The stability of magnetobipolarons in low-dimensional systems

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Received 7 March 2002 and Received in final form 22 April 2002 Published online 25 June 2002 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2002

Abstract. We investigate the stability condition of large bipolarons confined in a parabolic potential containing certain parameters and a uniform magnetic field. The variational wave function is constructed as a product form of electronic parts, consisting of center of mass and internal motion, and a part of coherent phonons generated by Lee-Low-Pines transformation from the vacuum. An analytical expression for the bipolaron energy is found, from which the ground and excited-state energies are obtained numerically by minimization procedure. The bipolaron stability region is determined by comparing the bipolaron energy with those of two separate polarons, which is already calculated within the same approximation. It is shown that the results obtained for the ground state energy of bipolarons reduce to the existing works in zero magnetic field. In the presence of a magnetic field, the stability of bipolarons is examined, for three types of low-dimensional system, as function of certain parameters, such as the magnetic-field, the electron-phonon coupling constant, Coulomb repulsion and the confinement strength. Numerical solutions for the energy levels of the ground and first excited states are examined as functions of the same parameters.

PACS. 73.21.-b Electron states and collective excitations in multilayers, quantum wells, mesoscopic, and nanoscale systems – 63.20.Kr Phonon-electron and phonon-phonon interactions – 71.38.-k Polarons and electron-phonon interactions

1 Introduction

The large bipolaron concept as usually understood arises from the consideration of the interaction of two electrons with the longitudinal optical phonon field of ionic lattices and their Coulomb repulsion. One of two electrons distorts and displaces its surrounding ions, establishing a polarization field in the crystal which in turn acts on the second electron. In the language of field theory these effects arise from the emission and reabsorption of virtual quanta of longitudinal optical phonon field of the material. Under certain conditions, the phonon mediated interaction may be strong enough to overcome the Coulomb repulsion between the two electrons, accordingly they end up in a bound state. A possibility of pairing of two electrons, or rather two large polarons, was first considered by Pekar (1951) [1] and a calculation of the large bipolaron binding energy was first achieved by Vinetskii and Gitterman(1957) [2].

The large bipolaron (polaron) can be dealt with thoroughly within the framework of Fröhlich approximation, in which the electron-phonon interaction is developed by treating the dielectric medium as a macroscopic continuum. This medium is represented by the static and the high frequency dielectric constants, ϵ_0 and ϵ_{∞} , respectively. In case of the bipolaron problem, the parameter $\eta = \epsilon_{\infty}/\epsilon_0$ plays a decisive role in the stability of the bipolaron.

The criterion for which a stable bipolaron forms can be derived by the requirement that the energy of two interacting polarons be lower than twice that of a single polaron. Apart from the other parameters, stable bipolarons exist in three dimension (3D) only for large values of electronphonon coupling strength, which takes place in the intermediate and strong coupling regions. A calculation for the bipolaron binding energy by using a variational wave function in a general form yields that the stability is fulfilled in 3D when $\alpha > 7.2$ [3]. Later, this value was found as $\alpha > 6.8$ [4–6]. It is also shown that this is reduced to $\alpha > 2.9$ for 2D systems [7] and $\alpha > 0.9$ for 1D systems [8], since the effects of the electron-phonon interaction are enhanced as the dimension is lowered. Ever since the discoverv of cuprate superconductors, the bipolaron problem in 2D formulation has become a common interest in connection with the high-temperature superconductivity, where it was thought that the pairing mechanism in real space can be realized by means of the bipolaron formation [9].

A large number of papers have been devoted to the investigation of the bipolaron stability in two and three dimensions; of these works, variational approaches [6,10-13], Feynman path integral techniques [5,14,15], and Bogolubov-Tyablikov adiabatic theory [16,17] are

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notable and give conclusively a stable bipolaron, where various results are found for the critical values of α and η .

In the presence of a magnetic field the bipolaron problem becomes more interesting due to the fact that characteristics of the bipolaron now are enhanced; indeed, it was shown that 3D bipolarons are equivalent to 1D bipolarons in a strong magnetic field [18]. Furthermore, it is possible to make a connection with cyclotron resonance experiments. There exist various works on large bipolarons in a magnetic field, investigated by a variational procedure [19–21] and on the basis of Feynman's path-integral approach [22,23], where the Jensen-Feynman inequality is used, whose range of validity is discussed conclusively in reference [24]. An overview of bipolaron research can be found in the proceedings of Pushchino Workshop [25] and in a book by Alexandrov and Mott [26], and furthermore, a detailed review of the subject is recently presented by Devreese(1996) [27].

Apart from a magnetic field it is also possible to enhance the characteristics of bipolarons through confining potentials. The presence of such a potential can limit the motion of the bipolarons in all directions and furthermore makes their formation more favorable. Recent technological advances in the fabrication of nanostructures have created low dimensional semiconductors such as quantum wells (QW)- quantum well wires (QWW) and quantum dots (QD) [28], therefore it is expected that theoretical interest in the bipolaron problem should arise in such systems.

In a recent paper [29], the stability of a strongcoupling singlet bipolaron is studied in a purely 2D and 3D parabolic QD's using the Landau-Pekar variational method, where it appears that the confining potential of the QD affects the stability of the bipolaron. More recently, a theory of bipolaron states in QD [30] and QWW [31] is developed applying the Feynman variational principle. For both cases, the number of phonons in the bipolaron cloud and the bipolaron radius are studied as functions of the confinement length.

In the present paper, we shall consider the bipolaron problem in a magnetic field and a parabolic confining potential with certain parameters, from which we shall obtain QD, QW and QWW as separate cases by changing the parameters accordingly. In this investigation we shall use a variational technique, which is recently developed for a single polaron and impurity polaron in the same potential and the magnetic field [32].

The layout of the present work is as follows. In Section 2, the formulation of the problem is presented in the framework of the variational approach parallel to the single polaron study in reference [32]. The ground- and firstexcited states of the magnetobipolaron are obtained by minimization procedures as three different physical cases in Section 3. Various properties of the magnetobipolarons are analyzed graphically in Section 4 and the paper ends with a conclusion.

