Journal of the Islamic University of Gaza, Vol.11, No.2, P115-P125, 2003

Energy Levels of Two-Dimensional Polaronic Donor

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مستويات الطاقة للمانح البولاروني ثنائي الأبعاد

ملخص: باستخدام طريقة التغيير تم دراسة مستويات الطاقة الأرضية والمثـارة الأولـى والثانيـة للمـانح 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 مجـال كولـوم فإن حالة الإنحلال بين مستويات الطاقة المثارة الأولى والثانية (2s و 2p) تنتهي عند قيم أصـغر لثابـت الإرتباط.

Abstract Using a variational approach, the ground and the first two excited states of a two-dimensional polaronic donor are studied over the entire range of the coupling constants. It is observed that the polaronic effects become more pronounced for strong Coulomb fields. The degeneracy between the two excited states (the 2s and the 2p) is found to be lifted at lower values of the polaronic coupling constant as the Coulomb strength increases.

Introduction

Due to the development achieved in 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 polarons [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 this paper, the energy of the ground and the first two excited states are calculated over the entire range of the coupling constant using a variational approach which was first used by Devreese et al [9].

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

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

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

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 with 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

$$S_Q = \langle \Phi_e | e^{\pm iq\cdot\rho} | \Phi_e \rangle \tag{5}$$

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

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

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

$$\eta_Q = e^{iq\cdot\rho} - S_Q \tag{7}$$

The ket $|0\rangle$ in Eq. [6] denotes the vacuum of the phonon.

Optimizing $\langle\Psi|H|\Psi\rangle$ 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

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

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

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

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

For the electronic part of the wavefunction (Φ_e in Eq. 3) we adopt the hydrogenic approximation and thus use for the ground state and the first two excited states we choose the variational hydrogenic 1s, 2s, and 2p wavefunctions:

$$\Phi_{1s} = \sqrt{8/\pi}\,\sigma\, e^{-2\sigma\rho} \tag{15}$$

$$\Phi_{2s} = \sqrt{8/27\pi}\left(\sigma - \frac{4\sigma^2}{3}\rho\right)e^{-2\sigma\rho/3} \tag{16}$$

$$\Phi_{2p} = \sqrt{16/81\pi}\,\sigma^2 \rho\, e^{i\theta}\, e^{-2\sigma\rho/3} \tag{17}$$

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

$$e_o = 4\sigma^2 - 4\beta\sigma \tag{18.a}$$

$$e_p = (3/4)\pi\alpha\sigma \tag{19.a}$$

$$S_Q = 1\Big/\sqrt[3]{1 + \frac{q^2}{16\sigma^2}} \tag{20.a}$$

$$f_Q = \left(q^2 + e_o\right)\left(1 - S_Q^2\right) + \frac{\beta q^2 S_Q^2}{2\sigma} \tag{21.a}$$

$$h_Q = 2e_p\left(1 + S_Q^2\right) - (8\alpha/\pi)S_Q \int_0^\infty \frac{S_{Q'}}{\upsilon_+ \upsilon_-^2} E(m)\, dq' \tag{22.a}$$

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 $m = \sqrt{qq'}/(2\upsilon + \sigma)$.

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

$$e_o = \frac{4}{9}\sigma^2 - \frac{4}{9}\beta\sigma \tag{18.b}$$

$$e_p = (53/512)\pi\alpha\sigma \tag{19.b}$$

$$S_Q = \mu^{-3} - 5\mu^{-5} + 5\mu^{-7} \tag{20.b}$$

$$f_Q = q^2 + e_o\left(1+S_Q^2\right) + S_Q\begin{Bmatrix}\left(\tfrac{16}{9}\sigma^2 - \tfrac{8}{9}\sigma\beta\right)\mu^{-1} - \left(\tfrac{56}{9}\sigma^2 - \tfrac{8}{3}\beta\sigma - \tfrac{2}{3}q^2\right)\mu^{-3} \\ + \left(\tfrac{88}{9}\sigma^2 - \tfrac{8}{3}\sigma\beta - \tfrac{22}{3}q^2\right)\mu^{-5} - \left(\tfrac{40}{9}\sigma^2 - \tfrac{25}{3}q^2\right)\mu^{-7}\end{Bmatrix} \tag{21.b}$$

