Original Research Article

Modified Lee-Low-Pines Polaron in Spherical Quantum Dot in an Electric Field. Part 2: Weak Coupling and Temperature Effect

Abstract

In this paper, we investigated the influence of electric field on the ground state energy of polaron in spherical semiconductor quantum dot (QD) using modified Lee Low Pines (LLP) method. The numerical results show the increase of the ground state energy with the increase of the electric field and the confinement lengths. The modulation of the electric and the confinement lengths lead to the control of the decoherence of the system. It's also seen that temperature is the decrease function of the electron-phonon coupling constant and longitudinal confinement length and it increase with the electric field strength.

Keywords:*Electric field, modified LLP, Polaron Energy, Quantum Dot, Weak coupling*

1- Introduction

Due to the recent progress achieved in nanotechnology, it has become possible to fabricate low dimensional semiconductor structures. Special interest is being devoted to the quasi zero dimensional structures, usually referred to as quantum dots (QD) [1-9]. In such nanometer QD's, some novel physical phenomena and potential electronic device applications have generated a great deal of interest. They may give theoretical physicists great challenges to develop the theory based on the quantum mechanical regime. Recently, much effort [10-12] has been focused on exploring the polaron effect of QD's. Roussignol et *al*. [10] have shown experimentally and explained theoretically that the phonon broadening is very significant in very small semiconductor QD's. Some have also observed [11-12] that the polaron effect is more important if the dot sizes are reduced to a few nanometers. More recently, the related problem of an optical polaron bound to a Coulomb impurity in a QD has also been considered in the presence of a magnetic field.

The theoretical investigation of the polaron properties was performed by using the standard perturbation techniques [13], by the variational Lee-Low-Pines method [14-15] and by modified LLP approach [16-17], by Feynman path integral method [18], by numerical diagonalization [19], or by Green function methods [20]. The experimental data [21] show, in particular, a large splitting width near the one-phonon and two-phonon resonance in aInAs/GaAs QD. This was accounted for by the theoretical model via a numerical diagonalization of the Fröhlich interaction

[19]. The required value of the Fröhlich constant was much larger (by a factor of two [19]), than measured in bulk. In [18] using the Feynman path integral method, the authors observed that the quadratic dependence of the magnetopolaron energy is modulated by a logarithmic function and strongly depend on the Fröhlich electron–phonon coupling constant structure and cyclotron radius. Furthermore the effective electron-phonon coupling is enhanced by high confinement or high magnetic field. In [21] the polaron energy in QD was calculated using a LLP approach and it was found that the polaronic effect is more pronounced for small dot sizes. In [16], using a modified LLP approach, the number of phonons around the electron, and the size of the polaron for the ground state, and for the first two excited states is calculated via the adiabatic approach.

It is important to note that, all works done are not used the modified LLP method to solve the problem of polaron subjected to an electric field. It is also instructive from the works presented above, to recall that polarons are often classified according to the Fröhlich electron-phonon coupling constant. Because it recovers simultaneously all couplings types characterizing Fröhlich electron-phonon coupling, the Feynman path integral method [18] has been seen as one of the best. The main feature of the method presented here is the modification of the LLP approach [16] by introducing a new parameter $b_1 \; and \, b_2$ in the traditional LLP approach, which permits us to obtain an "all coupling" polaron theory. Here the coupling is weak if $\boldsymbol{b_1 = b_2 \to 1}$, strong coupling if $\boldsymbol{b_1 = b_2 \to 0}$ and intermediate between these ranges.

In this work, we study the influence of the electric field on the polaron ground state energy. It has the following structure: In section two, we describe the Hamiltonian of the system while in section 3 the modified LLP method is presented and analytical results of the ground state energy, polaron effective mass are obtained. In section 4, the temperature effect on the average number of bulk LO phonons are given according to the quantum statistics theory is giving. In section 5, we present numerical results and discussions. Section 6 is devoted to the conclusion.

