

## The Optical Polaron versus the Effective Dimensionality in Quantum Well Systems

البولارون الضوئي مع الأبعاد الفعالة في أنظمة الحفر الكمية

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### Abstract

The confined optical polaron is investigated within the framework of an improved variational technique yielding a unified characterization of problem for all the coupling strengths. The ground state energy is studied as a function of the effective dimensionality of the quantum well to interpolate between all possible confinement geometries.

### ملخص

تم دراسة مسألة البولارون الضوئي المحصور باستخدام طريقة معدلة لنظرية LLP بحيث تكون الطريقة صالحة لجميع قيم ثابت الربط بين الإلكترونات والفونونات. تم دراسة تأثير الأبعاد الفعالة للحفر الكمية على طاقة المستوى الأرضي بهدف الربط بين جميع الأشكال.

### 1. Introduction

Despite the long history of polaron theory, the interest to the problem does not decrease. Different approaches have been used to study the problem according to the coupling strength [1-26].

The progress achieved in micro-fabrication make the growing of low dimensional semiconductor structures possible and this in turn opens a large area of research on two-, one-, and even zero-dimensional polarons. The common theoretical prediction reached is that the Polaronic effect

becomes more important as the dimensionality is reduced (Erçelebi, A. & Senger, R.T. 1994. Yildirim, T. Erçelebi, A. 1991. Yildirim, T. Erçelebi, A. (1991). Yu, Y.B. Shu, S.N. Guo, K.X. 2004. Xie, H.J. Chen, C.Y. Ma, B K 2000).

In a previous two reports (Samak, Z. Saqqa, B. 2009. Senger, R. T. & Erçelebi, A. 1997). we proposed a modification to the mixed coupling theory of Senger and Ercelebi (Senger, R. T. & Erçelebi, A. 1998) to study the optical polaron in a spherical quantum dot and in slab-like confinement, respectively. In this report we use the same approach to display a comprehensive theoretical model yielding an explicit track of the Polaronic effect as a function of the effective dimensionality in the overall range of the electron-phonon coupling strengths. Yildirim and Ercelebi (Yildirim, T. Erçelebi, A. 1991. Yildirim, T. Erçelebi, A. 1991) have already attacked the problem but for the strong and the weak coupling cases separately.

## 2. Theory

The model we use consists of an electron confined in an isotropic potential box with tunable dimensions immersed in the field of the bulk longitudinal optical (LO)-phonon modes. The dimensionless Hamiltonian describing the problem in Frohlich units ( $2m = \omega_{LO} = 1$ ) is given by (Erçelebi, A. & Senger R.T. 1994).

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

where  $H_e$  represents the electronic Hamiltonian and is given by

$$H_e = \frac{p^2}{2m} + \frac{1}{4}\omega_1^2 \rho^2 + \frac{1}{4}\omega_2^2 z^2 \quad (2)$$

with  $\vec{p}$  represents the momentum,  $\omega_1$  and  $\omega_2$  stand for the dimensionless measures of the degree of confinement in the  $x$ - $y$ -plane and the  $z$ -direction, respectively. By tuning  $\omega_1$  and/or  $\omega_2$  from zero to values much larger than unity one can trace the transition from the bulk

to all possible extremes of the effective dimensionality.  $H_{ph}$  is the phonon Hamiltonian defined to be as

$$H_{ph} = \sum_Q a_Q^\dagger a_Q \tag{3}$$

with  $a_Q^\dagger$  ( $a_Q$ ) are the creation (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 given by (Pekar S.I. 1954)

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

with  $\hbar\omega_{LO}$  being the energy of the phonons,  $V$  is the volume of the crystal which is taken as unity and

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

is the standard dimensionless coupling constant of the electron-phonon interaction with  $\epsilon_\infty$  ( $\epsilon_o$ ) is the high (static) dielectric constant of the medium.