$$h_Q = 2e_p\left(1+S_Q^2\right) - (4\alpha/\pi)S_Q\int_0^\infty dq'\,\frac{\sqrt{a+b}}{3\left(a^2-b^2\right)^3}S_{Q'} \begin{Bmatrix}E(r)\left[\left(46a^2+18b^2\right) - 40a\left(a^2-b^2\right) + 6\left(a^2-b^2\right)^2\right] \\ - K(r)(a+b)\left[16a+10\left(a^2-b^2\right)\right]\end{Bmatrix} \tag{22.b}$$

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

$$e_o = \frac{4}{9}\sigma^2 - \frac{4}{9}\beta\sigma \tag{18.c}$$

$$e_p = \left(245/2^{11}\right)\pi\alpha\sigma \tag{19.c}$$

$$S_Q = \tfrac{5}{2}\mu^{-7} - \tfrac{3}{2}\mu^{-5} \tag{20.c}$$

$$f_Q = q^2 + e_o\left(1+S_Q^2\right) - S_Q\left\{\left(\tfrac{4}{9}\sigma\beta - \tfrac{8}{9}\sigma^2\right)\mu^{-3} + \left(4\sigma^2 - \tfrac{4}{3}\beta\sigma - 3q^2\right)\mu^{-5} + \left(\tfrac{20}{9}\sigma^2 - 3q^2\right)\mu^{-7}\right\} \tag{21.c}$$

$$h_Q = 2e_p\left(1+S_Q^2\right) - (2\alpha/\pi)S_Q\int_0^\infty dq'\,\frac{\sqrt{a+b}}{3\left(a^2-b^2\right)^3}S_{Q'} \left\{E(r)\left[\left(46a^2+18b^2\right) - 24a\left(a^2-b^2\right)\right] - K(r)(a-b)\left[16a+10\left(a^2-b^2\right)\right]\right\} \tag{22.c}$$

Results and Discussion

First, let us test the validity of our formulation by making correspondence with some special limit 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 to

$$E_{1s} = -\beta^2 - \tfrac{3}{8}\pi\alpha\beta - \tfrac{1}{2}\pi\alpha \tag{23}$$

$$E_{2s} = -\tfrac{1}{9}\beta^2 - 0.052\pi\alpha\beta - \tfrac{1}{2}\pi\alpha \tag{24}$$

$$E_{2p} = -\tfrac{1}{9}\beta^2 - 0.060\pi\alpha\beta - \tfrac{1}{2}\pi\alpha \tag{25}$$

Comparing these results with that obtained in reference [13] (using the LLP-H method) we see that the present formalism yields lower energies for any values of α, and β.

In the strong coupling limit ($\alpha >> 1$), $S_Q \to 1$, and $\lambda \to 0$, as expected. For the energies we obtain

$$E_{1s} = -\left(\beta + \tfrac{3}{16}\pi\alpha\right)^2 \tag{26}$$

$$E_{2s} = -\left(\frac{\beta}{3} + 0.0776\pi\alpha\right)^2 \tag{27}$$

$$E_{2p} = -\left(\frac{\beta}{3} + 0.0897\pi\alpha\right)^2 \tag{28}$$

These results are identical to those obtained by [13] as it should be.

Calculation has to be performed numerically for all values of the coupling parameters. In Figure 1. we compare our results with that of the effective mass approximation (Equation 9 in reference [7]) by plotting the ground state polaron shift □*E* =|*E*(□)-*E*(□=0)| as a function of □ for □=0.07 (GaAs). As it is clear from the graph the two results match well for small □ values. For large □ the effective mass approximation loses its validity as it explained in [13].

In Figure 2. we display the variation of the ground state polaron shift □*E* with □ for □=1, 5, and 10. We at once note that the strength of the Coulomb field, greatly, enhances the polaronic effects on the binding energy. This is due to that with increasing □ the binding energy becomes larger making the localization of the electron more pronounced and this, in turn, increases the importance of the polaronic corrections.

