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The stability of two-dimensional magnetobipolarons in parabolic quantum dots

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Abstract. Using a variational procedure based on Lee-Low-Pines and Huybrechts canonical transformations, we study the stability region of two-dimensional bipolarons confined in a parabolic quantum dot, subject to a uniform magnetic field. In the framework of our approach, we calculate the ground-state energy for two-dimensional magnetobipolarons, together with the free polaron ground-state energy, by performing a self consistent calculation. We then obtain the binding energy for two-dimensional magnetobipolarons, in the usual way, to explore the properties of bipolaron formation in two-dimensional quantum dot structures. The stability region is found to be very sensitive to the confinement length of the parabolic potential and to the magnetic field strength, as well as to the material parameters α and η. The stability region is also found to be remarkably enhanced by increasing the degree of spatial confinement and magnetic field. Our results are both in qualitative and quantitative agreement with those found in the literature.

PACS. 71.38.Fp Large or Fröhlich polarons – 63.20.Kr Phonon-electron and phonon-phonon interactions

1 Introduction

It is a well-known fact that in nanostructures, such as quantum wells (QW), quantum well wires (QWW) and quantum dots (QD), in which the motion of electrons are restricted in various directions, polaronic effects [1] arising from the electron-phonon interaction as well as the effects caused by the size quantization [2,3] on electronic energy levels are enhanced due to the reduction of the dimensionality of the system. Thus, particularly in QDs wherein quantum confinement is imposed in all spatial dimensions, it is crucial to consider the possibility of pairing two polarons induced from the attractive interaction mediated by the electron-phonon coupling, since the most pronounced effects due to electron-phonon interactions are found in this system. Such a pairing is based on the fact that at certain values of the material parameters, the attractive electron-phonon interaction overcomes the repulsive Coulomb interaction between two electrons, and therefore induces polaron pairings, referred to as bipolarons. Accordingly, one may expect that it is more likely to observe stable bipolaron states in QDs than in QW and QWW type nanostructures since competition between these two types of interaction may result in favor of bipolaron formation. This is due to not only the fact that of having the lowest dimension among nanostructures, but also the possibility of decreasing its size in all directions, even if the electron-phonon coupling is weak.

The bipolaron problem was first considered by Pekar [4] and by Vinetskii and Gitterman [5]. Later, the possible relevance of bipolarons in the context of high temperature superconductivity was also suggested in various papers [6–10]. In these studies, several attempts by using different techniques have been made to investigate whether stable bipolaron states exist in three-(3D), two-(2D) and also in one-(1D)dimensional systems, or not. Following these works, systematic investigations on the bipolaron stability region (BPSR) have been performed, firstly by Adamowski [11] and subsequently by Verbist, Peeters and Devreese [12], and by Bassani and Geddo [13] in 2D and 3D bulk materials, and by many other authors [14–23] in various systems. An overview of bipolaron research can be found in the proceedings of the Pushchino Workshop [24], in a text-book by Alexandrov and Mott [25], and furthermore, in a detailed review by Devreese [26].

In the usual treatment of the large bipolaron theory, material parameters such as the dimensionless electron-phonon coupling strength α and the ratio of the high frequency (ϵ_∞) to static (ϵ_0) dielectric constants, $\eta = \epsilon_\infty/\epsilon_0$, all play a central role in determining the stability region. The procedure in determining the boundaries of this region is based on the fact that the energy of two interacting polarons should be lower than those of two free