2 Theory

We consider a system of two electrons, which are interacting with LO phonons and subjected to a confining QD potential. In the presence of a uniform magnetic field along the z-direction, the Hamiltonian describing the considered system, within the Fröhlich approach, is written as

$$H = H_E + \sum_{\mathbf{q}} \hbar \omega_0 b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{j=1,2} \sum_{\mathbf{q}} \left(V_{\mathbf{q}} b_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}_j} + \mathrm{h.c.} \right), \, (1)$$

where

$$H_E = \frac{1}{2\mu} \sum_{j=1,2} \left[\mathbf{p}_j + \frac{e}{c} \mathbf{A} \left(\mathbf{r}_j \right) \right]^2 + \frac{1}{2} \mu \sum_{j=1,2} \left(\omega_{\perp}^2 \mathbf{r}_{\perp j}^2 + \omega_{\parallel}^2 z_j^2 \right) + \frac{e^2}{\epsilon_{\infty} \left| \mathbf{r}_1 - \mathbf{r}_2 \right|}, \quad (2)$$

is the electronic part, and

$$|V_{\mathbf{q}}|^2 = (\hbar\omega_0)^2 \left(\frac{4\pi\alpha}{V}\right) \frac{r_0}{q_{\perp}^2 + q_z^2},$$
 (3)

is the electron-phonon interaction amplitude. In equation (1), $b_{\mathbf{q}}^{\dagger}(b_{\mathbf{q}})$ is the creation (annihilation) operator of an optical phonon with a wave vector $\mathbf{q} = (\mathbf{q}_{\perp}, q_z)$ and energy $\hbar\omega_0$, and \mathbf{p}_j and $\mathbf{r}_j \equiv (r_{\perp j}, z_j)$ denote the momentum and position operators of the electrons, respectively. α and r_0 are the electron-phonon coupling constant and polaron radius, respectively. In equation (2), the second term is a generic confining potential from which low dimensional systems can be obtained through the appropriate choice of parameters ω_{\perp} and ω_{\parallel} , and the last term represents the Coulomb repulsion between two electrons.

If we choose the symmetrical Coulomb gauge for vector potential $\mathbf{A} = B(-y, x, 0)/2$ and adopt the center of mass position operator $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and the relative position operator $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, with their canonically conjugate momenta $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{p} = \mathbf{p}_1 - \mathbf{p}_2$ respectively, then the Hamiltonian becomes

$$H = -\frac{\hbar^2}{4\mu} \nabla_{\mathbf{R}}^2 + \mu \omega^2 \mathbf{R}_{\perp}^2 + \mu \omega_{\parallel}^2 Z^2 + \frac{\omega_c}{2} L_Z - \frac{\hbar^2}{\mu} \nabla_{\mathbf{r}}^2 + \frac{1}{4} \mu \omega^2 \mathbf{r}_{\perp}^2 + \frac{1}{4} \mu \omega_{\parallel}^2 z^2 + \frac{\omega_c}{2} L_z + \frac{e^2}{\epsilon_{\infty} r}$$
(4)
$$+ \sum_{\mathbf{q}} \hbar \omega_0 b_{\mathbf{q}}^{\dagger} b_{\mathbf{q}} + \sum_{\mathbf{q}} 2 \cos\left(\frac{\mathbf{q} \cdot \mathbf{r}}{2}\right) \left(V_{\mathbf{q}} b_{\mathbf{q}} e^{i\mathbf{q} \cdot \mathbf{R}} + \text{h.c.}\right),$$

where $\omega_c = eB/\mu c$ is the cyclotron frequency, and $L_{Z(z)}$ is the Z(z) component of the angular momentum. The electronic part of equation (4) can be written as a sum of the center of mass and internal motion

$$H_E = H^{\mathbf{R}} \left(2\mu, \omega \right) + H^{\mathbf{r}} \left(\mu/2, \omega \right)$$

where $H^{\mathbf{r}}$ is given by

$$H^{\mathbf{r}} = H_{2D}^{\mathbf{r}_{\perp}}\left(\mu/2,\omega\right) + \frac{\omega_c}{2}L_z + H_{1D}^z\left(\mu/2,\omega_{\parallel}\right) + \frac{e^2}{\epsilon_{\infty}r} \cdot$$
(5)

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This is the sum of Hamiltonians for an isotropic 2D harmonic oscillator in the lateral plane with the mass $\mu/2$ and frequency $\omega = \left((\omega_c/2)^2 + \omega_{\perp}^2\right)^{1/2}$, and 1D oscillator along the z-axis with the mass $\mu/2$ and frequency ω_{\parallel} , plus terms of L_Z and electron-electron interaction. A similar expression can be written for the center of mass motion with the mass 2μ , but without the Coulomb repulsion.

The trial wave function in the variational approximation we choose is made up from direct products of electronic and phonon contributions

$$\left|\Psi_{\kappa;\kappa'}\right\rangle = \left|n_1, \mp m_1, \ell_1\right\rangle \otimes \left|n_2, \mp m_2, \ell_2\right\rangle \otimes D\left(f\right) \left|0\right\rangle_{ph}, (6)$$

where the first two products represent the states of the internal motion with quantum numbers $\kappa \equiv (n_1, \mp m_1, \ell_1)$ and those of center of mass with $\kappa^{'} \equiv (n_2, \mp m_2, \ell_2)$, respectively. In coordinate representation the states of the internal motion are given by

$$\left\langle \mathbf{r} \mid \kappa \right\rangle = \psi_{n_1, \mp m_1} \left(\mathbf{r}_{\perp} \right) \psi_{\ell_1} \left(z \right)$$

$$= N_{\kappa} \left(\gamma_1, \beta_1 \right) e^{-\gamma_1^2 \mathbf{r}_{\perp}^2 / 2} \left(x \mp \mathrm{i} y \right)^{m_1} L_{n_1}^{m_1} \left(\gamma_1^2 \mathbf{r}_{\perp}^2 \right)$$

$$\times e^{-\beta_1^2 z^2 / 2} H_{\ell_1} \left(\beta_1 z \right),$$

$$(7)$$

where the functions $L_{n_1}^{m_1}$ and H_{ℓ_1} are associated Laguerre polynomials and Hermite polynomials, respectively. N_{κ} is the normalization constant. A suitable choice of the trial wave function for the center of mass motion, which is to be consistent with equations (9) and (5) of the previous works [32], respectively, has a similar structure of equation (7) with new variational parameters γ_1 and β_1 . In equation (6), D(f) is the well-known Lee-Low-Pines (LLP) transformation , by which coherent boson states are generated through the application on the zero phonon states. This treatment is in accordance with the approach considered for a single polaron in reference [32], whose result for the energy will be used in the calculation of the bipolaron stability.