In Figure 3. We plot the two excited states as a function of □ for □□1, and □□1. 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 □□1, we see that the degeneracy is lifted at □□ 1.5, while it is lifted at □□0.5 when □□1. The small difference between the solid and the dashed curves in the figure is a measure of the induced Lamb shift.

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 all 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.

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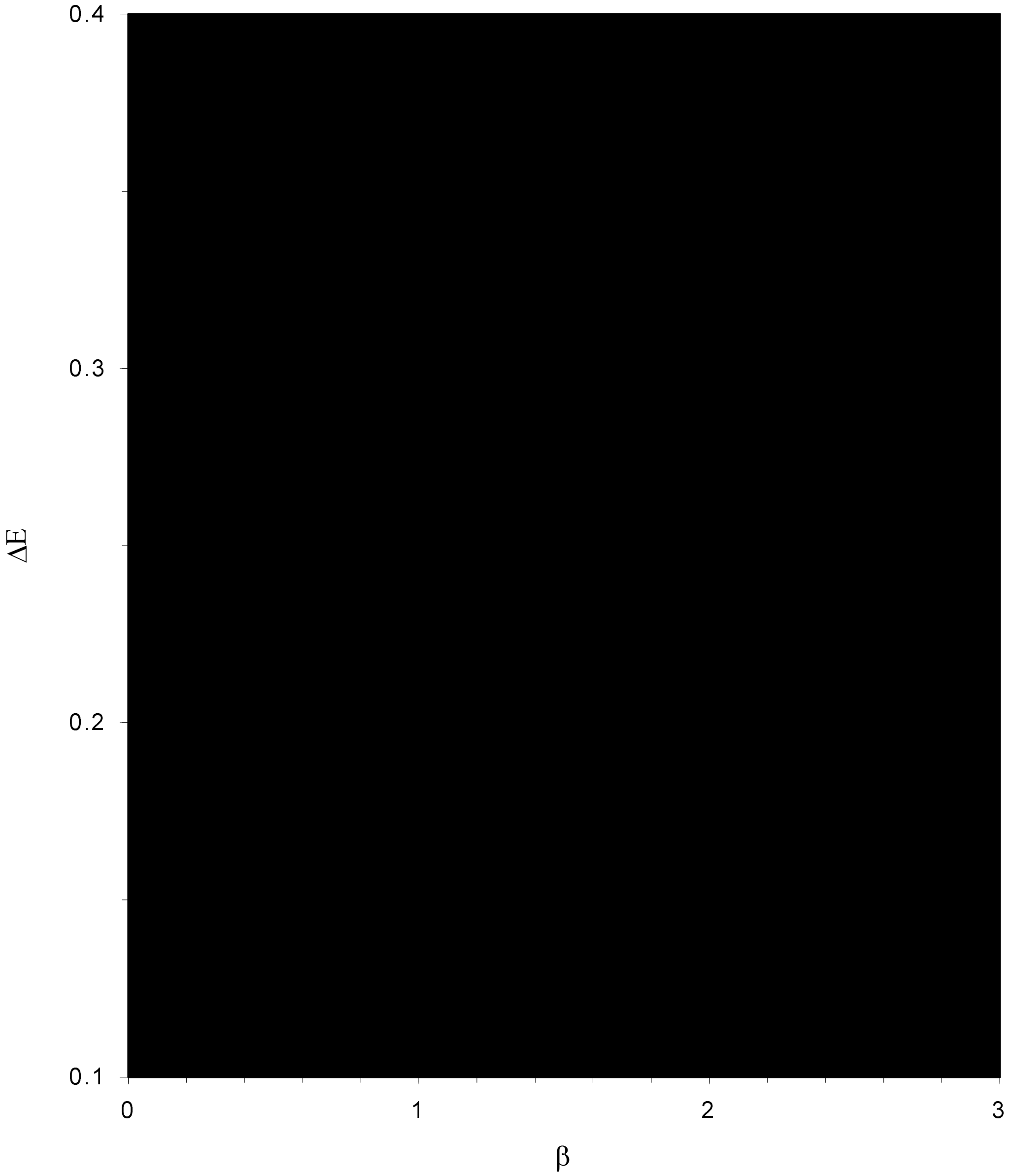

Figure 1. The ground state polaronic shift ΔE (in $\hbar\omega_{LO}$) as a function of β for α =0.07 (GaAs). The solid (dashed) curve correspond to the present (effective mass0 formalism.