2- Hamiltonian of system

The electron under consideration is moving in a polar crystal with three dimensional anisotropic harmonic potential, and interacting with the bulk LO phonons, under the influence of an electric field along the $\boldsymbol{\rho}-$ direction. The Hamiltonian of the electron-phonon interaction system can be written as [22]

$$H = H_e + H_{ph} + \sum_Q V_Q \left[a_Q e^{iQr} + a_Q^{+} e^{-Qr} \right] \qquad (2.1)$$

where $\boldsymbol{H_e}$ represents the electronic Hamiltonian and is given by

$$H_e = \frac{p^2}{2m} + \frac{1}{2} m \omega_1^2 \rho^2 + \frac{1}{2} m \omega_2^2 z^2 - e^* F \rho \; (2.2)$$

where p is the momentum, ω_1 and ω_2 measure the confinement in the $\rho -$ direction and $z -$ direction respectively.

H_{ph} is the phonon Hamiltonian defined as

$$H_{ph} = \sum_Q a_Q^+ a_Q \qquad (2.3)$$

Where $a_Q^+ (a_Q)$ are the creation (annihilation) operators for LO phonons of wave vector $Q = (q, q_z)$,

and V_Q and α is the amplitude of the electron-phonon interaction and the coupling constant respectively given by

$$V_q = i\left(\frac{\hbar\omega_{LO}}{q}\right)\left(\frac{\hbar}{2m\omega_{LO}}\right)^{1/4}\left(\frac{4\pi\alpha}{V}\right)^{1/2} \qquad (2.5)$$

$$\alpha = \left(\frac{e^2}{2\hbar\omega_{LO}}\right)\left(\frac{2m\omega_{LO}}{\hbar}\right)^{1/2} \qquad (2.6)$$

3- Modified LLP method and analytical results of ground state energy of the polaron

Adopting the mixed-coupling approximation of [23] we propose a modification to the first Lee-Low-Pines (LLP)-transformation by inserting two variational parameters b_1 and b_2 .

Our new unitary transformation is now

$$U_1 = \exp\left[i\left[(P_\rho - \boldsymbol{P}_\rho)\rho b_1 + (P_z - \boldsymbol{P}_\rho) z b_2 \right]\right] \qquad (3.1)$$

With

$$P = p + \sum_Q a_Q^+ a_Q \qquad (3.2)$$

is the total momentum of the polaron and

$$\boldsymbol{P} = \sum_{Q} Q a_Q^{+} a_Q \tag{3.3}$$

is the momentum of the phonon.

The two new variational parameters are supposed to trace the problem from the strong coupling case to the weak coupling limit and to interpolate between all possible geometries.

The second transformation is of the form [1]

$$\boldsymbol{U}_2 = \sum_{Q} u_Q (a_Q^{+} - a_Q) \tag{3.4}$$

where $\boldsymbol{u}_Q$ is a variational function. This transformation is called the displaced oscillator which is related to the phonon operators via the phonon wave vector through the relation

$$\varphi_{ph} = \boldsymbol{U}_2 \left| 0_{ph} \right\rangle \tag{3.5}$$

where $\left| 0_{ph} \right\rangle$ is the phonon vacuum state since at low temperature there will be no effective phonons.

Applying the transformation in (3.1) on the Hamiltonian (2.1), we obtained

$$\begin{aligned} H^{(1)} &= \boldsymbol{U}_1^{-1} H \boldsymbol{U}_1 \\ &= \frac{p^2}{2m} + \frac{1}{2} m\omega_1^2 \rho^2 + \frac{1}{2} m\omega_2^2 z^2 - e^* F\rho + b_1^2 (P_\rho - \boldsymbol{P}_\rho)^2 + \\ &+ 2b_1 p_\rho (P_\rho - \boldsymbol{P}_\rho) + b_2^2 (P_z - \boldsymbol{P}_z)^2 + 2b_2 p_z (P_z - \boldsymbol{P}_z) + \\ &+ \sum_Q a_Q^{+} a_Q + \sum_Q V_Q \left[a_Q e^{-i(b_1 q.\rho + b_2 q_z z)} e^{iQ.r} + a_Q^{+} e^{i(b_1 q\rho + b_2 q_z z)} e^{-iQ.r} \right] \end{aligned} \tag{3.6}$$