With this choice of wave functions, the expectation value of the bipolaron Hamiltonian becomes

$$E^{BP}_{(\kappa;\kappa')} = \left\langle \Psi_{\kappa;\kappa'} \right| H \left| \Psi_{\kappa;\kappa'} \right\rangle = E^{0}_{(\kappa;\kappa')} + E^{I}_{(\kappa;\kappa')}, \quad (8)$$

where $E^0_{(\kappa;\kappa')}$ represents the electronic part and is given by

$$\begin{aligned} E^{0}_{(\kappa;\kappa')} &= \\ \sum_{j=1,2} \left[\left(\frac{\hbar^{2}}{2\mu_{j}} \gamma_{j}^{2} + \frac{1}{2} \mu_{j} \omega^{2} \frac{1}{\gamma_{j}^{2}} \right) (2n_{j} + m_{j} + 1) \mp m_{j} \frac{\hbar \omega_{c}}{2} \right. \\ &+ \left. \left(\frac{\hbar^{2}}{2\mu_{j}} \beta_{j}^{2} + \frac{1}{2} \mu_{j} \omega_{\parallel}^{2} \frac{1}{\beta_{j}^{2}} \right) \left(\ell_{j} + \frac{1}{2} \right) \right] + \left\langle \frac{e^{2}}{\epsilon_{\infty} r} \right\rangle_{\kappa} \cdot \end{aligned}$$
(9)

Here, $\mu_1 = \mu/2$ is the reduced mass and $\mu_2 = 2\mu$ is the total mass of the system. $E^I_{(\kappa;\kappa')}$ in equation (8) represents

the contribution due to the phonon field and the electronphonon term and is given by

$$E^{I}_{(\kappa;\kappa')} = \sum_{\mathbf{q}} \left[\hbar \omega_{0} \left| f_{\mathbf{q}} \right|^{2} + 2V_{\mathbf{q}} f_{\mathbf{q}} \sigma_{\kappa} \left(\mathbf{q}, \gamma_{1}, \beta_{1} \right) \Sigma_{\kappa'} \left(\mathbf{q}, \gamma_{2}, \beta_{2} \right) \right. \\ \left. + 2V_{\mathbf{q}}^{*} f_{\mathbf{q}}^{*} \sigma_{\kappa}^{*} \left(\mathbf{q}, \gamma_{1}, \beta_{1} \right) \Sigma_{\kappa'}^{*} \left(\mathbf{q}, \gamma_{2}, \beta_{2} \right) \right], \quad (10)$$

with

$$\sigma_{\kappa} \left(\mathbf{q}, \gamma_{1}, \beta_{1} \right) = \left\langle n_{1}, \mp m_{1}, \ell_{1} \mid \cos\left(\frac{\mathbf{q} \cdot \mathbf{r}}{2}\right) \mid n_{1}, \mp m_{1}, \ell_{1} \right\rangle$$
(11a)

and

$$\Sigma_{\kappa'} \left(\mathbf{q}, \gamma_2, \beta_2 \right) = \left\langle n_2, \mp m_2, \ell \mid e^{\mathbf{i}\mathbf{q}\cdot\mathbf{R}} \mid n_2, \mp m_2, \ell_2 \right\rangle.$$
(11b)

By making use of the wave functions for the internal motion, one can easily calculate equation (11a), then finds the following implicit expression

$$\sigma_{\kappa} \left(\mathbf{q}, \gamma_1, \beta_1 \right) = \rho_{n_1, m_1} \left(\mathbf{q}_{\perp}/2, \gamma_1 \right) \rho_{\ell} \left(q_z/2, \beta_1 \right), \quad (12)$$

where each term on the right hand side is given, respectively, by

$$\rho_{n_1m_1} \left(\mathbf{q}_{\perp}, \gamma_1 \right) = \frac{1}{n_1! m_1!} \sum_{p=0}^{\infty} \frac{(m_1 + p)!}{\left[(p)! \right]^2} \left(-\frac{q_{\perp}^2}{16\gamma_1^2} \right)^p \Delta_{n_1m_1} \left(p \right) \quad (13a)$$

and

$$\rho_{\ell_1}\left(q_z/2,\beta_1\right) = e^{-q_z^2/16\beta_1^2} L_{\ell_1}\left(\frac{q_z^2}{8\beta_1^2}\right),\tag{13b}$$

in which $\Delta_{n_1m_1}(p)$ can be expressed in terms of the hypergeometric functions and its full description together with various values can be found in reference [32]. $\Sigma_{\kappa'}$ can be expressed by the same procedure as done for equations (12, 13a) and (13b) with the quantum numbers $n_2, \mp m_2, \ell_2$.

The last term in equation (9) which is the well-known average value of the Coulomb correlation can be written by means of equation (6) as

$$\left\langle \frac{e^2}{\epsilon_{\infty}r} \right\rangle_{\kappa} = \frac{e^2}{\epsilon_{\infty}} \frac{1}{2\pi} \int \frac{\mathrm{d}^3 \mathbf{k}}{k^2} \rho_{n_1 m_1} \left(\mathbf{k}_{\perp}, \gamma_1 \right) \rho_{\ell_1} \left(k_z, \beta_1 \right).$$
(14)

In the absence of the electron-phonon and electronelectron interactions if we minimize the resulting energy with respect to γ_j and β_j , then we obtain an expression of the energy for two non-interacting electrons in a magnetic field and a confining potential with $\gamma_j^2 = \mu_j \omega/\hbar$ and $\beta_j^2 =$ $\mu_j \omega_{\parallel}/\hbar$, (j = 1, 2). The corresponding energy consists of two parts: one is for the center-of-mass and the other for the internal motion, which are very much alike, except for quantum numbers

$$\overline{E}_{\left[\kappa;\kappa'\right]}^{BP}\Big|_{\alpha=0} = \sum_{j=1,2} \left[\left(2n_j + m_j + 1\right)\overline{\omega} \mp m_j \frac{\overline{\omega}_c}{2} + \left(\ell_j + \frac{1}{2}\right)\overline{\omega}_{\parallel} \right]. \quad (15)$$

In the above expression and hereafter, the energy and other parameters are expressed in terms of the LO-phonon frequency ω_0 , accordingly the dimensionless confinement frequencies $\overline{\omega}_{\perp(\parallel)}$ are directly related to the dimensionless confinement lengths $u_{\perp(z)} = \ell_{\perp(z)}/r_0 = \sqrt{2/\overline{\omega}_{\perp(\parallel)}}$. Equation (15) defines the well-known Fock-Darwin energy levels [33] for two electrons in a confining potential and a magnetic field. It should be noted that these are reduced to the Landau levels $\overline{E}_{[\kappa;\kappa']}^{BP}\Big|_{\alpha=0,\overline{\omega}_{\perp(\parallel)}=0} = \sum_{j=1,2} [n_j + (m_j \mp m_j)/2 + 1/2]\overline{\omega}_c$, in the absence of the confining potential.

