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

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Authors' contributions

This work is the fruit of teamwork. Author AJF and HF designed the study and wrote the protocol, NI and SCK wrote the first draft of the manuscript. Author MT and MPTD managed the analyses of the study and performed simulations. Author AVW managed the literature searches. Author LCF helped in the writing of the final draft. All authors read and approved the final manuscript.

Abstract

In this paper, we investigate the influence of an electric field on the ground state energy of a polaron in a spherical semiconductor quantum dot (QD) using the modified Lee Low Pines (LLP) method. The numerical results show an 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 enables the control of the decoherence of the system. It is also seen that the temperature is a decreasing function of the electron-phonon coupling constant and the longitudinal confinement length, whereas it increases with the electric field strength.

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

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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 QDs, some novel physical phenomena and potential electronic device applications have generated a great deal of interest. A great challenge has thus been laid on theoretical physicists, that of developing the theory based on the quantum mechanical regime. Recently, much effort [10-12] has been focused on exploring the polaron effect of QDs. Roussignol et *al*. [10] have shown experimentally and explained theoretically that the phonon broadening is very significant in very small semiconductor QD's. It has also been 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 has been performed using standard perturbation techniques [13], the variational Lee-Low-Pines method [14-15] the modified LLP approach [16-17], the Feynman path integral method [18], numerical diagonalization [19], and Green's function methods [20]. The experimental data [21] showed, in particular, a large splitting width near the one-phonon and two-phonon resonance in a InAs/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 that 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 depends on the Fröhlich electron–phonon coupling constant structure and the cyclotron radius. Furthermore, the effective electron-phonon coupling is enhanced by high confinement or a strong magnetic field. In [21] the polaron energy in a 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 the modified LLP method has not been used in any of the aforementioned works to solve the problem of a 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 types of coupling which characterize the Fröhlich electron-phonon coupling, the Feynman path integral method [19] has been seen as one of the best. The main feature of the method presented here is the modification of the LLP approach [17] by introducing new parameters 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 $b_1 = b_2 \to 1$, strong if $b_1 = b_2 \to 0$ 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 the analytical results of the ground state energy and the polaron's effective mass are obtained. In section 4, the temperature effect on the average number of bulk LO phonons is evaluated according to the quantum statistics theory. In section 5, we present numerical results and discussions. Section 6 is devoted to the conclusion.

2- Hamiltonian of the system

The motion of the electron under consideration is taking place in a polar crystal with a three dimensional anisotropic harmonic potential, and interacting with the bulk LO phonons, under the influence of an electric field along the $\rho -$ 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 H_e represents the electronic Hamiltonian and is given by

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

where p is the momentum while 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 $Q = (q, q_z)$,

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

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

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

3- Modified LLP method and analytical results of the 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

$$\boldsymbol{U}_1 = \exp\left[i\left[(P_\rho - \boldsymbol{P}_\rho)\rho b_1 + (P_z - \boldsymbol{P}_\rho) z b_2\right]\right] \quad (3.1)$$

With

$$\boldsymbol{P} = \boldsymbol{p} + \sum_{\boldsymbol{Q}} \boldsymbol{a}_{\boldsymbol{Q}}^{+}\boldsymbol{a}_{\boldsymbol{Q}} \quad (3.2)$$

being the total momentum of the polaron and

$$\boldsymbol{P} = \sum_{\boldsymbol{Q}} \boldsymbol{Q}\boldsymbol{a}_{\boldsymbol{Q}}^{+}\boldsymbol{a}_{\boldsymbol{Q}} \quad (3.3)$$

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]

$$\boldsymbol{U}_2 = \sum_Q u_Q (a_Q^+ - a_Q) \quad (3.4)$$

where $\boldsymbol{u}_{\boldsymbol{Q}}$ is a variational function. This transformation is called the displaced oscillator which is related to the phonon operators via the phonon wave vector by 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 temperatures there will be no effective phonons.

