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The Bound Polaron under the Effect of an External Magnetic Field

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Abstract: Using the adiabatic approach, the effect of an external magnetic field on the bound polaron is investigated. The energy, the number of phonons around the electron, and the size of the polaron are calculated for the ground state, and for the first two excited states. It is observed that, the magnetic field and the Coulomb field enhances the polaronic effect on the problem. The three fields: The polaronic, the Coulomb, and the magnetic fields affect each other in an interrelated manner.

مستويات الطاقة للمانح البولاروني ثنائي الأبعاد

ملخص: بإستخدام طريقة التغيير تم دراسة مستويات الطاقة الأرضية والمثارة الأولي والثانية للمانح البولاروني ثنائي الأبعاد لكل قيم ثابت الإرتباط البولاروني.

لقد وجد أن التأثير البولاروني يزداد مع زيادة شدة مجال كولوم. كما وجد أنه مع زيادة شدة مجال كولوم فإن حالة الإنشطار بين مستويات الطاقة المثارة الأولي والثانية (2s و 2p) تبدأ عند قيم أصغر لثابت الإرتباط.

1-Introduction

The subject of low dimensional polaron is receiving more interest among researchers in the last decades [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.

Bastard [5] was the first who study the problem for infinite potential barriers. Studies along the same line [6-15] revealed that the Coulomb interaction enhances the polaronic effects significantly. Furthermore, these effects grow at a much faster rate with reducing the dimensionality.

The application of an external magnetic field on the polaron puts a further confinement on the problem making the electron-phonon interaction more pronounced [16-19]. A part from the competition between the magnetic and the Coulomb fields, the polaronic effect introduces further complications. Reasonable simplifications however can be achieved on the extreme limits of the magnetic field. For sufficiently high magnetic fields, the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit [19]. Thus the most efficient coherent phonon state should be taken as centered on the orbit center rather than on the origin. For not too large magnetic fields and strong phonon coupling, the polaronic aspect dominates the magnetic field counterpart of the problem so that the lattice deformation should be thought as surrounding the mean charge density of the electron itself rather than it overall motion in a Landau orbit.

In a recently published papers [14, 15], we have studied the problem of bound polaron without the effect of the magnetic field. The energy, the number of phonons around the electron, and the radius of the polaron in the ground state, and the first two excited states, are calculated over the entire range of the coupling constant using a variational approach first used by Devreese et al [9]. It was found that the degeneracy of the two excited states is to be lifted at lower values of the coupling constant as the Coulomb strength decreases.

In this report our aim is to include the effect of an external magnetic field on the problem and investigate such effect on all the values calculated previously.

2-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

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

with H_e is the electronic part of the Hamiltonian. The operators $a_Q^\dagger$ and a_Q are, respectively, the creation and annihilation operators of a phonon of wavevector $\boldsymbol{Q} = (\boldsymbol{q}, \boldsymbol{q}_z)$, ω_{LO} is the frequency, $\Gamma_Q = \sqrt{4\pi\alpha/V}\,Q^{-1}$ is the amplitude of the electron-phonon interaction, V is the volume and α is the coupling constant. Using the symmetric gauge $\vec{A} = \frac{B}{2}(-y, x, 0)$ for the vector potential and assuming that the magnetic filed is along the z-axis, this electronic part of the Hamiltonian can be written as

$$H_e = p_x^2 + p_y^2 - \frac{b}{r} + \frac{1}{16}\Omega^2 r^2 + \tfrac{1}{2} L_z \Omega \,, \qquad \textbf{(2)}$$

where $\vec{r} = (x, y)$ denotes the electron position in the transverse plane, $\left(L_Z = xP_y - yP_x\right)$ is the angular momentum, and $\Omega = \left(eB/mcw_{LO}\right)$ is the dimensionless cyclotron frequency. The dimensionless parameter $b = \left(e^2/e_o\right)\sqrt{2m/\hbar^3 w_{LO}}$ 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]

$$\Psi = \Phi_e e^S |0\rangle \,, \qquad (3)$$

where

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

is a unitary displacement operator to set up the optimal lattice deformation around the mean charge density of the electron, and $|0\rangle$ is the phonon vacuum.

