An-Najah Univ. J. Res. (N. Sc.), Vol. 18(2), 2004

Polaronic Donor in a Strictly Two-Dimensional Quantum Well

المانح البولاروني ثنائي الأبعاد

Bassam Saqqa

Department of Physics, Faculty of Science, Islamic University, Gaza, Palestine

E-mail: bsaqqa@mail.iugaza.edu

Received: (24/4/2004), Accepted: (31/10/2004)

Abstract

The problem of a polaronic donor in a strictly two-dimensional quantum well is studied using the variational approach. The approach covers the overall range of the electron-phonon coupling and the Coulomb binding strengths. The energy, the number of phonons around the electron, and the size of the polaron are calculated for the ground, and for the first two excited states. It is observed that the polaronic effects become more pronounced for strong Coulomb fields. The size of the polaron is found to be mainly dependent on the polaronic field, as the Coulomb field becomes weak.

ملخص

باستخدام طريقة التغيير، تم دراسة المانح البولاروني ثنائي الأبعاد. وجد أن الطريقة صالحة لكل قيم ثابت الارتباط البولاروني و شدة مجال كولوم. في هذا البحث تم حساب الطاقة وعدد الفونونات حول الإلكترون وحجم البولارون للمستوى الأرضي والمستويين المثاريين الأول والثاني. لقد لوحظ أن التأثير البولاروني يزداد مع زيادة شدة مجال كولوم، كما لوحظ أن اعتماد حجم البولارون على التأثير البولاروني يكون أكبر كلما كان مجال كولوم أضعف.

I. Introduction

Due to the development of modern fabrication techniques, like molecular beam epitaxy and metal organic chemical-vapour deposition, it has become possible to grow low dimensional superstructures opening a large area of research on two-, one-, and even zero-dimensional polaron[1-4]. Particular emphasis has been devoted to the understanding of centers consisting of an electron bound to a charged impurity or a vacancy in a polar semiconductor or an ionic crystal. For example, the spectra of shallow impurities in polar semiconductors (III-V, II-VI compounds) are influenced by the polaronic effect. The bound polaron is also of some interest to the exciton problem as a limiting case where one of the masses tends to infinity.

Bastard [5] was the first to study the problem for infinite potential barriers. Studies along the same line[6-13] revealed that the Coulomb interaction enhances the polaronic effects significantly. Furthermore, these effects grow at a much faster rate with reducing the dimensionality. The effect of the magnetic field on the ground state level has been investigated in a previous work [12]. It was shown that the influence of the magnetic field on the polaronic effect becomes more pronounced for large phonon coupling and strong Coulomb potentials.

In a recently published paper [14], we have studied the energy of the ground state, and the first two excited states, over the entire range of the coupling constant using a variational approach first used by Devreese et al [9]. In this report our aim is to make the study more comprehensive by studying, in addition to the energy, the number of phonons around the electron, and the size of the polaron in the ground state and the first two excited states.

II. Theory

Scaling energy by $\hbar\omega_{LO}$ and length by $\sqrt{\hbar/2m\omega_{LO}}$, the Hamiltonian describing a donor electron confined in a strictly two-dimensional plane and interacting with the bulk optical phonon via the Fröhlich Hamiltonian can be expressed as

$$H = H_e + \sum_Q a_Q^\dagger a_Q + \sum_Q \Gamma_Q \left(a_Q e^{i\mathbf{q}\cdot\boldsymbol{\rho}} + hc \right) \tag{1}$$

$$H_e = p_x^2 + p_y^2 - \frac{\beta}{\rho} \tag{2}$$

where $a_Q^\dagger$ and a_Q are, respectively, the creation and annihilation operators of a phonon of wavevector $\boldsymbol{Q} = (\boldsymbol{q}, \boldsymbol{q}_z)$ and frequency ω_{LO}, and $\Gamma_Q = \sqrt{4\pi\alpha/V}Q^{-1}$ is the amplitude of the electron-phonon interaction, V is the volume and α is the coupling constant. The dimensionless parameter $\beta = (e^2/\varepsilon_o)\sqrt{2m/\hbar^3\omega_{LO}}$ stands for the strength of the Coulomb potential.