Applying the transformation (3.4) on (3.6), and express in Fröhlich unit i.e. $2m = \omega_{LO} = \hbar = 1$, we obtained the ground state energy ε_g

$$\begin{aligned}\varepsilon_g = & \langle 0_e | p^2 + \frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2 z^2 - e^* F\rho | 0_e \rangle + b_1^2 P_\rho^2 - 2b_1^2 P_\rho \boldsymbol{P}_\rho^{(0)} + b_1^2 \left(\boldsymbol{P}_\rho^{(0)}\right)^2 + \\ & + \sum_Q u_Q^2 \left(1 + b_1^2 q^2 + b_2^2 q_z^2\right) + \langle 0_e | \langle 0_{ph} | 2b_1 p_\rho \left(P_\rho - \boldsymbol{P}_\rho + \boldsymbol{P}_\rho^{(1)} - \boldsymbol{P}_\rho^{(0)}\right) | 0_{ph} \rangle | 0_e \rangle + \\ & + \sum_Q V_Q u_Q \langle 0_e | (\exp[-i(b_1 q.\rho + b_2 q_z z)] \exp(iQ.r) - \exp[i(b_1 q.\rho + b_2 q_z z)] \exp(-iQ.r)) | 0_e \rangle + \\ & + b_2^2 P_z^2 - 2b_2^2 P_z \boldsymbol{P}_z^{(0)} + b_2^2 \left(\boldsymbol{P}_\rho^{(0)}\right)^2 + \langle 0_e | \langle 0_{ph} | 2b_2 p_z \left(P_z - \boldsymbol{P}_z + \boldsymbol{P}_z^{(1)} - \boldsymbol{P}_z^{(0)}\right) | 0_{ph} \rangle | 0_e \rangle\end{aligned} \tag{3.7}$$

where

$$\boldsymbol{P}^{(1)} = \sum_Q Q u_Q \left(a_Q + a_Q^+\right) \tag{3.8}$$

And

$$\boldsymbol{P}^{(0)} = \sum_Q Q u_Q^2 \tag{3.9}$$

To evaluate this expression, we introduce the linear combination operators of the position and momentum of the electron by the following relation:

$$\begin{aligned} p_\mu &= \sqrt{\frac{m\hbar\lambda_1}{2}}(\sigma_\mu + \sigma_\mu^+) \\ x_\mu &= i\sqrt{\frac{\hbar}{2m\lambda_2}}(\sigma_\mu - \sigma_\mu^+) \\ p_z &= \sqrt{\frac{m\hbar\lambda_1}{2}}(\sigma_z + \sigma_z^+) \\ x_\mu &= -i\sqrt{\frac{\hbar}{2m\lambda_2}}(\sigma_z - \sigma_z^+) \end{aligned} \tag{3.10}$$

Where the index μ refers to the x and y directions, λ_1 and λ_2 are variational parameters, $\boldsymbol{\sigma}$ and $\boldsymbol{\sigma}^+$ are respectively the annihilation and creation operators for electron. Using the following commutator, $\left[x_\mu, p_\upsilon\right] = i\hbar\delta_{\mu\upsilon}$ and performing the required calculations, we may write the ground state energy as:

$$\begin{aligned}\varepsilon_g = & \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - 2\frac{e^* F}{\sqrt{\lambda_1}} + b_1^2 P_\rho^2 - 2b_1^2 P_\rho \boldsymbol{P}_\rho^{(0)} + b_1^2 \left(\boldsymbol{P}_\rho^{(0)}\right)^2 + \\ & + \sum_Q u_Q^2 \left(1 + b_1^2 q^2 + b_2^2 q_z^2\right) + b_2^2 P_z^2 - 2b_2^2 P_z \boldsymbol{P}_z^{(0)} + b_2^2 \left(\boldsymbol{P}_z^{(0)}\right)^2 - 2\sum_Q V_Q u_Q S_Q\end{aligned} \tag{3.11}$$

With

$$S_Q = \langle 0_e | \exp[\pm i(b_1 q.\rho + b_2 q_z z)] \exp(\pm iQ.r) | 0_e \rangle \quad (3.12)$$

this expression can be written as

$$S_Q = \exp\left[-(1-b_1)^2 \frac{q^2}{2\lambda_1}\right] \exp\left[-(1-b_2)^2 \frac{q_z^2}{2\lambda_2}\right] \qquad (3.13)$$

Minimizing (3.11) with respect to the variational function $\boldsymbol{u_Q}$ we obtain

$$\left[1 + b_1^2 q^2 + b_2^2 q_z^2 + 2b_1^2 q\left(\boldsymbol{P}_\rho^{(0)} - P_\rho\right) + 2b_2^2 q_z\left(\boldsymbol{P}_z^{(0)} - P_z\right)\right] u_Q = V_Q S_Q \qquad (3.14)$$

