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The Optical Polaron in Spherical Quantum Dot Confinement

البولارون الضوئي في نقطة كمية

Zher Samak, & Bassam Saqqa

زهر السمك، وبسام السقا

Department of Physics, Islamic University, Gaza, Palestine

E-mail: bsaqqa@iugaza.edu.ps

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Abstract

The problem of a polaron in quantum dot is retrieved using a modified LLP approach. The modification is intended to interpolate between the strong- and the weak-coupling limits of the problem. The polaronic effect is found to be more important for small dot sizes.

ملخص

درست مسألة البلارون في شريحة كمية باستخدام طريقة معدلة لنظريةLLP. التعديل المقترح يهدف إلى أن تكون النظرية صالحة لجميع قيم ثابت الربط بين الإلكترون و الفونون (حالة الربط الضعيفة وحالة الربط القوية). لقد وجد أن التأثير البولاروني يكون أكثر أهمية مع تقليل حجم النقطة .

1. Introduction

Due to the recent progress achieved in microfabrication, 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 [1-9]. The effect of the electron-phonon interaction on the energy levels and their variations versus the size of the dots is studied using different approaches. Using the LLP-H

approach Satyabrata Sahoo [10, 11], has calculated the energy of the ground state and the first two excited states. He concluded that the polaronic correction is more pronounced as the size of the quantum dot is decreased. The problem of a bound polaron in a quantum dot is studied separately by H. J. Xie and C.Y. Chen [12] and Li Zhang et al [13]. They showed that the phonon contribution to the binding energy is dependent on the size of the quantum dot as well as the position of the impurity in the quantum dot.

In this report we propose a modification to the mixed coupling method used by Senger and Erçelebi [1]. Using this modified LLP theory the binding energy of the polaron in a quantum dot is calculated. The modification is intended to cover all the values of the coupling constant. A comparison to well-known limits of the problem is made.

2. Theory

The usual Fröhlich polaron Hamiltonian describing an electron confined in a symmetric dot and interacting with the bulk optical phonon with a parabolic potential $V(r)$ is [14]

$$H = H_e + H_{ph} + \sum_Q V_Q \left[a_Q e^{(i\vec{Q}.\vec{r})} + a_Q^{\dagger} e^{(-i\vec{Q}.\vec{r})} \right] \quad , \tag{1}$$

where H_e represents the electronic Hamiltonian which is written as

$$H_e = p^2 + \frac{1}{4}\omega^2 r^2 \quad , \tag{2}$$

where $\vec{p}, \vec{r}$ represent the momentum and the position of the electron respectively, and ω represents the strength of the quantum dot potential that serves for the measure of the degree of confinement of the electrons, which is given by

$$\omega = (k/m\omega_{LO}^2)^{1/2} \quad ,$$

in which k denotes the force constant, and $(2m = \omega_{LO} = 1)$ [in Fröhlich

units], where m is the effective mass of the electron, ω_{LO} is the frequency of the longitudinal optical phonons (LO).

H_{ph} represents the phonon Hamiltonian which is written as

$$H_{ph} = \sum_Q a_Q^\dagger a_Q \qquad (3)$$

$a_Q^\dagger (a_Q)$ are the creation (and annihilation) operators for (LO) phonons of wave vector $\vec{Q} = (\vec{q}, q_z)$, and V_Q is the amplitude of the electron-phonon interaction which is given as [15, 16]

$$V_Q = -i\left(\frac{\hbar\omega_{LO}}{Q}\right)\left(\frac{4\pi\alpha}{V}\right)^{1/2}\left(\frac{\hbar}{2m\omega_{LO}}\right)^{1/4} , \qquad (4)$$

$\hbar\omega_{LO}$ is the energy of the phonons, V is the volume of the crystal which is taken as a unit and α is the standard dimensionless coupling constant of the electron-phonon interaction which is given as [15, 16]

$$\alpha = \frac{e^2}{2\hbar\varepsilon_0}\sqrt{\frac{2m}{\hbar\omega_{LO}}}\left(\frac{\varepsilon_\infty}{\varepsilon_0} - 1\right) , \qquad (5)$$

where $\varepsilon_\infty (\varepsilon_0)$ is the high frequency (static) dielectric constant of the medium.