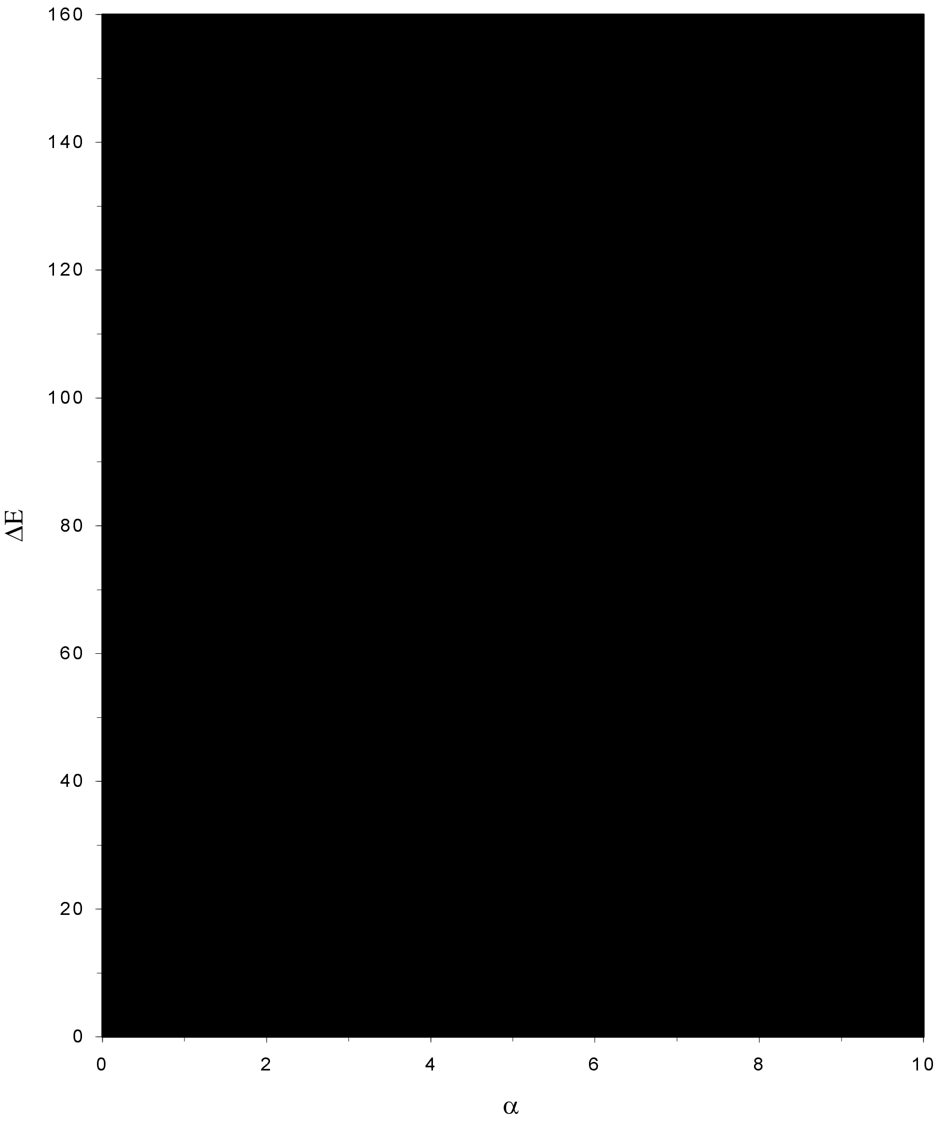

Figure 2. The ground state polaronic shift ΔE (in $\hbar\omega_{LO}$) as a function of α for different values of β.