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polarons over certain critical values of α and η. In 3D bulk materials, an upper bound for α and a lower bound for η of 7.3 and 0.14, respectively, have been provided by Adamowski [11] through a variational approach, and by Verbist, Peeters and Devreese [12], of 6.8 and 0.14, respectively, by using the Feynman path integral method. In the case of purely 2D systems, Verbist et al. [12] have performed binding energy calculations and found that the transition between polaron and bipolaron states can be realized in the region defined by the parameters $\alpha = 2.9$ and $\eta = 0.158$, while Luczak et al. [22] have predicted that this transition occurs at the values $\alpha = 3.5$ and $\eta = 0.158$ within a variational approach based on a comparison with Feynman free polaron energies. All the works cited above have concentrated on determining the stability criterion for bipolaron formation in 3D, 2D and also in 1D systems. However, there are a very few investigations in low dimensional structures [27–31], particularly in QD systems wherein in addition to the material parameters, one takes into account the size of QD as a determinative parameter to describe the bipolaron stability region. More recently, Pokatilov et al. have examined the bipolaronic mechanism in 3D spherical [28] and ellipsoidal [30] QDs with parabolic confinement by using the Feynman's path integral formalism. They have pointed out that in nanostructures having a size of the order of the polaron radius, it is possible to find the stable bipolaron states even for intermediate values of α ($\alpha \sim 2$).

The existence of a magnetic field in QDs is of particular importance since it enhances polaronic effects, and may therefore lead to a significant enlargement of the boundaries of the bipolaron stability region. It can also be used as an experimental probe to investigate both size and polaronic effects on electronic energy levels. In addition to the above references, there have also been studies that includes the effects of magnetic fields on the bipolaron formation in both 2D and 3D systems [32–41]. Among them, the Feynman-Haken path integral approach to the magnetic field effect on the binding energy of bipolaron was recently discussed in a series of papers [38,39]. A remarkable decrease of the critical value of α due to magnetic field was found. Magnetic field effects together with the effect of spatial confinement on BPSR have been analyzed in our previous paper [41], however the method that we used to get information on the stability region for QD, QWW and QW structures did not permit us to determine an upper critical value of α. Here I shall present a different method to overcome this problem.

In this paper, within the framework of Fröhlich large bipolaron theory, I propose a variational procedure to analyze the stability region of 2D bipolarons confined in a 2D parabolic QD potential subject to a uniform magnetic field, based on Lee, Low, Pines and Huybrechts (LLP-H) canonical transformations, where weak and strong coupling variational results can be interpolated by an additional variational parameter. These types of canonical transformations we use were originally suggested by Lee et al. [42], modified by Huybrechts [43], and widely used for describing electron-phonon interactions in several systems, such as the free and bound polaron problem [44], and very recently in a study on the ground- and first-excited states of magnetopolarons in two-dimensional QDs for all coupling strengths [45]. It is well-known that in attempting to calculate the binding energy of bipolarons as described above, a complete and satisfactory discussion of the stability region requires a self consistent calculation of free polaron energies from the bipolaron theory, or at least a calculation within the same technique as done for bipolaron energies. From this point of view, the main advantages of our approach are that firstly, it allows us to obtain the single polaron ground-state energy in a self consistent manner, as well as the bipolaron ground-state energy, and secondly, it gives results which valid for a whole range of electron-phonon coupling strengths.

The layout of the present paper is as follows. In Section 2 we discuss the Hamiltonian of the system consisting of two electrons coupled to LO phonons confined in a 2D parabolic potential subject to a uniform magnetic field using LLP-H transformations. Then we perform a variational calculation to the resulting effective Hamiltonian. In Section 3 we examine the stability of 2D magnetobipolarons by introducing a self consistent procedure to obtain the free polaron ground-state energy from the theory, and we summarize the main points of our discussions by comparing the results with those found in the literature. In Section 4 we present a brief conclusion.

2 Theory

We consider a system of two-interacting electrons coupled to LO-phonons and subject to both a homogeneous magnetic field and a parabolic QD potential. This results in the well-known Fröhlich bipolaron Hamiltonian

$$H = \sum_{j=1}^{2} \frac{1}{2m} \left\{ \left[\mathbf{p}_j + \frac{e}{c} \mathbf{A}\left(\mathbf{r}_j\right) \right]^2 + \frac{1}{2} m \omega_\bullet^2 \mathbf{r}_j^2 \right\} + \frac{e^2}{\epsilon_\infty \left|\mathbf{r}_1 - \mathbf{r}_2\right|} + \sum_{\mathbf{q}} \hbar\omega_0 b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + \sum_{j=1,2} \sum_{\mathbf{q}} \left(V_{\mathbf{q}} b_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}_j} + \text{h.c.} \right), \quad (1)$$