Adopting the mixed-coupling approximation of (Senger R. T. & Erçelebi A. 1998) 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

$$U_1 = \exp i \left[ (\vec{P}_\rho - \vec{\Pi}_\rho) \cdot b_1 \vec{\rho} + (P_z - \Pi_z) b_2 z \right] \tag{6}$$

with

$$\vec{P} = \vec{p} + \sum_Q \vec{Q} a_Q^\dagger a_Q \tag{7}$$

is the total momentum of the polaron and



$$\begin{aligned}
 H'' = & p^2 + \frac{1}{4}\omega_1^2\rho^2 + \frac{1}{4}\omega_2^2z^2 + b_1^2(P_\rho - \Pi_\rho)^2 + b_1^2(\Pi_\rho^{(0)})^2 \\
 & + 2b_1p_\rho(P_\rho - \Pi_\rho + \Pi_\rho^{(1)} - \Pi_\rho^{(0)}) + b_1^2(\Pi_\rho^{(1)} - 2\Pi_\rho)\Pi_\rho^{(1)} \\
 & + 2b_1^2(P_\rho - \Pi_\rho^{(0)})\Pi_\rho^{(1)} + 2b_1^2\Pi_\rho^{(0)}\Pi_\rho - 2b_1^2P_\rho\Pi_\rho^{(0)} \\
 & + b_2^2(P_z - \Pi_z)^2 + b_2^2(\Pi_z^{(0)})^2 + 2b_2p_z(P_z - \Pi_z + \Pi_z^{(1)} - \Pi_z^{(0)}) \\
 & + b_2^2(\Pi_z^{(1)} - 2\Pi_z)\Pi_z^{(1)} + 2b_2^2(P_z - \Pi_z^{(0)})\Pi_z^{(1)} + 2b_2^2\Pi_z^{(0)}\Pi_z \\
 & - 2b_2^2P_z\Pi_z^{(0)} + \sum_Q u_Q^2 + \sum_Q a_Q^\dagger a_Q + \sum_Q u_Q(a_Q + a_Q^\dagger) \\
 & + \sum_Q V_Q e^{-i(b_1\vec{q}\cdot\vec{\rho} + b_2q_z z)} e^{i\vec{Q}\cdot\vec{r}} (a_Q - u_Q) \\
 & + \sum_Q V_Q e^{i(b_1\vec{q}\cdot\vec{\rho} + b_2q_z z)} e^{-i\vec{Q}\cdot\vec{r}} (a_Q^\dagger - u_Q)
 \end{aligned} \tag{13}$$

with

$$\bar{\Pi}^{(1)} = \sum_Q \bar{Q} u_Q (a_Q + a_Q^\dagger) \tag{14}$$

and

$$\bar{\Pi}^{(0)} = \sum_Q \bar{Q} u_Q^2 \tag{15}$$

Using Eq. (13), the ground state energy given by Eq.(11) becomes

$$\begin{aligned}
E_g = & \langle 0_e | p^2 | 0_e \rangle + \langle 0_e | \left( \frac{1}{4} \omega_1^2 p^2 + \frac{1}{4} \omega_2^2 z^2 \right) | 0_e \rangle + b_1^2 P_\rho^2 - 2b_1^2 P_\rho \Pi_\rho^{(0)} \\
& + b_1^2 \left( \Pi_\rho^{(0)} \right)^2 + \sum_Q u_Q^2 \left( 1 + b_1^2 q^2 + b_2^2 q_z^2 \right) + \\
& + \langle 0_e | \langle 0_{ph} | 2b_1 p_\rho \left( \bar{P}_\rho - \bar{\Pi}_\rho + \bar{\Pi}_\rho^{(1)} - \bar{\Pi}_\rho^{(0)} \right) | 0_{ph} \rangle | 0_e \rangle \\
& + \sum_Q V_Q u_Q \langle 0_e | \left( e^{-i(b_1 \bar{q} \cdot \bar{\rho} + b_2 q_z z)} e^{i\bar{Q} \cdot \bar{r}} - e^{i(b_1 \bar{q} \cdot \bar{\rho} + b_2 q_z z)} e^{-i\bar{Q} \cdot \bar{r}} \right) | 0_e \rangle \\
& + b_2^2 P_z^2 - 2b_2^2 P_z \Pi_z^{(0)} + b_2^2 \left( \Pi_z^{(0)} \right)^2 \\
& + \langle 0_e | \langle 0_{ph} | 2b_2 p_z \left( \bar{P}_z - \bar{\Pi}_z + \bar{\Pi}_z^{(1)} - \bar{\Pi}_z^{(0)} \right) | 0_{ph} \rangle | 0_e \rangle
\end{aligned} \tag{16}$$

