R, then the GS energy can be written as $E_0 = V_0\cos^2 (m^*R^2E_0/2h^2)$. When R is small, the kinetic energy is large and therefore can be approximated by the kinetic energy on the right-hand side of the above equation and then as V_0 in increased, E_0 increases almost linearly. On the other hand, when R is large, the kinetic energy may be neglected and the particle can be expected to lie at the bottom of the potential well and so can be approximated by $[-V_0]$ on the right-hand side of the above equation. In this case, as V_0 increases, E_0 decreases, at least for the parameter values considered in this work.

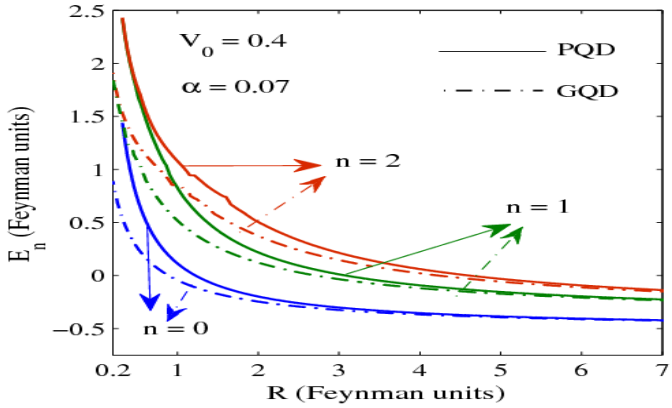

Fig. 3: Variation of E_0, E_1 and E_2 of a GaAs QD with GCP and PCP as a function of R for $V_0 = 0.4$

In Fig 3, we compare the energies of a GaAs QD obtained from the GCP and PCP models. It is clearly evident that the PCP model, in general, overestimates the energy. At large values of R, however, the results, as expected, become independent of the confinement potential models and consequently both the models give the same results which are, of course, the bulk limits. In the presence of the electron-phonon interaction, these degeneracies are lifted and the energy values are lowered. One can see from the figure that as approaches 1, the first ES energy (the solid curve) starts bending downward and with

further increase in ω gets pinned to the GS plus one-phonon energy. The removal of degeneracy by the electron-phonon interaction and the subsequent lowering of energy values are clear indications of the polaronic effects in a QD. Experimentally one should be able to observe the splitting and the pinning behavior of the energy levels and verify the existence of the polaronic effect in a QD.

IV. CONCLUSION

We have shown that the nearest-neighbour electron-phonon interaction has a stronger effect on PC than the onsite electron-phonon interaction has. In addition to this, we have shown that PC decreases with temperature and the PC curve becomes smoother with temperature. It is found that in the presence of electron-phonon interaction PC develops a sharp peak at low temperature. We have furthermore observed that the number of electrons in a QR can also change the magnitude and phase of the PC and therefore the chemical potential is expected to have a significant effect on PC.

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