where $|V_{\mathbf{q}}|^2 = (\hbar\omega_0)^2 (2\pi\alpha r_0/Vq)$ [46] is the electron-phonon interaction amplitude, $b_{\mathbf{q}}^\dagger (b_{\mathbf{q}})$ is the creation (annihilation) operator of an optical phonon with a wave vector $\mathbf{q}$ and energy $\hbar\omega_0$, while $\mathbf{p}_j$ and $\mathbf{r}_j$ denote the momentum and position operators of the electrons, respectively. α and $r_0 = \sqrt{\hbar/2m\omega_0}$ are the electron-phonon coupling constant and polaron radius, respectively. $\omega_\bullet$ characterizes the strength of a parabolic QD potential. By imposing the center of mass position operator $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ and the relative position operator $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$, along with their canonically conjugate momenta $\mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{p} = \mathbf{p}_1 - \mathbf{p}_2$, respectively, the Hamiltonian of the whole system can be divided in the usual way as $H = H_E + H_0$,

where

$$H_E = \frac{1}{2\mu}\left[\mathbf{p} + \frac{q}{c}\mathbf{A}\left(\mathbf{r}\right)\right]^2 + \frac{1}{2}\mu\omega_\bullet^2\mathbf{r}^2 + \frac{e^2}{\epsilon_\infty \mathbf{r}} + \frac{1}{2M}\left[\mathbf{P} + \frac{Q}{c}\mathbf{A}\left(\mathbf{R}\right)\right]^2 + \frac{1}{2}M\omega_\bullet^2\mathbf{R}^2 \quad (2)$$

and

$$H_0 = \sum_{\mathbf{q}} \hbar\omega_0 b_{\mathbf{q}}^\dagger b_{\mathbf{q}} + 2\sum_{\mathbf{q}} \cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right)\left(V_{\mathbf{q}} b_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}} + \text{h.c.}\right), \quad (3)$$

respectively. In equation (2) we introduce $\mu = m/2$, $M = 2m$, $q = e/2$ and $Q = 2e$. The ground-state trial wave function for the Hamiltonian H is chosen to be $|\Psi\rangle = U_1 U_2 |0\rangle_{PH} \otimes |\Psi(\mathbf{r},\mathbf{R})\rangle$, where $|0\rangle_{PH}$ is the vacuum state of phonons, and

$$U_1 = \exp\left[-i\lambda\mathbf{R}\cdot\sum_{\mathbf{q}} \mathbf{q}\; b_{\mathbf{q}}^\dagger b_{\mathbf{q}}\right], \quad (4)$$

and

$$U_2 = \exp\left\{\sum_{\mathbf{q}}\left[F_{\mathbf{q}}(\mathbf{r}) b_{\mathbf{q}} - F_{\mathbf{q}}^*(\mathbf{r}) b_{\mathbf{q}}^\dagger\right]\right\}, \quad (5)$$

are the well-known LLP-H transformations. These two successive canonical transformations provide results for the whole range of electron-phonon coupling strengths since they describe both weak and strong coupling variational solutions in the case of $\lambda = 1$ and $\lambda = 0$, respectively. The effect of transformations equations (4, 5) into the total Hamiltonian H can be observed by considering $U_1^{-1} b_{\mathbf{q}} U_1 = b_{\mathbf{q}} \exp[-i\lambda\mathbf{q}\cdot\mathbf{r}]$, $U_1^{-1}\mathbf{P}U_1 = \mathbf{P} - \lambda\hbar\sum_{\mathbf{q}} \mathbf{q} b_{\mathbf{q}}^\dagger b_{\mathbf{q}}$, and $U_2^{-1} b_{\mathbf{q}} U_2 = b_{\mathbf{q}} - F_{\mathbf{q}}^*(\mathbf{r})$. For the sake of simplicity, we restrict our attention to the diagonalized part of the effective Hamiltonian $U_2^{-1}U_1^{-1}HU_1U_2 = \widetilde{H}$, and we write down the phonon related part as