The variational theory we follow is based on utilizing a suitable modified adiabatic polaron state of the form [9]

$$\Psi = \Phi_e \, e^S \, \Phi_{ph} \tag{3}$$

where

$$S = \sum_Q \Gamma_Q S_Q \left(a_Q - a_Q^\dagger\right) \tag{4}$$

is a unitary displacement operator to set up the optimal lattice deformation around the mean charge density of the electron, and

$$S_Q = \left\langle \Phi_e \left| e^{\pm i\mathbf{q}\cdot\boldsymbol{\rho}} \right| \Phi_e \right\rangle \tag{5}$$

In the above, Φ_e is the electronic part of the wavefunction, and

$$\Phi_{ph} = \left\{ n - \sum_Q \Gamma_Q g_Q \eta_Q^* a_q \right\} \left|0\right\rangle \tag{6}$$

is the phonon part, g_Q is a variational parameter to interrelate the weak and the strong coupling counterparts of the problem, n is for normalization, and

$$\eta_Q = e^{i\mathbf{q}\cdot\boldsymbol{\rho}} - S_Q \tag{7}$$

The ket $\left|0\right\rangle$ in Eq. (6) denotes the vacuum of the phonon.

Optimizing $\left\langle \Psi \middle| H \middle| \Psi \right\rangle$ with respect to g_Q subject to the constraint that Ψ is normalized, we obtain for the energy

$$E = e_o - e_p + \lambda \tag{8}$$

Here λ is a Lagrange multiplier, which implicitly depends on α and β through the transcendental equation

$$\lambda = \sum_Q \Gamma_Q^2 \left(1 - S_Q^2\right)\left(g_Q / n\right) \tag{9}$$

where

$$\frac{g_Q}{n} = \frac{1 - S_Q^2}{\left(e_o - 2e_p - 1 + \lambda\right)\left(1 - S_Q^2\right) - f_q + h_Q} \tag{10}$$

in which

$$e_o = \langle \Phi_e | H_e | \Phi_e \rangle \tag{11}$$

$$e_p = \sum_Q \Gamma_Q^2 S_Q^2 \tag{12}$$

$$f_Q = \langle \Phi_e | \eta_Q H_e \eta_Q^* | \Phi_e \rangle \tag{13}$$

$$h_Q = \sum_{Q'} \Gamma_{Q'}^2 S_{Q'} \langle \Phi_e | \eta_Q \left(e^{iq'\cdot\rho} + e^{-iq'\cdot\rho}\right) \eta_Q^* | \Phi_e \rangle \tag{14}$$

The average number of phonons around the electron is calculated by finding the expectation value of the phonon part of the Hamiltonian (the second term of Eq. 1), that is,

$$N = \langle \Psi | \sum_Q a_Q^* a_Q | \Psi \rangle \tag{15}$$

The size of the polaron is the expectation value of the operator ρ, in other words

$$R = \langle \Psi | \rho | \Psi \rangle \tag{16}$$

For the electronic part of the wavefunction we choose the hydrogenic approximation and thus use for the ground state and the first two excited states the hydrogenic 1s, 2s, and 2p wavefunctions:

$$\Phi_{1s} = \sqrt{8/\pi}\,\sigma\, e^{-2\sigma\rho} \tag{17}$$

$$\Phi_{2s} = \sqrt{8/27\pi}\left(\sigma - \frac{4\sigma^2}{3}\rho\right)e^{-2\sigma\rho/3} \tag{18}$$

$$\Phi_{2p} = \sqrt{16/81\pi}\,\sigma^2\rho e^{i\theta}\, e^{-2\sigma\rho/3} \tag{19}$$

with σ is another variational parameter. Performing the required analytical calculations, Eq. (5), and Eqs. (11-14) become, for the ground state (1s),

$$e_o = 4\sigma^2 - 4\beta\sigma \tag{20.a}$$

$$e_p = (3/4)\pi\alpha\sigma \tag{21.a}$$

$$S_Q = 1\Big/\sqrt[3]{1 + \frac{q^2}{16\sigma^2}} \tag{22.a}$$

$$f_Q = \left(q^2 + e_o\right)\left(1 - S_Q^2\right) + \frac{\beta q^2 S_Q^2}{2\sigma} \tag{23.a}$$

$$h_Q = 2e_p\left(1 + S_Q^2\right) - (8\alpha/\pi)S_Q\int_0^\infty \frac{S_{Q'}}{\upsilon_+\upsilon_-^2}E(m)\,dq' \tag{24.a}$$

where $\upsilon_\pm = \sqrt{1 + \frac{1}{16\sigma^2}\left(q^2 \pm q'^2\right)^2}$, and $E(m)$ is the complete elliptic integral of the second kind with parameter $m = \sqrt{qq'}\big/(2\upsilon + \sigma)$.