Minimizing $\langle \Psi | H | \Psi \rangle$ with respect to the variational parameter S_Q we get

$$S_Q = \langle \Phi_e | e^{\pm i\mathbf{q}\cdot\mathbf{r}} | \Phi_e \rangle \,. \qquad \textbf{(5)}$$

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

For the energy we obtain

$$E = e_o - e_p \,, \qquad (6)$$

in which

$$e_o = \langle \Phi_e | H_e | \Phi_e \rangle , \tag{7}$$

and

$$e_p = \sum_Q \Gamma_Q^2 S_Q^2 \ . \tag{8}$$

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,

$$N = \langle \Psi | \sum_Q a_Q^* a_Q | \Psi \rangle . \tag{9}$$

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

$$R = \langle \Psi | r | \Psi \rangle \tag{10}$$

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:

$$\Phi_{1s} = \sqrt{8/p}\, s \ e^{-2sr} , \tag{11}$$

$$\Phi_{2s} = \sqrt{8/27p} \left(s - \frac{4s^2}{3} r \right) e^{-2sr/3} , \tag{12}$$

and

$$\Phi_{2p} = \frac{8s^2}{9\sqrt{3p}} \, r \, e^{iq} \ e^{-2sr/3} , \tag{13}$$

with s is another variational parameter. Performing the required analytical calculations, we obtain for the ground state (1s),

$$S_Q = \left(1 + \frac{q^2}{16s^2} \right)^{-\frac{3}{2}} , \tag{14.a}$$

$$E_{1s} = 4s^2 - 4bs + \frac{3}{128} \left(\frac{\Omega}{s} \right)^2 - \frac{3}{4} pas \ , \tag{15.a}$$

$$N_{1s} = (3/4) pas \ , \tag{16.a}$$

$$R_{1s} = \frac{1}{2s} . \qquad \textbf{(17.a)}$$

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

$$S_Q = m^{-3} - 5m^{-5} + 5m^{-7},\ m = \sqrt{1+\left(\tfrac{3q}{4s}\right)^2}\ , \qquad \textbf{(14.b)}$$

$$E_{2s} = \frac{4}{9}s^2 - \frac{4}{9}bs + \frac{117}{128}\left(\frac{\Omega}{s}\right)^2 - \frac{53}{512}pas\ , \qquad \textbf{(15.b)}$$

$$N_{2s} = (53/512)pas\ , \qquad \textbf{(16.b)}$$

$$R_{2s} = \frac{7}{2s} . \qquad \textbf{(17.b)}$$

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

$$S_Q = \tfrac{5}{2}m^{-7} - \tfrac{3}{2}m^{-5}, \qquad \textbf{(14.c)}$$

$$E_{2p} = \frac{4}{9}s^2 - \frac{4}{9}bs + \frac{45}{64}\left(\frac{\Omega}{s}\right)^2 - \frac{245}{2^{11}}pas\ , \qquad \textbf{(15.c)}$$

$$N_{2p} = \left(245/2^{11}\right)pas\ , \qquad \textbf{(16.c)}$$

$$R_{2p} = \frac{3}{s} . \qquad \textbf{(17.c)}$$

3-Results and Discussion

Before we present our results concerning the coupled effect of both the electron-phonon interaction and the magnetic field on the problem, we would like to discuss some special cases where the situation is more clear and well-known. For the bare two-dimensional polaron (β=Ω=0) we get E=-0.347α^2 which differ from the standard strong coupling value $\left(-a^2/3p^2\right)$ about 11% . The discrepancy here is due to the wave function adopted. The Hydrogen-like wave function used in this work is suitable only for bound problem and so for β=0, the Gaussian wave function is supposed to be more appropriate.