For the mixed-coupling approximation to be adopted for such a problem we propose a modification to the first LLP-transformation. Our proposed U_1 is

$$U_1 = \exp[i(\vec{P} - \vec{\Pi}).b\vec{r}] , \qquad (6)$$

where U_1 is the unitary transformation which is related to the electron operators, $\vec{P}$ is the total-momentum operator of the polaron, and is given by

$$\vec{P} = \vec{p} + \sum_Q \vec{Q} a_Q^\dagger a_Q , \qquad (7)$$

$\vec{\Pi}$ represents the momentum of phonon

$$\vec{\Pi} = \sum_Q \vec{Q} u_Q^\dagger u_Q \quad , \quad (8)$$

The modification we made is by inserting another variational parameter b in equation (6). This parameter is supposed to trace the problem from the strong-coupling limit ($b = 0$) to the weak-coupling limit ($b = 1$).

$\vec{r}$ denote to the position of electron, this transformation eliminates the electron operators from the electron-phonon Hamiltonian part.

The second transformation is of the form:

$$U_2 = \exp[\sum_Q u_Q (a_Q^\dagger - a_Q)] \quad , \quad (9)$$

The u_Q is treated as a variational function. The unitary transformation U_2 is called the displaced-oscillator which is related to the phonon operators via equation (9). The phonon wave function is [15]

$$\Phi_{ph} = U_2 |0_{ph}\rangle \quad , \quad (10)$$

where the ket $|0_{ph}\rangle$ is the phonon vacuum state, simply because at low temperature ($KT << \hbar\omega_{LO}$), there will be no effective phonons, (K is Boltzmann's constant and T the absolute temperature) [16, 17].

The ground-state energy of the polaron can be obtained as

$$E_g = \langle 0_{ph}|\langle 0_e|U_2^{-1}U_1^{-1}HU_1U_2|0_e\rangle|0_{ph}\rangle \quad (11)$$

$$= \langle 0_{ph}|\langle 0_e|U_2^{-1}H'U_2|0_e\rangle|0_{ph}\rangle \quad ,$$

where

$$H' \rightarrow U_1^{-1}HU_1 \quad ,$$

and $|\vartheta_e\rangle$ is the electron state [15].

Applying the first LLP transformation to each part of the Hamiltonian, we get [1]

$$H' = U_1^{-1} H U_1 \quad (12)$$

$$= b^2(P-\Pi)^2 + p^2 + 2bp(P-\Pi) + \tfrac{1}{4}\omega^2 r^2 + \sum_Q a_Q^\dagger a_Q$$

$$+ \sum_Q V_Q [a_Q e^{i(1-b)\vec{Q}.\hat{r}} + a_Q^\dagger e^{-i(1-b)\vec{Q}.\hat{r}}] \quad .$$

From equation (12) it is clear that when $b = 1$, the terms $e^{\pm i\vec{Q}.\hat{r}}$ will be eliminated, leading to the weak-coupling approach [14].

Now applying the second LLP-transformation U_2 of equation (9), the Hamiltonian of equation (12) transforms as [1]

$$H'' = U_2^{-1} H' U_2 \quad (13)$$

$$= p^2 + \tfrac{1}{4}\omega^2 r^2 + b^2(P-\Pi)^2 + b^2[\Pi^{(0)}]^2 + \sum_Q a_Q^\dagger a_Q$$

$$+ \sum_Q u_Q^2 + b^2(\Pi^{(1)} - 2\Pi)\Pi^{(1)} + 2b^2(P - \Pi^{(0)})\Pi^{(1)} + 2b^2\Pi^{(0)}\Pi - 2b^2 P\Pi^{(0)}$$
$$- \sum_Q V_Q u_Q [e^{i(1-b)\vec{Q}.\hat{r}} + e^{-i(1-b)\vec{Q}.\hat{r}}] + 2bp(P - \Pi + \Pi^{(1)} - \Pi^{(0)})$$

$$+ \sum_Q [V_Q e^{i(1-b)\vec{Q}.\hat{r}} - u_Q] a_Q + \sum_Q [V_Q e^{-i(1-b)\vec{Q}.\hat{r}} - u_Q] a_Q^\dagger \quad ,$$

where $\vec{\Pi}$ is given in equation (8), and

$$\vec{\Pi}^{(1)} = \sum_Q \vec{Q} u_Q (a_Q^\dagger + a_Q) \quad , \qquad (14)$$

$$\vec{\Pi}^{(0)} = \sum_Q \vec{Q} u_Q^2 \quad , \qquad (15)$$

The ground-state energy can be obtained as

$$E_g = \langle 0_e|p^2|0_e\rangle + \langle 0_e|\frac{1}{2}\omega^2 r^2|0_e\rangle + b^2P^2 - 2b^2P\Pi^{(0)} \quad (16)$$

$$+b^2[\Pi^{(0)}]^2 + \sum_Q u_Q^2(1+b^2Q^2) + \langle 0_e|\langle 0_{ph}|2bp(P-\Pi+\Pi^{(1)}-\Pi^{(0)})|0_{ph}\rangle|0_e\rangle$$

$$-\sum_Q V_Q u_Q \langle 0_e|e^{-i(1-b)\vec{Q}.\hat{r}}|0_e\rangle - \sum_Q V_Q u_Q \langle 0_e|e^{i(1-b)\vec{Q}.\hat{r}}|0_e\rangle \quad .$$