For the first excited state (2s), we obtain for the above equations

$$e_o = \frac{4}{9}\sigma^2 - \frac{4}{9}\beta\sigma \tag{20.b}$$

$$e_p = (53/512)\pi\alpha\sigma \tag{21.b}$$

$$S_Q = \mu^{-3} - 5\mu^{-5} + 5\mu^{-7} \tag{22.b}$$

$$f_Q = q^2 + e_o\left(1 + S_Q^2\right) + S_Q\left\{\begin{array}{l}\left(\frac{16}{9}\sigma^2 - \frac{8}{9}\sigma\beta\right)\mu^{-1} - \left(\frac{56}{9}\sigma^2 - \frac{8}{3}\beta\sigma - \frac{2}{3}q^2\right)\mu^{-3} \\ + \left(\frac{88}{9}\sigma^2 - \frac{8}{3}\sigma\beta - \frac{22}{3}q^2\right)\mu^{-5} - \left(\frac{40}{9}\sigma^2 - \frac{25}{3}q^2\right)\mu^{-7}\end{array}\right\} \tag{23.b}$$

$$h_Q = 2e_p\left(1+S_Q^2\right)-(4\alpha/\pi)S_Q\int_0^\infty dq'\frac{\sqrt{a+b}}{3\left(a^2-b^2\right)^3}S_{Q'}$$
$$\begin{Bmatrix} E(r)\left[\left(46a^2+18b^2\right)-40a\left(a^2-b^2\right)+6\left(a^2-b^2\right)^2\right] \\ -K(r)(a+b)\left[16a+10\left(a^2-b^2\right)\right] \end{Bmatrix} \quad (24.b)$$

where $\mu=\sqrt{1+\left(\frac{3q}{4\sigma}\right)^2}$, $a=1+\frac{9}{16\sigma^2}\left(q^2+q'^2\right)$, $b=\frac{9}{8\sigma^2}qq'$ and $K(r)$ is the complete elliptic integral of the first kind with parameter $r=\sin^2\sqrt{2b/(a+b)}$.

For the second excited state (2p), the corresponding equations are

$$e_o=\frac{4}{9}\sigma^2-\frac{4}{9}\beta\sigma \quad (20.c)$$

$$e_p=\left(245/2^{11}\right)\pi\alpha\sigma \quad (21.c)$$

$$S_Q=\tfrac{5}{2}\mu^{-7}-\tfrac{3}{2}\mu^{-5} \quad (22.c)$$

$$f_Q=q^2+e_o\left(1+S_Q^2\right)- S_Q\left\{\left(\tfrac{4}{9}\sigma\beta-\tfrac{8}{9}\sigma^2\right)\mu^{-3}+\left(4\sigma^2-\tfrac{4}{3}\beta\sigma-3q^2\right)\mu^{-5}+\left(\tfrac{20}{9}\sigma^2-3q^2\right)\mu^{-7}\right\} \quad (23.c)$$

$$h_Q=2e_p\left(1+S_Q^2\right)-(2\alpha/\pi)S_Q\int_0^\infty dq'\frac{\sqrt{a+b}}{3\left(a^2-b^2\right)^3}S_{Q'}$$
$$\left\{E(r)\left[\left(46a^2+18b^2\right)-24a\left(a^2-b^2\right)\right]-K(r)(a-b)\left[16a+10\left(a^2-b^2\right)\right]\right\} \quad (24.c)$$

III. Results and Discussion

First, let us test the validity of our formulation by considering some special limiting cases. For the weak-coupling limit ($\alpha,\beta<<1$) $S_Q\to 0$, and this leads to $f_Q=e_o+q^2$, and $h_Q=2e_p$. To first order in α, energies are approximated as

$$E_{1s}=-\beta^2-\tfrac{3}{8}\pi\alpha\beta-\tfrac{1}{2}\pi\alpha \quad (25)$$

$$E_{2s} = -\tfrac{1}{9}\beta^2 - 0.052\pi\alpha\beta - \tfrac{1}{2}\pi\alpha \tag{26}$$

$$E_{2p} = -\tfrac{1}{9}\beta^2 - 0.060\pi\alpha\beta - \tfrac{1}{2}\pi\alpha \tag{27}$$