Minimization of $\overline{E}^{BP}_{(\kappa;\kappa')}$ with respect to $f_{\mathbf{q}}^*$ yields

$$f_{\mathbf{q}} = -\frac{2V_{\mathbf{q}}^{*}}{\hbar\omega_{0}}\sigma_{\kappa}^{*}(\mathbf{q},\gamma_{1},\beta_{1})\Sigma_{\kappa'}^{*}(\mathbf{q},\gamma_{2},\beta_{2})$$
(16)

and after substituting $f_{\mathbf{q}}$ into equation (10), $\overline{E}_{(\kappa;\kappa')}^{l}$ becomes

$$\overline{E}_{\left(\kappa;\kappa'\right)}^{I} = -\frac{4}{\left(\hbar\omega_{0}\right)^{2}}\sum_{\mathbf{q}}\left|V_{\mathbf{q}}\right|^{2}\left|\sigma_{\kappa}\left(\mathbf{q},\gamma_{1},\beta_{1}\right)\Sigma_{\kappa'}\left(\mathbf{q},\gamma_{2},\beta_{2}\right)\right|^{2}.$$
 (17)

With the change of variables $q_{\perp}/\sqrt{2}\gamma_1 = x$ and $q_z/2\sqrt{2}\beta_1 = y$ in equation (17) and similarly $k_{\perp}/\sqrt{2}\gamma_1 = x$ and $k_z/\sqrt{2}\beta_1 = y$ in equation (14), the dimensionless bipolaron energy simplifies to the following form

$$\overline{E}_{\left(\kappa;\kappa'\right)}^{BP} = \sum_{j=1,2} \left[\left(\frac{1}{\overline{\gamma}_{j}^{2}} + \frac{1}{4} \overline{\omega}^{2} \overline{\gamma}_{j}^{2} \right) (2n_{j} + m_{j} + 1) \\
\mp m_{j} \frac{\hbar \omega_{c}}{2} + \left(\frac{1}{\overline{\beta}_{j}^{2}} + \frac{1}{4} \overline{\omega}_{\parallel}^{2} \overline{\beta}_{j}^{2} \right) (\ell_{j} + \frac{1}{2}) \right] \\
+ \frac{2\sqrt{2}}{\pi} \frac{e^{2}}{\epsilon_{\infty} \hbar \omega_{0}} \left(\frac{m \omega_{0}}{\hbar} \right)^{1/2} \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} I_{\kappa}^{(1)} \left(\overline{\Omega} \right) \\
- \frac{16}{\pi} \alpha \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} I_{\kappa\kappa'}^{(2)} \left(\overline{\Omega}; \overline{\gamma}_{2}, \overline{\beta}_{2} \right),$$
(18)

where $\overline{\Omega}$ is given by $\overline{\Omega}^2 = \overline{\beta}_1^2 / \overline{\gamma}_1^2$ and the relevant integrals are defined as

$$I_{\kappa}^{(1)}\left(\overline{\Omega}\right) = \int_{0}^{\infty} x \mathrm{d}x \rho_{n_{1}m_{1}}\left(x^{2}/2\right)$$
$$\times \int_{0}^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-y^{2}/2}}{\overline{\Omega}^{2}x^{2} + y^{2}} L_{\ell_{1}}\left(y^{2}\right) \qquad(19)$$

and

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$$\begin{split} T^{(2)}_{\kappa;\kappa'}\left(\overline{\Omega};\overline{\gamma}_{2},\overline{\beta}_{2}\right) &= \\ \int_{0}^{\infty} x \mathrm{d}x \left| \rho_{n_{1}m_{1}}\left(x^{2}/2\right) \right|^{2} \left| \times \rho_{n_{2}m_{2}}\left(\overline{\gamma}_{2}^{2}x^{2}/2\overline{\gamma}_{1}^{2}\right) \right|^{2} \\ &\times \int_{0}^{\infty} \mathrm{d}y \frac{\mathrm{e}^{-y^{2}\left(1+\overline{\beta}_{2}^{2}/\overline{\beta}_{1}^{2}\right)}}{\overline{\Omega}^{2}x^{2}+y^{2}} L^{2}_{\ell_{1}}\left(y^{2}\right) L^{2}_{\ell_{2}}\left(\overline{\beta}_{2}^{2}y^{2}/\overline{\beta}_{1}^{2}\right). \end{split}$$
(20)

It should be noted that in equation (18) the coupling constant α , the amplitude of the Coulomb repulsion $U = e^2 (\mu \omega_0 / \hbar)^{1/2} / \epsilon_{\infty} \hbar \omega_0$ and the material parameter $\eta = \epsilon_{\infty} / \epsilon_0$ are connected by the relation $U = \sqrt{2}\alpha/(1-\eta)$.

Equation (18) is our fundamental result, from which we obtain the ground- and excited-state energies of bipolaron according to the values of $\overline{\Omega}$. It should be pointed out that the values of $\overline{\Omega}$ play a decisive role in the determination of the features of low dimensional systems. For example, under certain conditions which will be discussed in the next section, the case $\overline{\Omega}^2 = 1$ ($\overline{\omega} = \overline{\omega}_{\parallel}$) defines a QD which represents a 3D confinement, that is, quasizero dimensional motion, embedded in a three dimensional material, whereas $\overline{\Omega}^2 > 1$ ($\overline{\omega} > \overline{\omega}_{\parallel}$) and $\overline{\Omega}^2 < 1$ ($\overline{\omega} < \overline{\omega}_{\parallel}$) correspond to a QWW and QW which are 2D confinement (quasi-one dimensional motion) and 1D confinement (quasi-two dimensional motion), respectively, where all confinements are embedded in a 3D material.

3 The ground and first excited states

3.1 Ground state

The ground-state energy for the large bipolaron can be easily obtained from equation (18) and is given by

$$\overline{E}_{(0;0)}^{BP} = \sum_{j=1,2} \left[\left(\frac{1}{\overline{\gamma}_{j}^{2}} + \frac{1}{4} \overline{\omega}^{2} \overline{\gamma}_{j}^{2} \right) + \frac{1}{2} \left(\frac{1}{\overline{\beta}_{j}^{2}} + \frac{1}{4} \overline{\omega}_{\parallel}^{2} \overline{\beta}_{j}^{2} \right) \right] \\
+ \frac{2\sqrt{2}}{\pi} U \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} I_{\mathbf{0}}^{(1)} \left(\overline{\Omega} \right) - \frac{16}{\pi} \alpha \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} I_{\mathbf{0},\mathbf{0}}^{(2)} \left(\overline{\Omega}; \overline{\gamma}_{2}, \overline{\beta}_{2} \right),$$
(21)

where the relevant integrals are calculated in detail according to three different cases $\overline{\Omega}$ in reference [32], and (0;0) represents the state with quantum numbers $n_j = 0$, $m_j = 0$ and $\ell_j = 0$. Hence, the energy expression in compact form becomes

$$\overline{E}_{(0;0)}^{BP} = \sum_{j=1,2} \left[\left(\frac{1}{\overline{\gamma}_{j}^{2}} + \frac{1}{4} \overline{\omega}^{2} \overline{\gamma}_{j}^{2} \right) + \frac{1}{2} \left(\frac{1}{\overline{\beta}_{j}^{2}} + \frac{1}{4} \overline{\omega}_{\parallel}^{2} \overline{\beta}_{j}^{2} \right) \right] \\
- \frac{2}{\sqrt{\pi}} \alpha \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} \frac{1}{\overline{\Omega}^{2}} \left[\frac{4\mathcal{F}^{0} \left(\overline{D}^{2} \right)}{\left(1 + \overline{\beta}_{2}^{2} / \overline{\beta}_{1}^{2} \right)^{1/2}} - \frac{\sqrt{2}}{1 - \eta} \mathcal{F}^{0} \left(\overline{\Omega}^{2} \right) \right],$$
(22)