$$\widetilde{H}_0 = \sum_{\mathbf{q}}\left\{\hbar\Omega_{\mathbf{q}}(\lambda)\left|F_{\mathbf{q}}(\mathbf{r})\right|^2 + \frac{1}{2\mu}\left|\left[\mathbf{p} + \frac{q}{c}\mathbf{A}\left(\mathbf{r}\right), F_{\mathbf{q}}(\mathbf{r})\right]\right|^2 - 2\cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right)\left[V_{\mathbf{q}} F_{\mathbf{q}}^*(\mathbf{r}) e^{i(1-\lambda)\mathbf{q}\cdot\mathbf{R}} + \text{c.c.}\right]\right\}, \quad (6)$$

and we discard all the terms including $b_{\mathbf{q}}(b_{\mathbf{q}}^\dagger)$, and higher orders, since they vanish when applied to the vacuum. In equation (6) $\Omega_{\mathbf{q}}(\lambda)$ is defined as

$$\Omega_{\mathbf{q}}(\lambda) = \omega_0 + \frac{\lambda^2\hbar}{2M}\mathbf{q}^2 - \frac{\lambda\hbar}{M}\mathbf{q}\cdot\left[\mathbf{P} + \frac{Q}{c}\mathbf{A}\left(\mathbf{R}\right)\right] + \frac{\lambda^2\hbar}{2M}\mathbf{q}\cdot\sum_{\mathbf{q}'}\mathbf{q}'\left|F_{\mathbf{q}'}(\mathbf{r})\right|^2, \quad (7)$$

and the last term on the right hand side of equation (7) gives no contribution to equation (6), i.e., $\sum_{\mathbf{q}} \mathbf{q}\;\left|F_{\mathbf{q}}(\mathbf{r})\right|^2 = 0$ due to the symmetry of the QD. The next step in our variational scheme is to minimize equation (6) with respect to $F_{\mathbf{q}}(\mathbf{r})$. This can be done in several ways as pointed out in reference [44]. A very convenient way to do this is to take an Ansatz

$$F_{\mathbf{q}}(\mathbf{r}) = Q_{\mathbf{q}} \cos\left(\frac{\mathbf{q}\cdot\mathbf{r}}{2}\right) + G_{\mathbf{q}}, \quad (8)$$

where $Q_{\mathbf{q}} = \lambda_1 V_{\mathbf{q}}/(1 + \lambda_2 r_0^2 q^2)$ and λ_1, λ_2 and $G_{\mathbf{q}}$ are the variational parameters to be determined. This type of choice for $F_{\mathbf{q}}(\mathbf{r})$ is analogous to that of Adamowski [11], but for the $\mathbf{r}$ independent part of the trial wave function, we follow a variational procedure to obtain the $\mathbf{q}$ dependence of $G_{\mathbf{q}}$ as opposed to predicting it. After substituting equation (8) into equation (6) we find

$$\begin{aligned}\widetilde{H}_0 = \sum_{\mathbf{q}}\Big\{\hbar\Omega_{\mathbf{q}}(\lambda)\Big[\left|Q_{\mathbf{q}}\right|^2\sigma(\mathbf{q}) + \left|G_{\mathbf{q}}\right|^2 + Q_{\mathbf{q}}^*\sigma_1^*(\mathbf{q})\,G_{\mathbf{q}} \\ + Q_{\mathbf{q}}\sigma_1(\mathbf{q})\,G_{\mathbf{q}}^*\Big] + \frac{\hbar^2\mathbf{q}^2}{8\mu}\left|Q_{\mathbf{q}}\right|^2\left(1 - \sigma(\mathbf{q})\right)\Big\} \\ - \sum_{\mathbf{q}}\Big\{2V_{\mathbf{q}}\left[Q_{\mathbf{q}}^*\sigma^*(\mathbf{q})\,\rho(\mathbf{q}) + \sigma_1(\mathbf{q})\,\rho(\mathbf{q})\,G_{\mathbf{q}}^*\right] \\ + 2V_{\mathbf{q}}^*\left[Q_{\mathbf{q}}\sigma(\mathbf{q})\,\rho^*(\mathbf{q}) + \sigma_1^*(\mathbf{q})\,\rho^*(\mathbf{q})\,G_{\mathbf{q}}\right]\Big\}, \end{aligned} \quad (9)$$