Expressing the coordinates and momenta of the electron as [18]

$$p_\mu = \lambda_1^{\frac{1}{2}}(\sigma_\mu + \sigma_\mu^\dagger) \quad , \quad (17)$$

$$x_\mu = i/\lambda_1^{\frac{1}{2}}(\sigma_\mu - \sigma_\mu^\dagger) \quad , \quad (18)$$

$$p_z = \lambda_2^{\frac{1}{2}}(\sigma_z + \sigma_z^\dagger) \quad , \quad (19)$$

$$z = i/\lambda_2^{\frac{1}{2}}(\sigma_z - \sigma_z^\dagger) \quad , \quad (20)$$

where the index μ refers to the x and y directions, λ_1, λ_2 are variational parameters, and $\sigma^\dagger, (\sigma)$ are the creation (and annihilation) operators for electron, and after performing straightforward calculations we obtain the ground-state energy of the polaron as

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} + b^2P^2 - 2b^2P\Pi^{(0)} \quad (21)$$

$$+b^2[\Pi^{(0)}]^2 + \sum_Q u_Q^2(1+b^2Q^2) - 2\sum_Q V_Q u_Q S_Q \quad ,$$

where

$$S_Q = \langle 0_e|e^{\pm i(1-b)\vec{Q}.\hat{r}}|0_e\rangle \quad , \quad (22)$$

which is found to be

$$S_Q = e^{-(1-b)^2 q^2/2\lambda_1} e^{-(1-b)^2 q_z^2/2\lambda_2} \quad . \tag{23}$$

Minimizing equation (21) with respect to the variational function u_Q we get

$$[1 + b^2 Q^2] u_Q - V_Q S_Q = 0 \quad . \tag{24}$$

So we can write u_Q as

$$u_Q = \frac{V_Q S_Q}{1+b^2 Q^2} \quad . \tag{25}$$

The momentum $\tilde{\Pi}^{(0)}$ differs from the total momentum by a scalar factor as

$$\tilde{\Pi}^{(0)} = \eta \tilde{P} \quad . \tag{26}$$

In which the unknown scalar, η is determined by the equation

$$\tilde{\Pi}^{(0)} = \Sigma_Q \tilde{Q} u_Q^2 \quad ,$$

$$\eta \tilde{P} = \frac{\tilde{Q} v_Q^2 s_Q^2}{[1+b^2 Q^2]^2} \quad . \tag{27}$$

Substituting back in equation (21), we obtain the following result:

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \Sigma_Q \frac{s_Q^2 v_Q^2}{[1+b^2 Q^2]^2} + b^2 (1-\eta)^2 P^2 \quad . \tag{28}$$

But E_g may be well represented by the first two terms of a power series expansion in P^2 as [17]

$$E_g = E_g(0) + \beta P^2/2 + \ldots O(P^4) + \ldots \tag{29}$$

The effective mass of the polaron is then β^{-1}.

By comparing equation (28) and equation (29) we get the expression for the ground-state energy of the polaron as

$$E_g(0) = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 S_Q^2}{[1+b^2Q^2]} \quad , \tag{30}$$

and the mass of the polaron is

$$m_g = \frac{1}{4[b^2(1-\eta)^2]} \quad . \tag{31}$$

Using the expression for S_Q in equation (23), the ground-state of the energy becomes

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 e^{-(1-b)^2 q^2/\lambda_1} e^{-(1-b)^2 q_z^2/\lambda_2}}{[1+b^2Q^2]} \quad , \tag{32}$$

This last equation gives the general formula for the ground-state energy of the confined polaron. This formula enables us to find the binding energy of the 3D polaron in both weak- and strong-coupling range.