where

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$$\frac{1}{2} \frac{\chi}{\sqrt{\chi^2 - 1}} \ln \frac{\chi + \sqrt{\chi^2 - 1}}{\chi - \sqrt{\chi^2 - 1}} \qquad \chi^2 > 1$$

$$D^{0}(\chi^{2}) = \begin{cases} 1 & \chi^{2} = 1 \\ \chi & \chi^{1-\chi^{2}} & \chi^{2} = 1 \end{cases}$$

$$\left(\frac{\chi}{\sqrt{1-\chi^2}} \arctan \frac{\sqrt{1-\chi}}{\chi} \qquad \chi^2 < 1$$
(23)

with

$$\overline{D}^2 = \overline{\Omega}^2 \frac{1 + \overline{\beta}_2^2 / \overline{\beta}_1^2}{1 + \overline{\gamma}_2^2 / \overline{\gamma}_1^2} \cdot \tag{24}$$

It should be mentioned that for the case $\overline{\Omega}^2 = 1$, there are three possibilities for \overline{D}^2 , which are $\overline{D}^2 > 1$, $\overline{D}^2 < \overline{D}^2$ 1, $\overline{D}^2 = 1$; however, only the last one is acceptable for optimal results from the variational calculations to obtain a bound bipolaron in a box-type confinement. Likewise, for the case $\overline{\Omega}^2 < 1(>1)$ there are again three possible values for \overline{D}^2 as mentioned for the box case, and only $\overline{D}^2 < 1(>1)$ now gives the optimal results for the QWW (QW). The other limits can also exist mathematically, but are not acceptable physically.

In order to have a stable bipolaron it is necessary that the ground-state energy of two interacting polarons should be lower than twice that of a single polaron; this defines the bipolaron stability region, which is expressed as $W(\eta, \alpha; \omega, \omega_{\parallel}, \omega_c) = 2\overline{E}_{(0)}^P - \overline{E}_{(0;0)}^{BP} \ge 0$ where $\overline{E}_{(0)}^P$ is the single polaron ground-state energy, calculated within the same framework as for the bipolaron system and can be readily available from reference [32].

$$3.1.1 \ \overline{\Omega}^2 = \overline{\mathsf{D}}^2 = 1$$

This condition allows us to consider parabolic potentials in the lateral plane and the z-direction so that we are free to adjust the relevant parameters to restrict the motion of electrons in a box. Therefore, this case defines a box-type confinement and represents a quantum dot embedded in a three-dimensional material. It corresponds to taking $\overline{\omega} = \overline{\omega}_{\parallel}$ in equation (22), since $\overline{\beta}_1^2 = \overline{\gamma}_1^2 = \overline{\beta}^2$, $\overline{\beta}_2^2 = \overline{\gamma}_2^2 = \overline{B}^2$ and $\mathcal{F}^0(1) = 1$, so one obtains the result for the bipolaron ground-state energy

$$\overline{E}_{(0;0)}^{BP} = \frac{3}{2} \left(\frac{1}{\overline{\beta}^2} + \frac{1}{\overline{B}^2} \right) + \frac{1}{4} \left(\overline{\omega}^2 + \frac{1}{2} \overline{\omega}_{\parallel}^2 \right) \left(\overline{\beta}^2 + \overline{B}^2 \right) \\ + 2 \sqrt{\frac{2}{\pi}} \frac{\alpha}{1 - \eta} \frac{1}{\overline{\beta}} - \frac{8}{\sqrt{\pi}} \alpha \frac{1}{\sqrt{\overline{\beta}^2 + \overline{B}^2}}.$$
 (25)

Before starting to give a detailed discussion of equation (25), it is useful firstly to analyze it for simpler and known problems. For example, when we take $\overline{\omega}_c = \overline{\omega}_{\perp} =$

 $\overline{\omega}_{\parallel} = 0$ in the last equation it gives a simpler expression from which one can obtain exactly the same result by using the oscillator wave functions proposed by Verbist et al. [6] for both relative and center-of-mass motions, just by substituting $2/\overline{\beta}^2$ with $\hbar\Omega/\mu\omega_0$ and $2/\overline{B}^2$ with $\hbar\Omega_1/\mu\omega_0$; likewise, by substituting $1/\sqrt{2\beta}$ with γ and $\sqrt{2}/\overline{B}$ with β in reference [10], and $1/\overline{\beta}$ with b and $1/\sqrt{1+\overline{B}^2/\overline{\beta}^2}$ with λ in reference [11], one obtains equation (22) of Bassani *et al.* and equation (10) of Luczak *et al.*, respectively, whose results are generally accepted fundamental for variational approach with Gaussian-Gaussian type trial functions.

$3.1.2 \overline{\Omega}^2 > 1$

The condition $\overline{\Omega}^2 > 1$ implies $\overline{D^2} > 1$, as mentioned be-fore, which require $\overline{\beta}_1^2 > \overline{\gamma}_1^2$ and $\overline{\beta}_1^2 + \overline{\beta}_2^2 > \overline{\gamma}_1^2 + \overline{\gamma}_2^2$. This condition allows us to keep the confining potential only in the lateral plane and to remove that of its perpendicular part, *i.e.* $\overline{\omega}_{\parallel} = 0$, so that electrons are free to move along the z-axis. Therefore, this case defines a 2D confinement, quasi-one dimensional motion and represents a QWW embedded in a 3D material. If one substitutes $\mathcal{F}^0(\chi^2 > 1)$ into equation (22) one obtains the bipolaron ground state energy as

$$\overline{E}_{(0;0)}^{BP} = \sum_{j=1,2} \left(\frac{1}{\overline{\gamma}_{j}^{2}} + \frac{1}{4} \overline{\omega}^{2} \overline{\gamma}_{j}^{2} + \frac{1}{2} \frac{1}{\overline{\beta}_{j}^{2}} + \frac{1}{8} \overline{\omega}_{\parallel}^{2} \overline{\beta}_{j}^{2} \right) - \frac{\alpha}{\sqrt{\pi}} \left[\frac{4}{(V-Y)^{1/2}} \ln \left(\frac{\sqrt{V} + \sqrt{V-Y}}{\sqrt{V} - \sqrt{V-Y}} \right) - \frac{\sqrt{2}}{1-\eta} \frac{1}{\sqrt{Z}} \ln \left(\frac{\overline{\beta}_{1} + \sqrt{Z}}{\overline{\beta}_{1} - \sqrt{Z}} \right) \right], \quad (26)$$

where $V = \overline{\beta}_1^2 + \overline{\beta}_2^2$, $Y = \overline{\gamma}_1^2 + \overline{\gamma}_2^2$ and $Z = \overline{\beta}_1^2 - \overline{\gamma}_1^2$. This energy is minimized numerically to determine optimal values of the parameters $\overline{\gamma}_j$ and $\overline{\beta}_j$ (j = 1, 2). The single polaron energy in W is obtained by the same method as in reference [32]. The change of W with respect to η , with and without a magnetic field can be obtained in a similar way as in the previous one. The results show that the overall picture is the same as those in the previous case.