To evaluate Eq. (16) we express the coordinates and momenta of the electron in terms of its creation (annihilation) operators  $\sigma^\dagger$  ( $\sigma$ ) as

$$p_\mu = \sqrt{\lambda_1} (\sigma_\mu + \sigma_\mu^\dagger) \tag{17}$$

$$x_\mu = i\sqrt{\lambda_1} (\sigma_\mu - \sigma_\mu^\dagger) \tag{18}$$

$$p_z = \sqrt{\lambda_2} (\sigma_z + \sigma_z^\dagger) \tag{19}$$

$$p_\mu = i\sqrt{\lambda_2} (\sigma_z - \sigma_z^\dagger) \tag{20}$$

where the index  $\mu$  refers to the  $x$  and  $y$  coordinates, and  $\lambda_1$  and  $\lambda_2$  are another variational parameters. Performing the required calculations we get for the ground state energy

$$\begin{aligned}
 E_g = & \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} + b_1^2 P_\rho^2 \\
 & - 2b_1^2 P_\rho \Pi_\rho^{(0)} + b_1^2 \left(\Pi_\rho^{(0)}\right)^2 \\
 & + b_2^2 P_z^2 - 2b_2^2 P_z \Pi_z^{(0)} + b_2^2 \left(\Pi_z^{(0)}\right)^2 \\
 & + \sum_Q u_Q^2 \left(1 + b_1^2 q^2 + b_2^2 q_z^2\right) - 2 \sum_Q V_Q u_Q S_Q
 \end{aligned} \tag{21}$$

with

$$S_Q = \langle 0_e | e^{\pm i(b_1 \vec{q} \cdot \vec{p} + b_2 q_z z)} e^{\pm i \vec{Q} \cdot \vec{r}} | 0_e \rangle \tag{22}$$

which can be written as

$$S_Q = e^{-(1-b_1)^2 q^2 / 2\lambda_1} e^{-(1-b_2)^2 q_z^2 / 2\lambda_2} . \tag{23}$$

Minimizing Eq. (21) with respect to the variational function  $u_Q$  we obtain

$$\left[ 1 + b_1^2 q^2 + b_2^2 q_z^2 + 2b_1^2 q \left(\Pi_\rho^{(0)} - P_\rho\right) + 2b_2^2 q_z \left(\Pi_z^{(0)} - P_z\right) \right] u_Q = V_Q S_Q \tag{24}$$

Solving for  $u_Q$ , with the assumption that  $\vec{\Pi}^{(0)}$  differs from the total momentum by a scalar factor  $\eta$  ( $\vec{\Pi}^{(0)} = \eta \vec{P}$ ), we get

$$u_Q = \frac{V_Q S_Q}{1 + b_1^2 q^2 + b_2^2 q_z^2 - 2b_1^2 q P_\rho (1 - \eta) - 2b_2^2 q_z P_z (1 - \eta)} . \tag{25}$$

Substituting Eq. (25) into Eq. (21) we obtain





### 3. Results and Discussions

To examine the present approach we, in the following, make correspondence with common geometries of the problem and display comparison of our results with well-known strong-coupling and the perturbation theories. In the limit  $b_1 = b_2 \rightarrow 0$  the problem is expected to be turned to the pure strong-coupling regime. In this limit, the ground state energy of Eq. (30) reduces to

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q V_Q^2 e^{-q^2/2\lambda_1} e^{-q_z^2/2\lambda_2}. \quad (31)$$

For  $\omega_1 = \omega_2 = 0$ , we obtain numerically  $\lambda_1 = \lambda_2 = \frac{4\alpha^2}{9\pi}$ . Defining the binding energy as

$$\varepsilon_p = \omega_1 + \frac{1}{2}\omega_2 - E_g \quad (32)$$

we obtain the 3D binding energy as

$$\varepsilon_p^{3D} = \frac{\alpha^2}{3\pi}, \quad (33)$$

which is exactly the strong-coupling result obtained in (Erçelebi, A. & Senger, R. T. 1995).