Solving (3.14) with respect to $\boldsymbol{u_Q}$, with the assumption that $\boldsymbol{P}^{(0)}$ differ from the total momentum by a scalar factor $\eta\left(\boldsymbol{P}^{(0)} = \eta P\right)$, we get

$$u_Q = \frac{V_Q S_Q}{1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1-\eta) - 2b_2^2 q_z P_z (1-\eta)} \qquad (3.15)$$

Substituting (3.15) into (3.11) we obtain

$$\begin{aligned} \varepsilon_g = {} & \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - 2\frac{e^* F}{\sqrt{\lambda_1}} + b_1^2 P_\rho^2 (1-\eta)^2 + b_2^2 P_z^2 (1-\eta)^2 + \\ & + \sum_Q \frac{V_Q^2 S_Q^2 \left(1 + b_1^2 q^2 + b_2^2 q_z^2\right)}{\left[1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1-\eta) - 2b_2^2 q_z P_z (1-\eta)\right]^2} - \\ & - 2\sum_Q \frac{V_Q^2 S_Q^2}{\left[1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1-\eta) - 2b_2^2 q_z P_z (1-\eta)\right]} \end{aligned} \qquad (3.16)$$

But $\boldsymbol{\varepsilon_g (P)}$ may be well represented by the first two terms of a power series expansion in $\boldsymbol{P^2}$ as in [23]

$$\varepsilon_g(P) = \varepsilon_g(0) + \beta \frac{P^2}{2} + 0\left(P^4\right) + \ldots \qquad (3.17)$$

with $\boldsymbol{\beta^{-1}}$ gives the effective mass of the polaron. Comparing (3.16) and (3.17) we obtain for the ground state energy

$$\varepsilon_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - 2\frac{e^* F}{\sqrt{\lambda_1}} - \sum_Q \frac{V_Q^2 S_Q^2}{\left[1 + b_1^2 q^2 + b_2^2 q_z^2\right]} \qquad (3.18)$$

Substituting (3.13) in the ground state energy (3.18), we obtained

$$\varepsilon_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - 2\frac{e^* F}{\sqrt{\lambda_1}} - \sum_Q \frac{V_Q^2 \exp\left[-(1-b_1)^2 \frac{q^2}{\lambda_1}\right] \exp\left[-(1-b_2)^2 \frac{q_z^2}{\lambda_2}\right]}{\left[1 + b_1^2 q^2 + b_2^2 q_z^2\right]} \qquad (3.19)$$

re-arranging this expression, we finally obtained the ground state energy

$$\varepsilon_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{1}{2\lambda_1 l_1^4} + \frac{1}{4\lambda_2 l_2^2} - 2\frac{e^* F}{\sqrt{\lambda_1}} - \sum_Q \frac{V_Q^2 \exp\left[-(1-b_1)^2 \frac{q^2}{\lambda_1}\right] \exp\left[-(1-b_2)^2 \frac{q_z^2}{\lambda_2}\right]}{\left[1 + b_1^2 q^2 + b_2^2 q_z^2\right]} \qquad (3.20)$$

where $l_1 = \sqrt{\frac{\hbar}{m\omega_1}}$ *and* $l_2 = \sqrt{\frac{\hbar}{m\omega_2}}$ are the confinement length in $\boldsymbol{x} - \boldsymbol{y}$ $-$plane and $\boldsymbol{z}$ $-$ direction respectively

4- Temperature Effect

The polaron is no longer in the ground state when it’s in the ground state at a finite temperature. The properties of polaron are described by the statistical average of the phonons number. The average number of bulk LO phonons are given according to the quantum statistics theory as