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

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

Applying the transformation (3.4) on (3.6), and expressing in Fröhlich units i.e. $\boldsymbol{2m = \omega_{LO} = \hbar = 1}$, we obtain the ground state energy $\boldsymbol{\varepsilon_g}$

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

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:

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

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

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

With

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

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 $\boldsymbol{P}^{(0)}$ differs from the total momentum by a scalar factor $\eta\left(\boldsymbol{P}^{(0)} = \eta P\right)$, we get

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

Substituting (3.15) into (3.11) we obtain

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

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]

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

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

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

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

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

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

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

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

4- Temperature Effect

The polaron is no longer considered to be in the ground state when it is at a non-zero temperature. The properties of the polaron are then described by the statistical average of the phonon number. The average number of bulk LO phonons is given according to the quantum statistics theory as

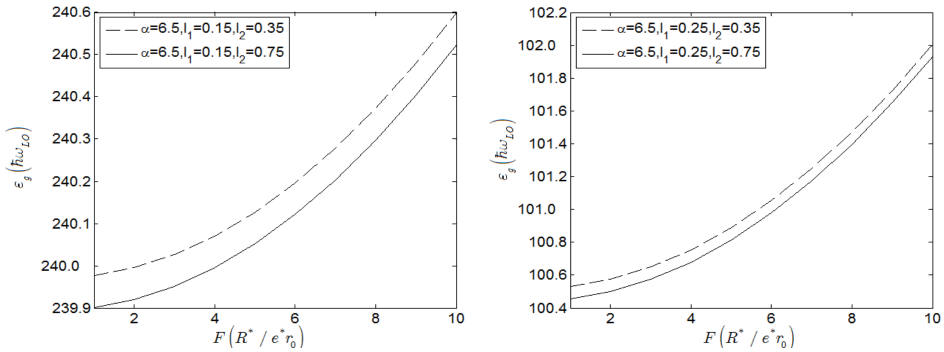
$$\overline{N}_0 = \left[\exp\left(\frac{\varepsilon_g}{K_B T}\right) - 1\right]^{-1}$$

(4.1)

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

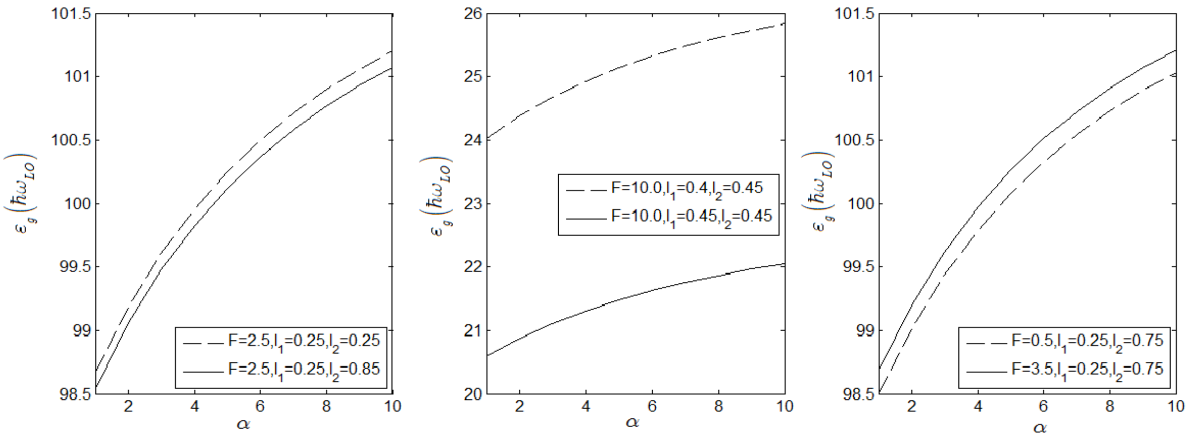
5- Numerical results and discussions

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 $r_0 = \left(\hbar/2m^*\omega_{LO}\right)^{1/2}$