Without the polaronic effect and in the absence of the magnetic field (α=0,Ω=0) we trivially obtain E=- β^2 which is the 2D-Rydberg which is four times that for the 3D case.

For the bare donor in a magnetic field (α=0) we refer to the paper by MacDonald and Richeie [20]. In the high magnetic field limit they obtain

$$E = 2b^2 g\left(0.5 - c - 0.04401c^2 - 0.02331c^3 - 0.00727c^4 ....\right)$$

where,

$$c = \sqrt{\frac{p}{8g}} \quad \text{and} \quad g = \frac{\Omega}{2b^2} \;,$$

Are the a measure of the strength of the magnetic field relative to the 2D-effective Rydberg, β^2, and for weak magnetic field γ≤0.1, they obtain $E = -b^2\left(1 - \frac{3}{8}g^2\right)$. In table 3.1 we tabulate our results with that of [20] for Ω=0.1. As it is clear from the table the agreement is exact between the two results for Ω>β. The discrepancy between the two results comes from the choice of the wave function. For Ω>β the H-like wave function lose its validity.

Table 3.1 Comparison between our results without polaronic coupling with that of Macdonald Richeie (E_M) [20] for Ω=0.1 and different values of β.

b	b=**0.1**	b=**0.5**	b=**1.0**	b=**5.0**
E_M	0.08375	-0.2463	-0.99906	-25.00
E_{1s}(Present work)	0.02332	-0.2463	-0.99906	-25.00

Taking the remaining case (β=0) the problem reduces to the 2D, magnetopolaron which was studied in detail by Ercelebi and Saqqa [19].

We now turn back to the donor problem and study the polaronic effect together with the additional enhancement coming from the magnetic field on the ground state and the first two excited states.

To show the effect of the external magnetic field on the problem we plot in Figure 3.1 the ground state energy as a function of the strength of the magnetic field for two different values of the coulomb strength. As it is clear from the graph, the importance of the Coulomb strength becomes more important as Ω is increased. Moreover, the effect of the magnetic field on the energy is more clear for larger values of β. The reason behind this feature is that the strength of the three fields, (the polaronic, the Coulomb and the magnetic field) do not enter the problem independently, but affect the contributions one another in a somewhat involved and interrelated manner. The same feature shows up in Figure 3.2 where we plot the two excited states as a function of Ω for the same values of β.

In Figure 3.3 and Figure 3.4 we plot, respectively the number of phonons and the polaron size in the ground state versus Ω again for β=1 and β=10. For a given value of Ω, the bound polaron cloud appears to contains a smaller number of phonons when β=1 than β=10. The Ω-dependence in the size of the polaron becomes more prominent as β gets smaller.

In Figure 3.5 and Figure 3.6 we display the effect of the magnetic field on the number of phonons and the size of polaron, respectively for the two excited states. The polaron size in the excited states exhibits qualitatively the same behavior as the ground state. For large value of β we note that the size does not change appreciably over a wide range of Ω. The effect of the magnetic field on the number of phonons is more solid for β=10.

It should be noted that for too large values of the magnetic field, the coherent state we adopt in this work may be not fit to reflect a correct description of the problem, specially for smaller values of the polaronic constant α. In this limit the lattice can only respond to the mean charge density of the rapidly orbiting electron and hence acquire a static deformation over the entire Landau orbit rather than about the origin.

Conclusion

In this work we have retrieved the problem of a two dimensional bound polaron using the strong coupling approach. The effect of an external magnetic field on the problem is studied. The energy of the first three-levels has been calculated in addition to the average number of phonons around the electron and the size of the polaron in the three states. It is found that the polaronic effect becomes more important as the Coulomb field increases. The strength of the three fields: the polaronic field, the Coulomb field and the magnetic field do not enter the problem independently but rather affect each other in an involved and interrelated manner.