3.1.3 $\overline{\Omega}^2 < 1$

The characteristic condition of this case is $\overline{D}^2 < 1$ as well as $\overline{\beta}_1^2 < \overline{\gamma}_1^2$ and $\overline{\beta}_1^2 + \overline{\beta}_2^2 < \overline{\gamma}_1^2 + \overline{\gamma}_2^2$. Here, it is possible to take $\overline{\omega}_{\perp} = 0$, that is, a confining potential along the zaxis keeps the electrons moving in the lateral plane freely. Therefore, this case defines a slab-type confinement (or 1D confinement) and quasi-two dimensional motion, and represents a QW embedded in 3D material. If one sub-stitutes $\mathcal{F}^0(\chi^2 < 1)$ into equation (22), one obtains the

$$\mathcal{F}^{1}(\chi^{2}) = \begin{cases} \frac{1}{2} \frac{\chi^{3}}{\chi^{2} - 1} \left[\chi \frac{1}{2} \frac{1}{\sqrt{\chi^{2} - 1}} \ln \frac{\chi + \sqrt{\chi^{2} - 1}}{\chi - \sqrt{\chi^{2} - 1}} \right] & \chi^{2} > 1 \\ \frac{1}{3} & \chi^{2} = 1 \end{cases}$$
(31)

$$\left[\frac{1}{2}\frac{\chi^3}{1-\chi^2}\left[\frac{1}{\sqrt{1-\chi^2}}\arctan\frac{\sqrt{1-\chi^2}}{\chi}-\chi\right] \qquad \chi^2 < 1$$

$$\mathcal{F}^{2}(\chi^{2}) = \begin{cases} \frac{1}{4} \frac{\chi^{5}}{\chi^{2} - 1} \left[2\chi + \frac{3}{2} \frac{1}{(\chi^{2} - 1)^{3/2}} \ln \frac{\chi + \sqrt{\chi^{2} - 1}}{\chi - \sqrt{\chi^{2} - 1}} \frac{3\chi}{\chi^{2} - 1} \right] & \chi^{2} > 1 \\ \frac{2}{5} & \chi^{2} = 1 \\ \frac{1}{4} \frac{\chi^{5}}{1 - \chi^{2}} \left[\frac{1}{(1 - \chi^{2})^{3/2}} \arctan \frac{\sqrt{1 - \chi^{2}}}{\chi} \frac{3\chi}{1 - \chi^{2}} - 2\chi \right] & \chi^{2} < 1 \end{cases}$$
(32)

bipolaron ground-state energy as

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$$\overline{E}_{(0;0)}^{BP} = \sum_{j=1,2} \left(\frac{1}{\overline{\gamma}_{j}^{2}} + \frac{1}{4} \overline{\omega}^{2} \overline{\gamma}_{j}^{2} + \frac{1}{2} \frac{1}{\overline{\beta}_{j}^{2}} + \frac{1}{8} \overline{\omega}_{\parallel}^{2} \overline{\beta}_{j}^{2} \right)$$
$$- \frac{2\alpha}{\sqrt{\pi}} \left[\frac{4}{\left(Y - V\right)^{1/2}} \arctan\left(\frac{\sqrt{Y - V}}{\sqrt{V}}\right) - \frac{\sqrt{2}}{1 - \eta} \frac{1}{\sqrt{-Z}} \arctan\left(\frac{\sqrt{-Z}}{\overline{\beta}_{1}}\right) \right].$$
(27)

This expression, together with the single polaron energy of reference [32], is minimized numerically to determine optimal values of the parameters $\overline{\gamma}_{j}$ and $\overline{\beta}_{j}$ (j = 1, 2).

3.2 Excited states

The excited-state energies for the large magnetobipolaron in low dimensional systems can be easily obtained from equation (18) by choosing certain quantum numbers and calculating the related integrals $I_{\kappa}^{(1)}$ and $I_{\kappa,\kappa'}^{(2)}$, and then applying the variational techniques to the resulting equation. Such a set of quantum numbers we choose is $(0 \mp 10; 0), (0; 0 \mp 10)$ and (001; 0) and for these states the interaction parts of the bipolaron energy of equation (18) become

$$\overline{E}_{(0\mp10;0)}^{I} = \frac{4}{\sqrt{2\pi}} \frac{\alpha}{1-\eta} \frac{1}{\overline{\Omega}^{2}} \overline{\overline{\gamma}_{1}^{2}} \left[\mathcal{F}^{0} \left(\overline{\Omega}^{2} \right) - \frac{1}{\overline{\Omega}^{2}} \mathcal{F}^{1} \left(\overline{\Omega}^{2} \right) \right]
- \frac{8}{\sqrt{\pi}} \alpha \frac{1}{\overline{\Omega}^{2} \sqrt{\Delta}} \overline{\overline{\gamma}_{1}^{2}} \left[\mathcal{F}^{0} \left(\overline{D}^{2} \right) - \frac{1}{\Delta \overline{\Omega}^{2}} \mathcal{F}^{1} \left(\overline{D}^{2} \right)
+ \frac{1}{4\Delta^{2} \overline{\Omega}^{2}} \mathcal{F}^{2} \left(\overline{D}^{2} \right) \right]$$
(28)

$$\overline{E}_{(0;0\mp10)}^{I} = \frac{4}{\sqrt{2\pi}} \frac{\alpha}{1-\eta} \frac{1}{\overline{\Omega}^{2}} \overline{\overline{\gamma}_{1}^{2}} \mathcal{F}^{0}\left(\overline{\Omega}^{2}\right) - \frac{8}{\sqrt{\pi}} \alpha \frac{1}{\overline{\Omega}^{2} \sqrt{\Delta}} \overline{\overline{\gamma}_{1}^{2}} \\
\times \left[\mathcal{F}^{0}\left(\overline{D}^{2}\right) - \frac{1}{\Delta \overline{\Omega}^{2}} \overline{\overline{\gamma}_{1}^{2}} \mathcal{F}^{1}\left(\overline{D}^{2}\right) \\
+ \frac{1}{4\Delta^{2} \overline{\Omega}^{2}} \overline{\overline{\gamma}_{1}^{4}} \mathcal{F}^{2}\left(\overline{D}^{2}\right) \right]$$
(29)