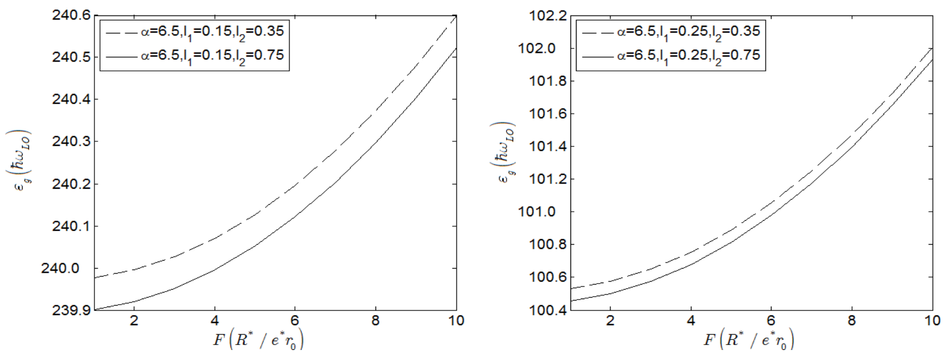
$$\overline{N}_0 = \left[\exp\left(\frac{\varepsilon_g}{K_B T}\right) - 1\right]^{-1}$$

(4.1)

where K_B is the Boltzmann constant and T is the temperature of the system.

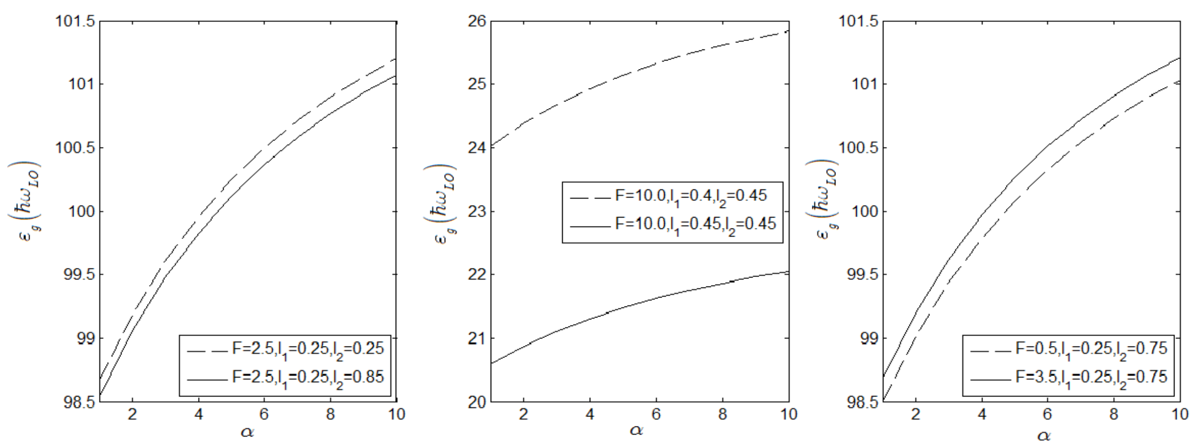
5- Numerical results and discussions

For the numerical results, we consider the weak coupling case, i.e. $b_1 = b_2 = 1$. In this part, we show the numerical results of the ground state energy versus the electron-phonon coupling strength, the cyclotron frequency and the confinement lengths with the following polaron units: $R^* = \hbar\omega_{LO}$ and $r_0 = \left(\hbar/2m^*\omega_{LO}\right)^{1/2}$



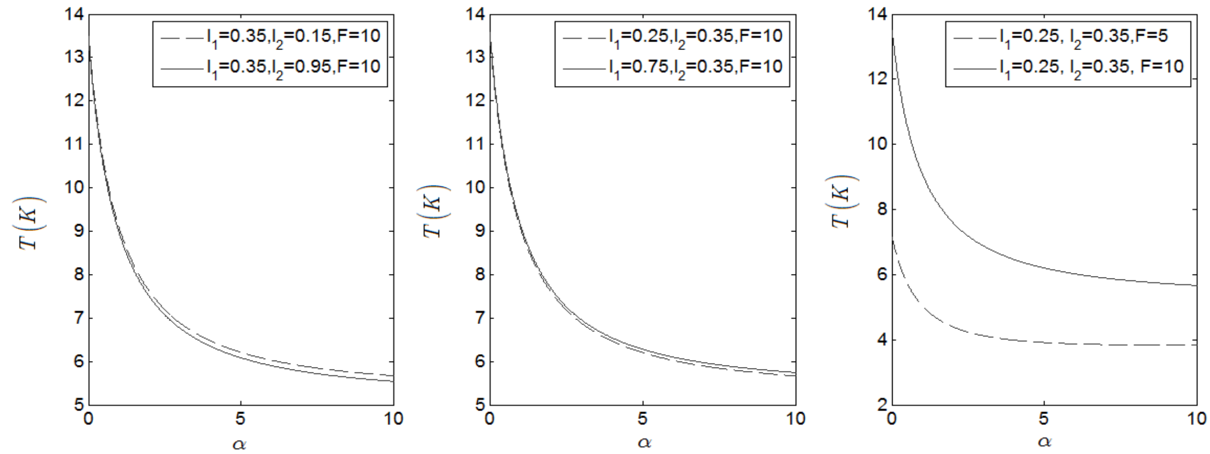
(a)