In the limit  $b_1 = b_2 \rightarrow 1$  (the weak-coupling limit) the ground state energy becomes

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q \frac{V_Q^2}{1+Q^2}. \quad (34)$$

Again for  $\omega_1 = \omega_2 = 0$ , we get  $\lambda_1 = \lambda_2 \rightarrow 0$  and for the 3D binding energy we have

$$\varepsilon_p^{3D} = \alpha \quad (35)$$

Which agrees with the corresponding weak-coupling result obtained in (Senger, R. T. & Erçelebi, A. 1997).

To obtain the strong coupling result in the strict 2D limit we put  $\omega_2 = \lambda_2 \rightarrow \infty$  in Eq. (30). The value of  $\lambda_1$  which minimizes  $E_g$  in this case can be obtained numerically as  $\lambda_1 = \frac{\pi\alpha^2}{4}$ . The binding energy in this limit is then

$$\varepsilon_p^{2D} = \frac{\pi\alpha^2}{8} \quad , \quad (36)$$

which is the result obtained in (Erçelebi, A. & Senger, R. T. 1995) using the strong coupling theory.

The weak coupling result in the 2D limit is obtained by putting  $b_1 = 1$  and  $b_2 = 0$  in Eq.(30) to give for the ground state energy

$$E_g = \frac{\lambda_1}{2} + \frac{\lambda_2}{4} + \frac{\omega_1^2}{2\lambda_1} + \frac{\omega_2^2}{4\lambda_2} - \sum_Q \frac{V_Q^2 e^{-q^2/\lambda_2}}{1+q^2} \quad . \quad (37)$$

Again in the strict 2D limit we have  $\omega_2 = \lambda_2 \rightarrow \infty$  and  $\lambda_1 \rightarrow 0$ . The binding energy in this limit is found to be

$$\varepsilon_p = \sum_Q \frac{V_Q^2}{1+q^2} \quad (38)$$

Projecting out the summation in the last equation we obtain

$$\varepsilon_p^{2D} = \frac{\pi\alpha}{2} \quad (39)$$

This is the same result for the weak coupling case obtained in (Senger, R. T. & Erçelebi, A. 1997).

In Figure (1) we plot the binding energy as a function of the degree of confinement for the wire-like ( $\omega_2 = 0$ ) and for the slab-like ( $\omega_1 = 0$ )

configuration for a weak coupling value ( $\alpha = 0.9$ ). Setting  $\omega_1 = 0$  and varying  $\omega_2$  we can trace the problem from the bulk case to the strictly 2D limit. On the other hand, deleting the confining potential along the z-axis  $\omega_2 = 0$  and varying  $\omega_1$  the theory reflects the problem in a quantum well-wire.

In Figure (2) we display the binding energy as a function of the degree of confinement for the wire- and slab-like confinement for a rather strong value of the coupling constant ( $\alpha = 5$ ). Correspondence is also made for the bulk and the strict 2D limits.