Comparing these results with those obtained in reference [13] (using the LLP-H method) we see that the present formalism yields lower energies for the values of α, and β under consideration.. For the average number of phonons and the size of the polaron, we obtain

$$N_{1s} = 0.375\pi\alpha\beta + \tfrac{1}{4}\pi\alpha \tag{28}$$

$$N_{2s} = 0.052\pi\alpha\beta + \tfrac{1}{4}\pi\alpha \tag{29}$$

$$N_{2p} = 0.060\pi\alpha\beta + \tfrac{1}{4}\pi\alpha \tag{30}$$

$$R_{1s} = \frac{1}{\beta} - 0.1875\pi\alpha \tag{31}$$

$$R_{2s} = \frac{7}{\beta} - 1.630\pi\alpha \tag{32}$$

$$R_{2p} = \frac{6}{\beta} - 1.615\pi\alpha \tag{33}$$

As is obvious from these equations, in the limit ($\alpha \to 0,\ \beta \to 0$), the average number of phonons mainly depends on α, while the polaron size is governed mainly by β and that agrees with what is found by [13].

In the strong coupling limit ($\alpha >> 1$), $S_Q \to 1$, and $\lambda \to 0$, we get

$$E_{1s} = -\left(\beta + \tfrac{3}{16}\pi\alpha\right)^2 \tag{34}$$

$$E_{2s} = -\left(\frac{\beta}{3} + 0.0776\pi\alpha\right)^2 \tag{35}$$

$$E_{2p} = -\left(\frac{\beta}{3} + 0.0897\pi\alpha\right)^2 \tag{36}$$

$$N_{1s} = 0.75\pi\alpha\left(\frac{\beta}{2} + \tfrac{3}{32}\pi\alpha\right) \tag{37}$$

$$N_{2s} = 0.104\pi\alpha\left(\frac{\beta}{2} + 0.116\pi\alpha\right) \tag{38}$$

$$N_{2p} = 0.120\pi\alpha\left(\frac{\beta}{2} + 0.135\pi\alpha\right) \tag{39}$$

$$R_{1s} = \left(\beta + \tfrac{3}{16}\pi\alpha\right)^{-1} \tag{40}$$

$$R_{2s} = 7(\beta + 0.058\pi\alpha)^{-1} \tag{41}$$

$$R_{2p} = 6(\beta + 0.269\pi\alpha)^{-1} \tag{42}$$

These results are identical to those obtained by [(13)] as they should be.

For all values of the coupling parameters the calculation has to be performed numerically. In Figure 1. we display the ground state energy as a function of α for $\beta = 1$ and $\beta = 10$. It is clearly evident that the effect of the polaronic interaction on the binding energy becomes more pronounced as β is increased. To show this feature in more details, we plot, in Figure 2., the average number of phonons around the electron in the ground state as a function of α for the same values of β. Here, again, we conclude that the polaronic effects are greatly enhanced in the strong coupling fields. The reason for this lies in that with increasing β the binding energy becomes larger making the localization of the electron more pronounced and this, in turn, increases the importance of the polaronic correction.

Figure 3. gives a description of the polaron size in the ground state as a function of α, again, for $\beta = 1$ and $\beta = 10$. We note that the α-dependence on the size becomes more prominent as β gets smaller. This result shows that, what is claimed by [(13)] that in the extended-state limit (α and β is very small) the size is governed by β only, is only valid for very small values of the coupling constants.

In figure 4. We plot the energies of the two excited states as a function of α for β=1, and β=10. From the graph we conclude that the polaronic coupling lifts the degeneracy of the two states and once again the Coulomb strength plays the role of enhancing the polaronic effect.

Taking β=1, we see that the degeneracy is lifted at $\alpha \sim$ 1.5, while it is lifted at $\alpha \sim$ 0.5 when β=10. The small difference between the solid and the dashed curves in the figure is a measure of the induced Lamb shift. In Figures 5 and 6. We display, respectively, the α-dependence of the average number of phonons and the size of the polaron for the excited states. For a given value of α, the bound polaron cloud appears to contain a smaller number of phonons when β=1 than when β=10. For the excited states, the polaron size exhibits qualitatively the same behavior as the ground state. For β=10, we again note that the size does not change appreciably over a wide range of α.

IV. Conclusion

In this paper we have reformulated the problem of the 2D bound polaron using the variational approach of Devreese et al [9]. We have calculated the energy of the first 3-levels for a large range of the coupling constant. Lower values for the energies are obtained compared with that obtained in [13] using the LLP-H approximation. The degeneracy of the two excited states is found to be lifted at lower values of α as β decreases.

The number of phonons around the electron and the size of the polaron in the three states are also calculated. It is observed that the polaronic effect becomes more important as the Coulomb field increases.