3. Results and Discussions

First, let us test our theory for some limiting cases. In the limit $b \to 0$, the ground-state energy gives the adiabatic (strong) limit as

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \sum_Q V_Q^2 e^{-q^2/\lambda_1} e^{-q_z^2/\lambda_2} \quad , \tag{33}$$

Projecting out the $\vec{Q}$-summation in equation (33) we obtain

$$E_g = \frac{\lambda_1}{2} + \frac{\omega^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\omega^2}{4\lambda_2} - \frac{\alpha}{\sqrt{\pi}} \sqrt{\frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1}} \tan^{-1} \sqrt{\frac{\lambda_2}{\lambda_1} - 1} \quad , \tag{34}$$

and for the polaron binding energy, we have

$$\varepsilon_p = \frac{3}{2}\omega - E_g \quad . \tag{35}$$

For $\omega = 0$, we obtain numerically that

$$\lambda_1 = \lambda_2 = \frac{4\alpha^2}{9\pi} \quad ,$$

and

$$\varepsilon_p^{(3D)} = \frac{\alpha^2}{3\pi} \quad , \tag{36}$$

which is the strong-coupling result obtained from our modified method and agreed with the result obtained in [18] using strong-coupling theory.

Also, in the limit $b \to 1$, the ground-state energy describes the case of weak-coupling as

$$E_g = \frac{\lambda_1}{4} + \frac{\alpha^2}{2\lambda_1} + \frac{\lambda_2}{4} + \frac{\alpha^2}{4\lambda_2} - \sum_Q \frac{V_Q^2}{[1+Q^2]} \quad . \tag{37}$$

For $\omega = 0$, we obtain $\lambda_1 = \lambda_2 \to 0$, and

$$\varepsilon_p^{(2D)} = \alpha \quad , \tag{38}$$

This is the result obtained from our modified method and agreed with the result obtained in [19] using perturbation theory.

For $0 < b < 1$ we expect that our formula of equation (32) can describe the ground state energy of the problem for the whole range of the coupling constant (α).

To compare our results with that of the strong-coupling, and the weak-coupling theories, we, in Figure (1), display the binding energy as a

function of (α) for $\omega = 0$ together with the results of the two theories. As it is clear from the graph we have a good matching to those approaches in the extreme values of (α).

To study the effect of the confinement length of the quantum dot $l = (\hbar/m\omega)^{\frac{1}{2}}$ [20] in the binding energy we plot, in Figure (2) the binding energy versus α for two different values of the length of the quantum dot (l). As expected, the binding energy increases with increasing α. Furthermore, for small values of l the effect of the polaronic effect becomes more important. This is because by decreasing l the problem becomes more confined and this increases the effect of the electron-phonon interaction.

To show the effect of the confinement length on the polaronic aspect we display, in Figure (3) the polaronic correction to the ground state energy as a function of (l).

The Figure again shows that the correction is large for small value of (l). It decreases exponentially with increasing the dot size. As $l \to \infty$, the result approaches the 3D result as expected.

4. Conclusion

A modification in the LLP approach is proposed by imposing a further variational parameter intended to interpolate between the strong- and the weak-coupling aspects of the polaron problem in a quantum dot.

The polaronic correction in the ground state energy is found to be more pronounced for small values of the size of the dot.

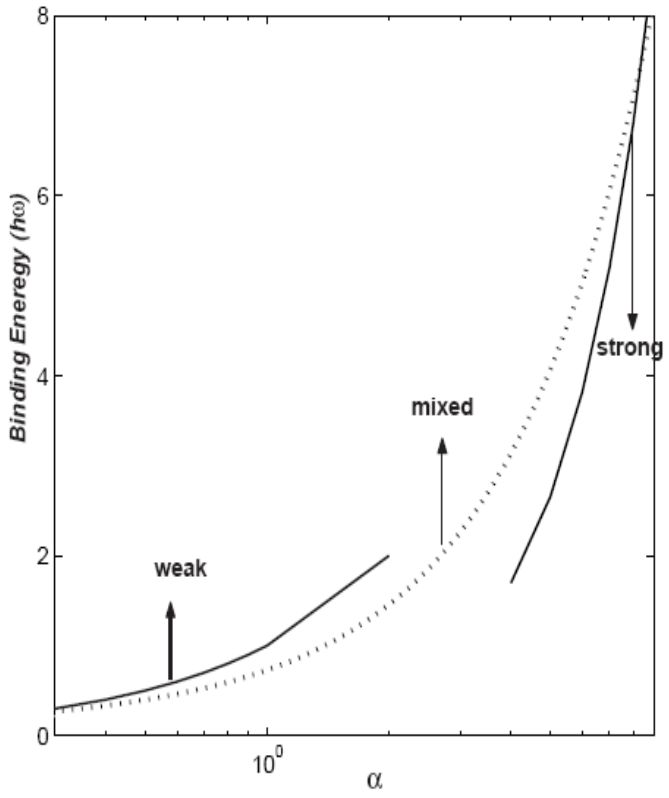

Fig. (1): The binding energy ε_p versus the coupling constant (α) in unites of $(\hbar\omega)$. The solid lines, from the left, and the right are for the weak and the strong coupling limits.