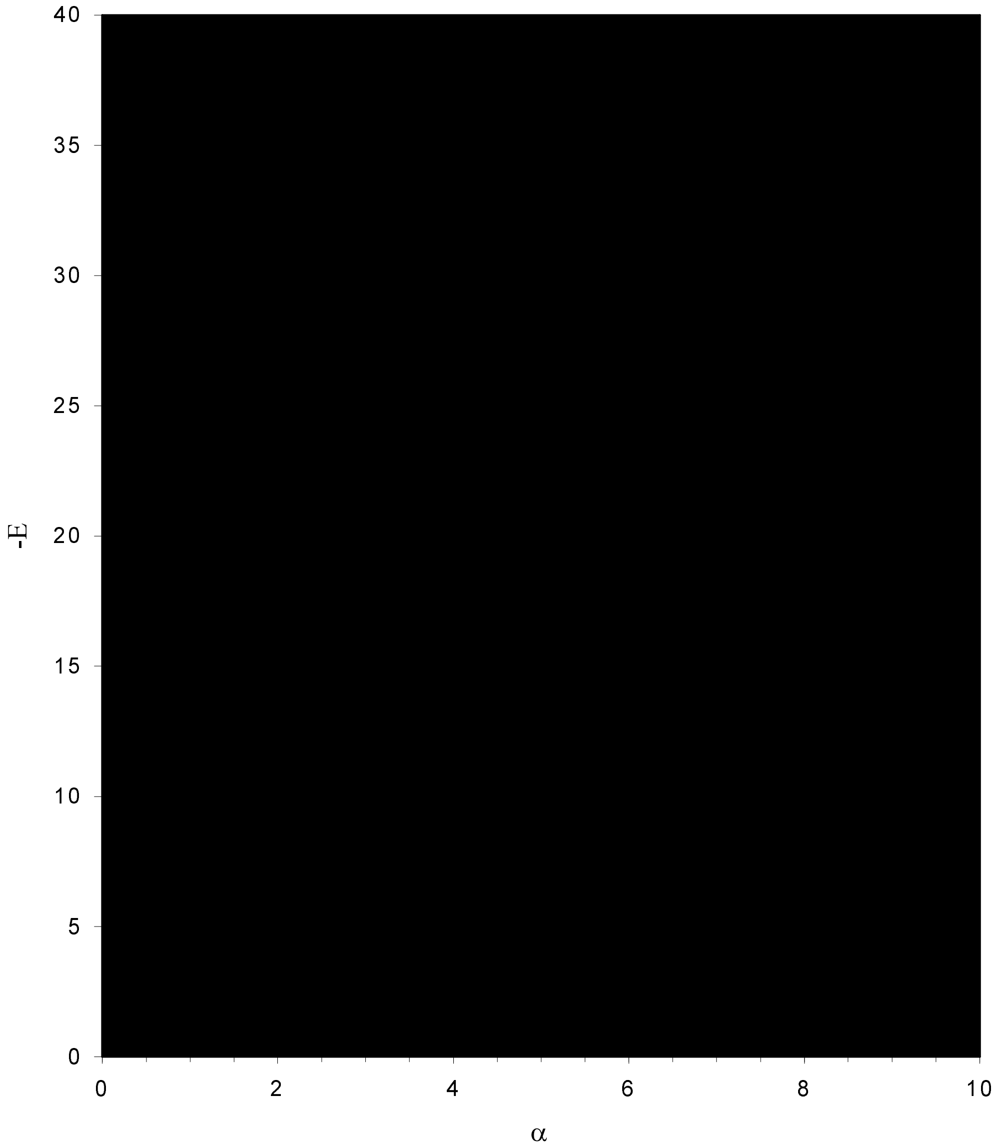

Figure 3. The excited energies (in $\hbar\omega_{LO}$) as a function of α for β=1 and β=10. The dashed and the solid curves correspond to the 2s and 2p states, respectively.