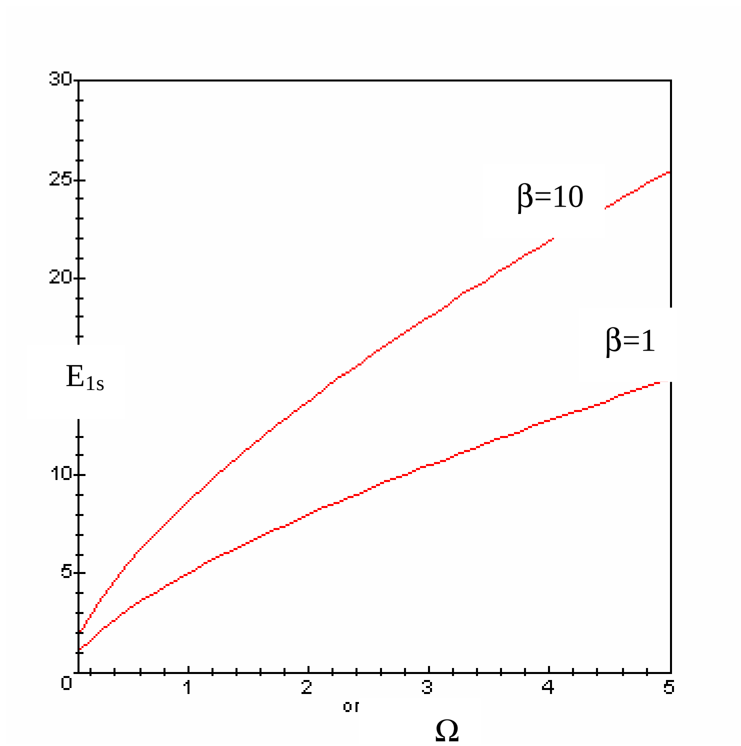

Fig.3.1. The ground state energy in $\hbar\omega$ (in the presence of magnetic field) as a function of Ω for β=1 and β=10 and α=10.

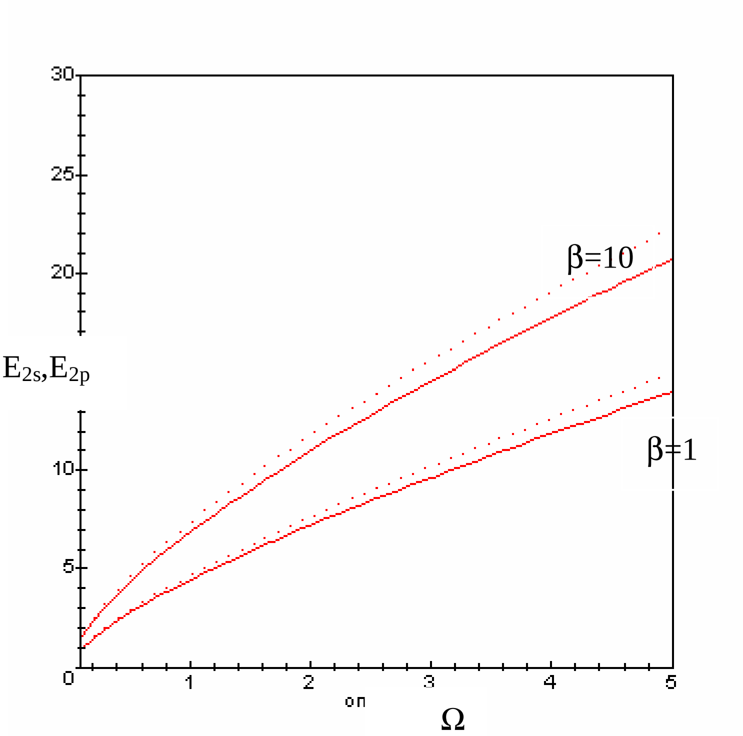

Fig.3.2. The excited energies in hw (in the presence of magnetic field) as a function of W for b=1 and b=10 and a=10. The dashed and the solid curves correspond to the 2s and 2p states respectively.