$$\overline{E}_{(001;0)}^{I} = \frac{4}{\sqrt{2\pi}} \frac{\alpha}{1-\eta} \frac{1}{\overline{\Omega}^{2}} \frac{\beta_{1}}{\overline{\gamma}_{1}^{2}} \left[\mathcal{F}^{0} \left(\overline{\Omega}^{2} \right) + 2\mathcal{F}^{1} \left(\overline{\Omega}^{2} \right) - \overline{\Omega}^{2} \right] \\
- \frac{8}{\sqrt{\pi}} \alpha \frac{1}{\overline{\Omega}^{2} \sqrt{\Delta}} \frac{\overline{\beta}_{1}}{\overline{\gamma}_{1}^{2}} \\
\times \left[\mathcal{F}^{0} \left(\overline{D}^{2} \right) + \frac{1}{\Delta} \mathcal{F}^{1} \left(\overline{D}^{2} \right) - \frac{\overline{\Omega}^{2}}{2\Gamma} \right] \quad (30)$$

with

see equations (31, 32) above

where $\Delta = 1 + \overline{\beta}_2^2 / \overline{\beta}_1^2$, $\Gamma = 1 + \overline{\gamma}_2^2 / \overline{\gamma}_1^2$ and $\mathcal{F}^0(\chi^2)$ is given by equation (23). Obtaining the remaining parts of the bipolaron energy is trivial, as such giving the values of related set of quantum numbers in equation (18). As we mentioned in the formulation of the ground state part, there are again three possibilities depending on the choice of $\overline{\Omega}$ and \overline{D} , yielding the formation of QW's,QWW's and QD's.

One can easily extend what we achieved for the ground state to the excited states, *i.e.*, the dependence of W on the confinement lengths (u_{\perp}, u_z) , magnetic field $(\overline{\omega}_c)$, η and α , just by optimizing the energy equation (18) with equations (19–20). In the present work, regarding for excited states, we will focus only on QD's embedded in a 3D material, which is equivalent to take $\overline{\Omega}^2 = \overline{D}^2 = 1$.

4 Results and discussions

We can now examine closely each case we have considered in the previous section. Since analytical minimization of $\overline{E}_{(0;0)}^{BP}$ is not possible, the optimal values of parameters $\overline{\beta}$, \overline{B} , η will be determined by numerical treatment and throughout the discussion for QD we set $u_{\perp} = u_z = u$ in order to facilitate the calculations. With appropriate choice for the values of α , η and Ω , equation (25), together with equation (24) of reference [32], have been minimized with respect to $\overline{\beta}$ and \overline{B} in such a way that the condition



Fig. 1. Dependence of the binding energy W of the bipolaron in the ground-state on cyclotron frequency (a) at $\eta = 0.01$ and (b) at $\eta = 0.02$; dashed line- $u = \infty$; thin line-u = 2; thick line-u = 1.

for the formation of bipolaron, *i.e.* $W \ge 0$, is satisfied. In Figure 1, we analyze dependencies of W on magnetic field $\overline{\omega}_c$ and confinement length u graphically, where we plot W with respect to $\overline{\omega}_c$ for fixed values of η and u at $\alpha = 4$. The dashed lines in Figure 1a and 1b show the effect of magnetic field without any confinement and are agree with references [6,10] at $\overline{\omega}_c = 0$. From Figure 1b one can also observe that both magnetic field and confinement enhance the formation of a bipolaron up to a certain value of the magnetic field when η takes larger values. Beyond this value of the magnetic field the binding energy decreases (Fig. 1b) compared to that of the smaller values of η (Fig. 1a). This effect can be clearly seen on the plot of the binding energy with respect to η for different values of magnetic field at a constant confinement length and $\alpha = 4$ (Fig. 2). The thin line in Figure 2 is the result in the absence of a magnetic field and gives the known critical value of η ($\eta_c = 0.079$) just as found in reference [6], whereas the other lines show the pronounced effect of the



Fig. 2. Dependence of the binding energy W of the bipolaron in the ground-state on η , at a fixed confinement length u = 2; thin line- $\overline{\omega}_c = 0$; thick line- $\overline{\omega}_c = 5$; bold line- $\overline{\omega}_c = 10$.



Fig. 3. The binding energy W of the bipolaron in the groundstate as a function of the confinement length u for a QD; dashed lines- $\overline{\omega}_c = 0$; solid lines- $\overline{\omega}_c = 5$.

magnetic field on W, up to a certain value of η , beyond which W remains under the result for $\overline{\omega}_c = 0$ (thin line), although the formation of a bipolaron is still possible. It should also be noted that the critical value of η decreases with increasing magnetic field, for instance η_c is about 0.054 at $\overline{\omega}_c = 10$.

To further the effects in Figure 1, we plot the binding energy W with respect to the confinement parameter in Figure 3, to describe the effects of the coupling constant α , the material parameter η and the magnetic field $\overline{\omega}_c$ on W. There it appears that the binding energy W increases with increasing confinement, which is realized with the decreasing confinement length u. The curves show a general trend that the binding energy increases with increasing α and $\overline{\omega}_c$, and is very sensitive on the values of η , which are agree with the other works. When η goes to smaller values, the confinement effect on the binding energy Wis more pronounced and the stability of the bipolaron becomes more favorable. It should be noted that these curves are meaningful only for the values above u = 1, since this is the region where the polaron radius is at the same order of the confinement length.

Before analyzing excited states, it may be worthy of considering the above mentioned excited states with and without electron-phonon interaction, equation (15). Firstly, in the absence of the electron-phonon and electron-electron interactions, one can obtain the Fock-Darwin energy levels for two non-interacting electrons, Such as the ground-state energy $\overline{E}_{[0;0]}^{BP}\Big|_{\alpha=0} = 2\overline{\omega} + \overline{\omega}_{\bullet}$ and the first excited state energies $\overline{E}_{[0\mp10;0]}^{BP}\Big|_{\alpha=0} = \overline{E}_{[0;0\mp10]}^{BP}\Big|_{\alpha=0} = 3\overline{\omega} + \overline{\omega}_{\bullet} \mp \overline{\omega}_{c}/2$ and $\overline{E}_{[001;0]}^{BP}\Big|_{\alpha=0} = 2\overline{\omega} + 2\overline{\omega}_{\bullet}$; where for convenience $\overline{\omega}_{\perp} = \overline{\omega}_{\parallel} = \overline{\omega}_{\bullet}$ is taken, and $\overline{\omega} = (\overline{\omega}_{\bullet}^{2} + \overline{\omega}_{c}^{2}/4)^{1/2}$ represents the hybrid frequency. Secondly when we switch on the electron phenom $\overline{\omega}_{\perp}$ Secondly, when we switch on the electron-phonon and electron-electron interactions, these levels will be shifted down and split, respectively. In Figure 4a we plot the bipolaron energy as a function of $\overline{\omega}_c$ in the absence of a confining potential, where the labels of energy levels are put according to an admixture set of quantum numbers of center-of-mass and relative motions, such as $(n_1, m_1, \ell_1; n_2, m_2, \ell_2)$. It is evident that center-of-mass and relative motions are separated by the electron-phonon interaction, which are further split for $m_1 = \pm 1$ and $m_2 = \pm 1$ by the magnetic field. It should be noted that the states with $m_1 = -1$ and $m_2 = -1$ go asymptotically parallel to the ground state [0;0] and those with $m_1 = +1$ and $m_2 = +1$ parallel to the first excited states. Figure 4b illustrates the bipolaron energy as a function of $\overline{\omega}_c$ in the presence of a confining potential as for the case of QD. When the electron-phonon and electron-electron interactions are neglected, we obtain the ground state energy of an isotropic oscillator specified as [0; 0] and the first excited states as [001; 0], [010; 0], [0; 010], [0 - 10; 0]and [0; 0-10] which are split by the magnetic field. If the electron-phonon interaction is now switch on, the center of mass and relative motions are separated, and we obtain the same asymptotic behavior as in Figure 4a for high magnetic fields.