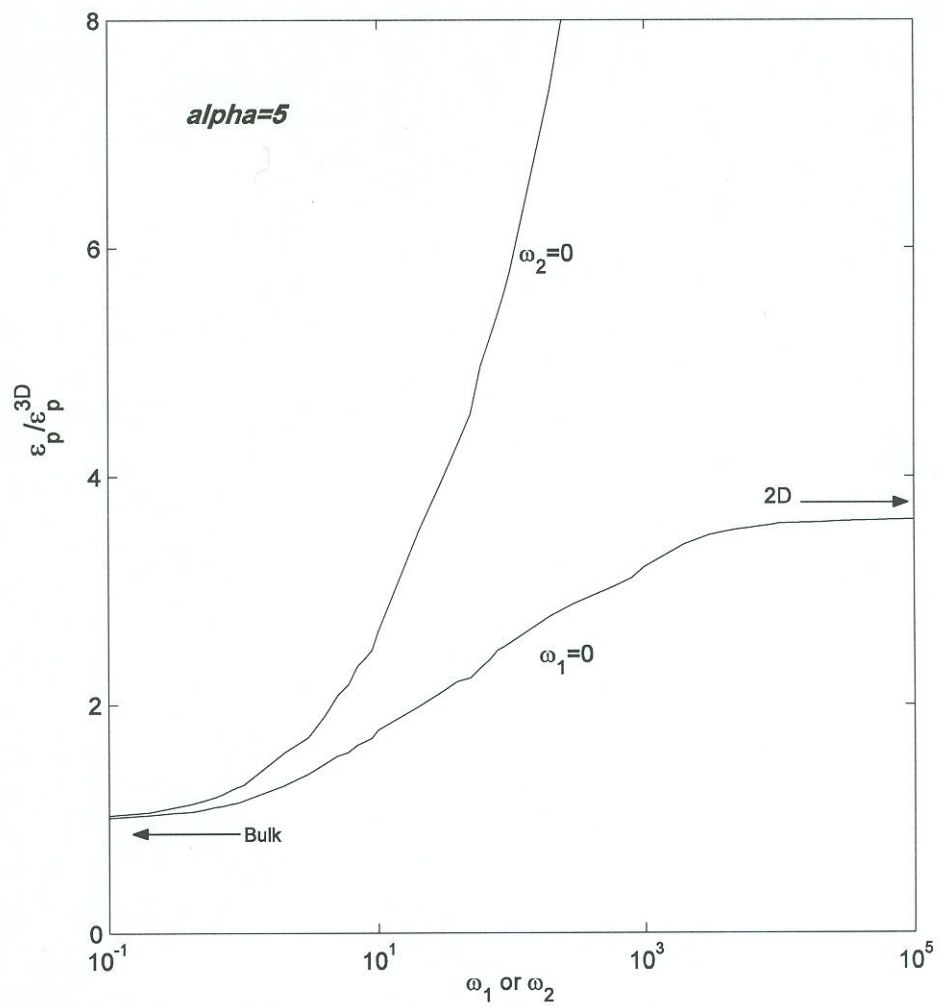
From the two graphs we find that with increasing the barrier slopes of the confining potential, the binding energy for the wire geometry becomes larger than for the quazi-2D configuration. This follows essentially from the fact that in the wire geometry the polaron cloud is squeezed towards the wire axis in all transverse directions resulting in a much stronger effective electron-phonon coupling than that for the slab-like configuration.

To explain the relation between the variational parameters  $b_1$  and  $b_2$  with the coupling constant, we plot in Figure (3) the variational parameter  $b = b_1 = b_2$  with  $\alpha$ . As expected, the value of  $b$  varies between 0 and 1. For large values of the coupling constant  $b \rightarrow 0$  which conforms the problem to the strong coupling theory. In the other hand, for small values of  $\alpha$   $b \rightarrow 1$  which turns the problem to the weak-coupling limit.

#### 4. Conclusion

A modification to the LLP-theory is proposed to study the polaron problem. We proposed the insertion of two variational parameters intended to trace the problem from the strong coupling case to the weak coupling limit and to interpolate between all possible geometries. The formalism is supposed to set up a weighted admixture between the strong and the weak coupling counterparts of the problem such that the adiabatic results can conform successfully to those attained from the perturbation theory. It is supposed to display a comprehensive theoretical model





**Figure (2):** The binding energy  $\epsilon_p$  as a function of the degree of  $\omega_1$  or  $\omega_2$ , for  $\alpha = 5$ .



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