Figure 1: Ground state energy ε_g as a function of electric field F for (a) $\alpha = 6.5, l_1 = 0.15, l_2 = 0.35$; (b) $\alpha = 6.5, l_1 = 0.25, l_2 = 0.35$



(a)

Figure 2: Ground state energy ε_g as electron-phonon coupling constant α for (a) $F = 2.5$ and $l_1 = 0.25$; (b) $F = 10.0$ and $l_2 = 0.45$; (c) $l_1 = 0.25$ and $l_2 = 0.75$



(a)

Figure 3: Temperature as electron-phonon coupling constant α for

(a) $F = 10.0 \text{ and } l_1 = 0.35$;(b) $F = 10.0 \text{ and } l_2 = 0.35$; (c) $l_1 = 0.25 \text{ and } l_2 = 0.35$

In figure 1, we have plotted the ground state energy ε_g of polaron as a function of electric field F for $\alpha = 6.5, l_1 = 0.15, l_2 = 0.35 \text{ and } l_2 = 0.75$ (figure (1a)) and $\alpha = 6.5, l_1 = 0.25, l_2 = 0.35 \text{ and } l_2 = 0.75$ (figure (1b)). The ground state energy is the increase function of electric field. This is because the electric field leads to the electron energy increment and makes the electrons interact with more phonons. This indicates a new way to control the QD energies via the electric field. In fact, the electric field plays an important role in low-dimensional materials. For example, both the quantum decoherence process and the electron's probability density are affected by it. Thus, here we find a suitable two-state system by adjusting the electric field, which is crucial in constructing a qubit [24-26].

In figure 2, we have plotted the ground state energy ε_g as electron-phonon coupling constant α for(a) $F = 2.5 \text{ and } l_1 = 0.25$; (b) $F = 10.0 \text{ and } l_2 = 0.45$; (c) $l_1 = 0.25 \text{ and } l_2 = 0.75$. These figures show that the ground state energy increase with the increase of electron-phonon coupling constant and the decrease with the increase the confinement length. With the increase of the harmonic potential($\omega_1 \text{ and } \omega_2$), the energy of the electron and the interaction between the electron and the phonons, which take phonons as the medium, are enhanced because of the smaller particle motion range. The larger the electron-phonon coupling constant, the stronger the ground state energy of polaron. This result is similar to the one obtained in [27-28].

In figure 3, we have plotted the Temperature as electron-phonon coupling constant α for (a) $F = 10.0 \text{ and } l_1 = 0.35$;(b) $F = 10.0 \text{ and } l_2 = 0.35$;(c) $l_1 = 0.25 \text{ and } l_2 = 0.35$

In weak coupling range, the temperature is the decrease function of the electron-phonon coupling constant and the decrease function of the confinement lengths strength. When the electron motion range decrease, the energy of interaction increase and the motion of electron and phonons make the medium hot. The temperature is the increase function of the electric field strength; this is because the electric field is a an external perturbation source and it acceleration in motions of particles (electron and phonons) in the QD. The result is in according to the result obtained by Jing-Lin Xiao[29-30]

6- Conclusion

In conclusion, with the use of modified LLP method, we have study the energy levels of strong polaron in spherical quantum dot (QD)a weak coupling polaron in an anisotropic QDsubject the electric field. It is found that the ground state energy of the polaron is the increase function of the electric field; this is because the presence of electric field make phonons interact more with the electron. It’s also see that, with the good control of the confinement length and the electron coupling constant we can control the decoherence of the system. The enhancement of the coupling strength is very important in the construction of quantum computers since it leads to the conservation of its internal properties such as its superposition states against the influence of its environment, which can induce the construction of coherent states and cause coherence quenching. The temperature is the increase function of electric field and the decrease function of confinement lengths.

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