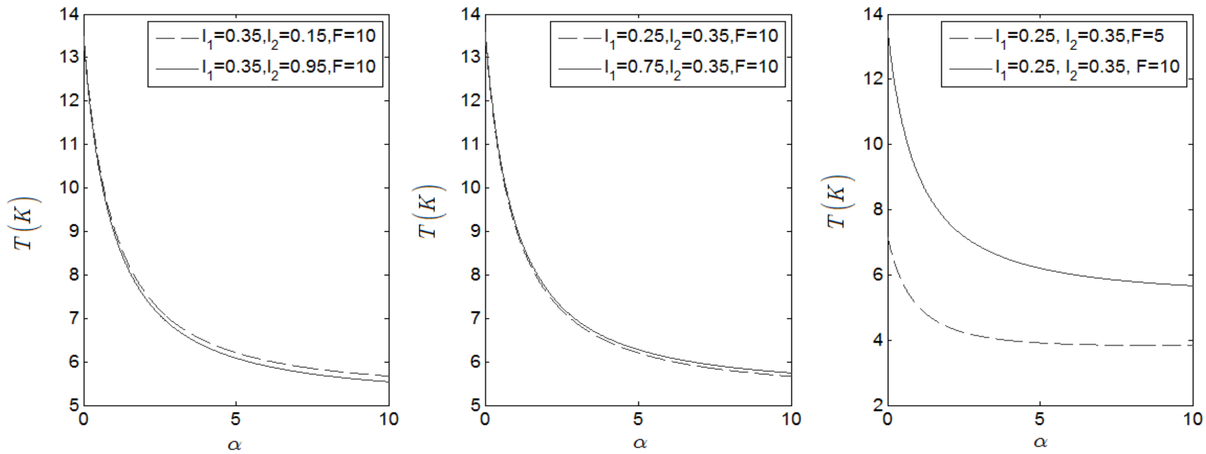
(a)

Figure 1: Ground state energy ε_g as a function of the 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 a function of the 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 a function of the 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 the polaron as a function of the 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 an increasing function of the electric field. This is because the electric field brings about an increase in the electron energy and makes the electrons to interact with more phonons. This is a novel approach to controlling the QD energies via the electric field. In fact, the electric field plays an important role in low-dimensional materials. For example, it affects both the quantum decoherence process and the electron's probability density are affected. 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 a function of the 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 increases with the electron-phonon coupling constant and decreases with an increase in 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 the polaron. This result is similar to that obtained in [27-28].
In figure 3, we have plotted the Temperature as a function of the 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 the weak coupling range, the temperature is a decreasing function of the electron-phonon coupling constant and a decreasing function of the confinement length strength as well. When the electron motion range decreases, the energy of interaction increases. As such, the motion of electrons and phonons heats up the medium. The temperature is an increasing function of the electric field strength; this is because the electric field is an external perturbation source which accelerates the motion of particles (electron and phonons) in the QD. The mesoscopic phenomena have gained more importance as a basis for novel electronic and optical devices. It is necessary to formulate models that describe physical phenomena associated with Nano crystals. This study is in accordance with this philosophy. Therefore, from our study and results, it is clear that the coupling between the electron and the phonon can explain properties of novel electric and optical devices. Temperature effect and the application of the electric field enhance the polaron ground state energy and the polaron tends to a highly localized state. This gives the possibility for the most favorable condition for a stable bipolaron and bipolaron superconductivity [29-34].The result is in in accordance with that obtained by Jing-Lin Xiao[35-36]

6- Conclusion

With the use of the modified LLP method, we have studied the energy levels of a weak coupling polaron in a spherical quantum dot (QD) and a weak coupling polaron in an anisotropic QD subjected to an electric field. It is found that the ground state energy of the polaron is an increasing function of the electric field; this is because the presence of the electric field makes phonons to interact more with the electrons. It is also seen that, with a 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 the superposition states against the influence of its environment, which can induce the construction of coherent states and cause coherence quenching. The temperature is an increasing function of the electric field and a decreasing function of the confinement lengths.

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