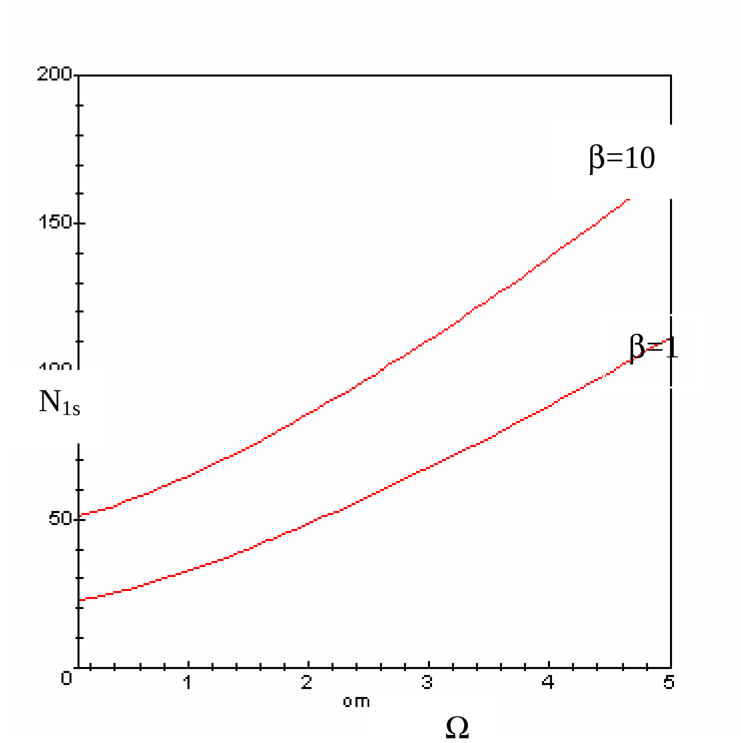

Fig.3.3. The average number of phonons (in the presence of magnetic field) around the electron in the ground state as a function of W for b=1 and b=10 and a=10.

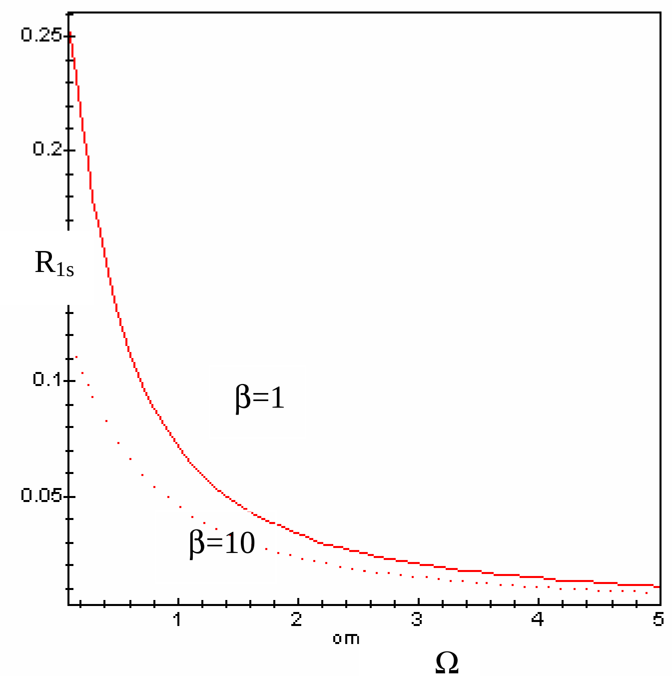

Fig.3.4. The size of the polaron (in the presence of magnetic field) in the ground state as a function of W for b=1 and b=10 and a=10.