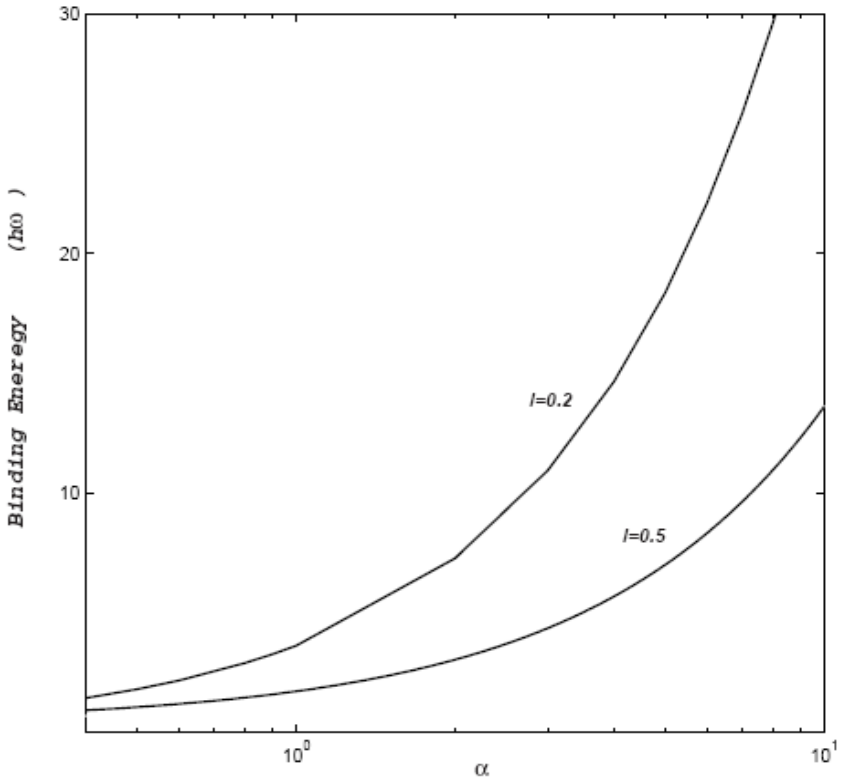

Fig. (2): The binding energy (ε_p) versus the coupling constant (α) at confinement length ($l = 0.2, 0.5$) in unites of ($\hbar\omega$).

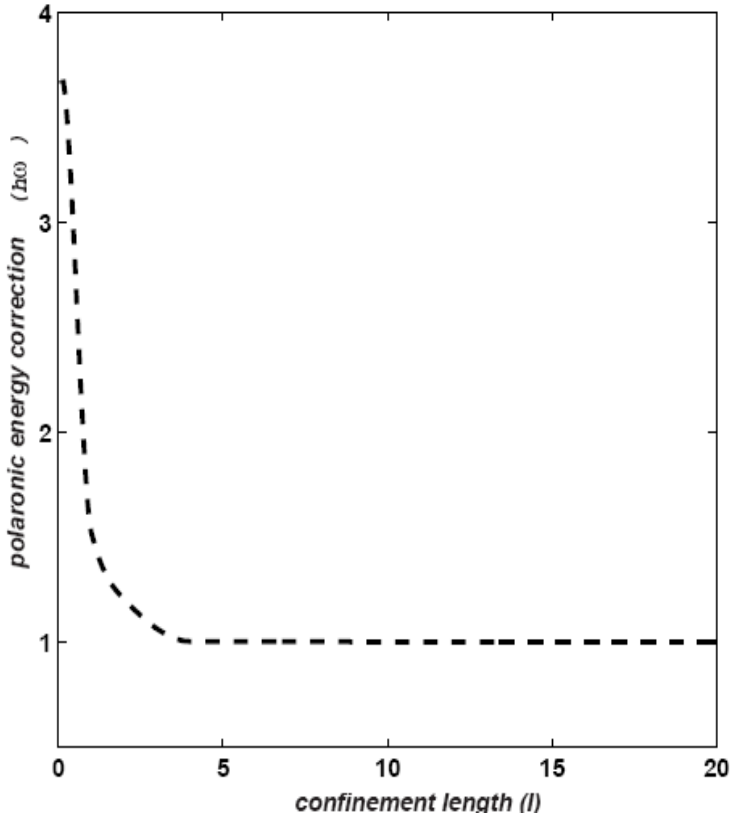

Fig. (3): The polaronic energy correction ($-\Delta E$) versus confinement length (l) in unites of ($\hbar\omega$).

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