Similar to the spatial confinement arising from the confining potential, it is also possible to remark a confinement due to magnetic fields, which affects in the lateral plane when the field is along the z-direction. In regard with the competition between the spatial and magnetic confinement we can observe that, when the spatial confinement is much less than the magnetic confinement length, the energy spectrum approaches smoothly that of a free particle, when it is much greater, then the Landau levels are recovered [34]. Furthermore, if there exists an additional effect such as electron-phonon interaction, then the energy levels are shifted down and split to produce relaxed excited states (RES) [35].

The change of the binding energy of bipolarons, for $\eta = 0.01$ and $\alpha = 4$, as a function of confining parameters is displayed in Figure 5a, in the absence of a magnetic field. As expected, the confinement becomes more effective when the dimension is further restricted. The curves



Fig. 4. Cyclotron frequency dependence of the bipolaron energies in a QD (a) at $u = \infty$ and (b) u = 2. The solid and dashed lines represent the unperturbed $[n_1 \mp m_1 \ell_1; n_2 \mp m_2 \ell_2]$ and perturbed $(n_1 \mp m_1 \ell_1; n_2 \mp m_2 \ell_2)$ energy levels, respectively.

in Figure 5a, from top to bottom, describe a QD system with quasi-zero-dimensional motion in 3D confinement, a QWW with quasi-one-dimensional motion in 2D confinement and a QW with quasi-two dimensional motion in 1D confinement. It should be noted that all these three cases reach asymptotically to the energy of a bipolaron without spatial and magnetic confinements (dashed line in the figure), which is depicted by the work of Bassani *et al.* [10]. If we keep $\alpha = 4$ and $\overline{\omega}_c = 0$, but increase η to a higher value, for instance, to 0.05, then the stability region is reversed as seen in Figure 5b. This is due to the fact that the least adversely affected system is the least confined one, which is the QW. Here again, the dashed



Fig. 5. Dependence of the binding energy W of the bipolaron in the ground-state on confinement lengths (a) at $\eta = 0.01$ and (b) at $\eta = 0.05$.

line is the binding energy of a free bipolaron [10]. The other important point is that, in the region $u, u_{\perp}, u_z < 1$, the curves in Figure 5a turn down to zero after maxima, whereas those in Figure 5b decrease to zero in the same region, which is not shown in our plots since this region is not meaningful due to the large polaron concept. However, the same behaviour has been obtained by applying the Feynman variational principle with path integrals [30].

In Figure 6 we plot the curves for the three systems showing the variation of the Coulomb repulsion parameter normalized by α , $U/\sqrt{2\alpha}$, as a function of α without (a) and with (b) a magnetic field. The region below each curve describes the stability region of a bipolaron. Note that the existence of a magnetic field brings the exchange of the curves of QW and QWW. This is because of the introduction of an extra term into the Hamiltonian aris-



Fig. 6. Stability region for bipolaron formation in QD, QW and QWW type structures (a) at $\overline{\omega}_c = 0$ and (b) at $\overline{\omega}_c = 5$, with a fixed confinement length u = 2

ing from the magnetic confinement in the lateral plane and accordingly the QW case, in a sense, becomes a 3Dconfinement in quasi-zero dimensional motion similar to a QD.

It is an interesting fact that our results are reduced to those of references [6,10,11] found for the ground-state energy, when one removes the magnetic field and the confinement. The approaches of those references use Gaussian type trial wavefunctions for both center-of-mass and the relative motions, and reproduce the leading term in the strong coupling expansion. From the point of view of judging the validity region of our and those works cited above, it is important to realize that polaron and bipolaron energies obtained in these approaches are proportional to α^2 , which do not allow one to get an optimum value for α . Therefore, it is a well-known and common fact that the only drawback in these approaches is the failure to predict a critical value for α . As seen from Figure 3, in the absence of a magnetic field, when one increases u to its larger values, the bipolaron binding energy does not change with u and eventually becomes independent of u, as expected. This is essentially bulk limit, where the binding energies are proportional to α^2 , arising from a strong coupling approach where it is well-known that there is no binding below $\alpha < 6.8$ [4–6] for bulk materials. There is, however, a part of confinement region beyond which the bipolaron binding energy reach to its asymptotic value; it is about up to $u \sim 4$ (Fig. 6). In fact, this region depends sensitively on the choice of the parameters η , α and $\overline{\omega}_c$, and it broadens when η decreases, and α and $\overline{\omega}_c$ increases as mentioned before. It is shown that the reduction of dimensionality of the system to two and one dimensions yields an enlargement in the bipolaron stability region [7,8]. In order to have a stable bipolaron, it is found that the minimum value of α should be 2.9 [7] in 2D systems and 0.9 [8] in 1D systems. In particular, Pokatilov et al. [30,31] conclude that the stable bipolaron states are possible even for intermediate values of α ($\alpha \sim 2$) in nanostructures whose size are of the same order as the polaron radius. Thus, it is reasonable to expect that the present results obtained in the framework of strong coupling approach are valid for the above critical values of α which are obtained in the path integral formalism.

5 Conclusion

In summary, we have concluded from our present investigations that the complicated dependencies of the groundand first-excited-state energies of the magnetobipolarons on confinement parameters arising from a magnetic field and a confining potential apart from the material parameters α and η , can be examined within a variational approach as function of these parameters. We have found that our results for the ground state of a bipolaron are completely equivalent to those obtained in the simplest case, *i.e.*, in the absence of spatial and magnetic confinements. Thus, the method we have used here not only generalize those of references [6,10] but also enables us to discuss the excited-state energies of a magnetobipolaron in a parabolic QD together with the ground-state energy.

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