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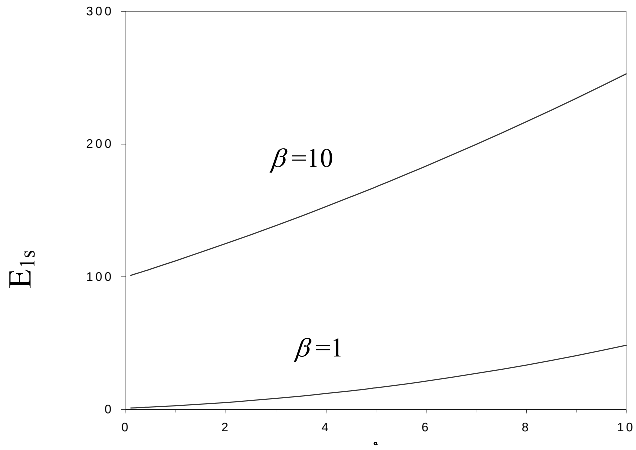

Figure (1): The ground state energy (in $\hbar\omega_{LO}$) as a function of α. for β=1 and β=10.

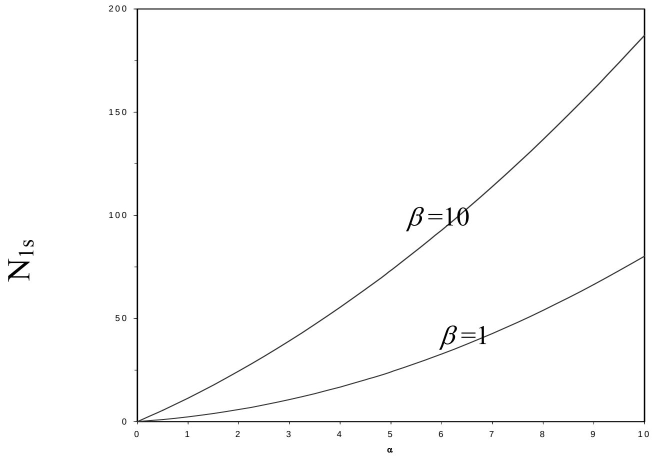

Figure (2): The average number of phonons around the electron in the ground state as a function of α for β=1 and β=10.

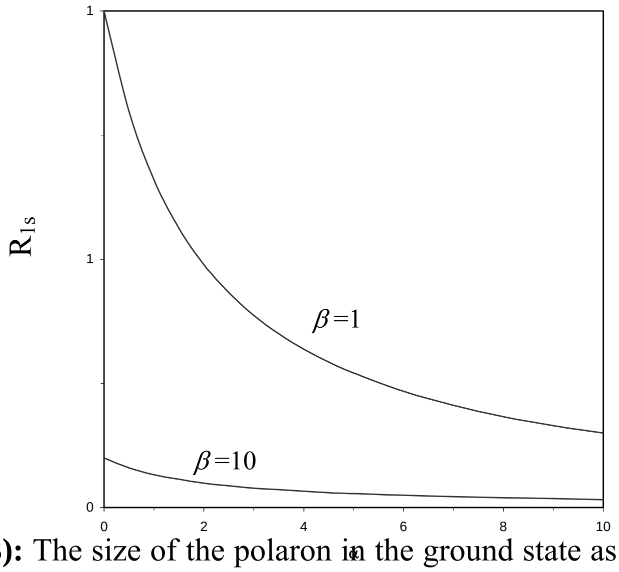

Figure (3): The size of the polaron in the ground state as a function of α for β=1 and β=10.

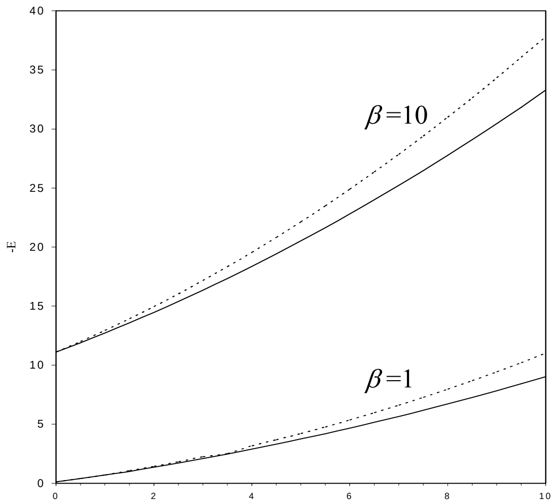

Figure (4): The excited energies (in $\hbar\omega_{LO}$) as a function of α for β=1 and β=10. The dashed and the solid curves correspond to the 2s and 2p states, respectively.