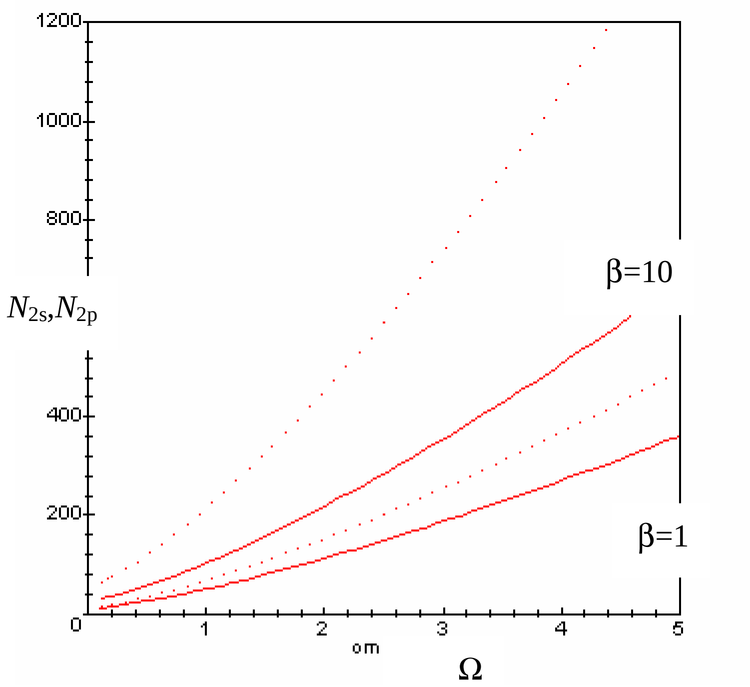

Fig.3.5. The average number of phonons (in the presence of magnetic field) around the electron in the (2s and 2p) states as a function of W for b=1 and b=10 and a=10. The dashed and the solid curves correspond to the 2s and 2p states respectively.

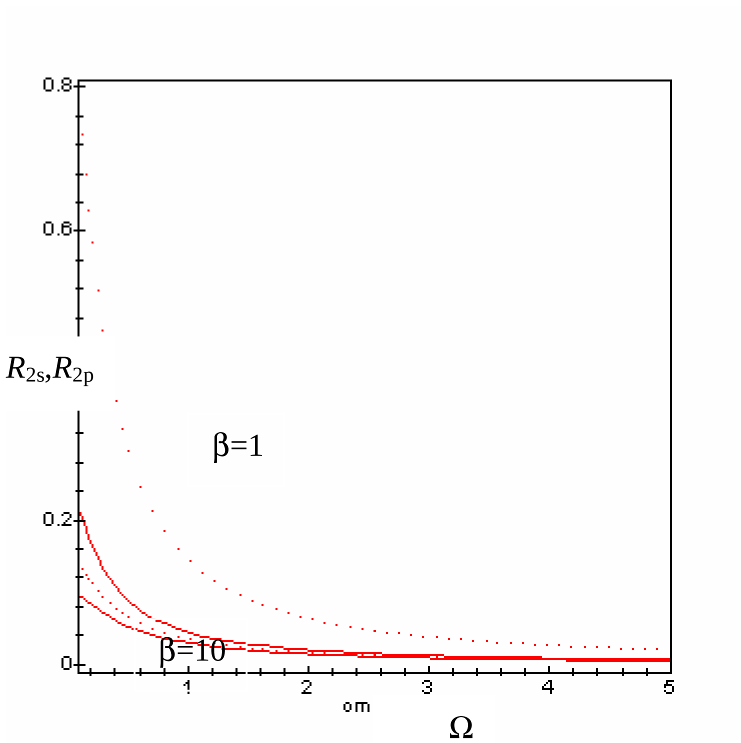

Fig.3.6. The size of polaron (in the presence of magnetic field) in the (2s and 2p) states as a function of W for b=1 and b=10 and a=10. The dashed and the solid curves correspond to the 2s and 2p states respectively.

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