where $\sigma_1(\mathbf{q}) = \langle\cos(\mathbf{q}\cdot\mathbf{r}/2)\rangle$, $\sigma(\mathbf{q}) = \left\langle\cos^2(\mathbf{q}\cdot\mathbf{r}/2)\right\rangle$, $\rho(\mathbf{q}) = \langle\exp(i(1-\lambda)\mathbf{q}\cdot\mathbf{R})\rangle$, and $\langle\cdots\rangle$ denotes the expectation value with respect to the electronic coordinates. For the electronic part, if we choose the 2D harmonic oscillator ground-state wave functions for both center of mass and relative parts, i.e.,

$$\Psi(\mathbf{r},\mathbf{R}) = N(\gamma,\beta)\exp[-\left(\gamma^2\mathbf{r}^2 + \beta^2\mathbf{R}^2\right)/2], \quad (10)$$

and impose a symmetrical Coulomb gauge for the vector potential, (as done in Ref. [41]), then every term including the electronic average in equations (2) and (9) can easily be calculated in terms of confluent hypergeometric functions as such: $\sigma_1(\mathbf{q}) = {}_1F_1(1,1;-q^2/16\gamma^2)$, $\rho(\mathbf{q}) = {}_1F_1(1,1;-q^2/16\beta^2)$ and $\sigma(\mathbf{q}) = \left[1 + \sigma_1(q^2/4\gamma^2)\right]/2$, where γ and β are variational parameters. After the minimization of $\widetilde{H}_0$ with respect to $G_{\mathbf{q}}$ we find the expression

$$G_{\mathbf{q}}^* = -Q_{\mathbf{q}}^*\sigma_1^*(\mathbf{q}) + \frac{2V_{\mathbf{q}}^*}{\hbar\Omega_{\mathbf{q}}(\lambda)}\sigma_1^*(\mathbf{q})\,\rho^*(\mathbf{q}). \quad (11)$$

Substituting this result back into equation (9) and combining the results with H_E of equation (2), we find the ground-state energy for the 2D magnetobipolaron system to be:

$$\begin{aligned}E = \frac{\hbar^2}{2\mu}\gamma^2 + \frac{1}{2}\mu\omega^2\frac{1}{\gamma^2} + \frac{e^2}{\epsilon_\infty}\gamma\sqrt{\pi} + \frac{\hbar^2}{2M}\beta^2 + \frac{1}{2}M\omega^2\frac{1}{\beta^2} \\ + \sum_{\mathbf{q}}\Bigg\{\left|Q_{\mathbf{q}}\right|^2\Bigg[\hbar\Omega_{\mathbf{q}}\left[\sigma(\mathbf{q}) - \left|\sigma_1(\mathbf{q})\right|^2\right] \\ + \frac{\hbar^2}{8\mu}q^2\left[1 - \sigma(\mathbf{q})\right]\Bigg] - 4\frac{\left|V_{\mathbf{q}}\right|^2}{\hbar\Omega_{\mathbf{q}}}\left|\sigma_1(\mathbf{q})\right|^2\left|\rho(\mathbf{q})\right|^2\Bigg\} \\ - \sum_{\mathbf{q}}\Big\{2Q_{\mathbf{q}}V_{\mathbf{q}}^*\left[\sigma(\mathbf{q})\rho(\mathbf{q}) - \left|\sigma_1(\mathbf{q})\right|^2\rho^*(\mathbf{q})\right] \\ + 2Q_{\mathbf{q}}^*V_{\mathbf{q}}\left[\sigma^*(\mathbf{q})\rho(\mathbf{q}) - \left|\sigma_1(\mathbf{q})\right|^2\rho(\mathbf{q})\right]\Big\}, \end{aligned} \quad (12)$$

in which $\omega^2 = \omega_\bullet^2 + \omega_c^2/4$ and $\omega_c = qB/\mu c = QB/Mc = eB/mc$ are the hybrid and cyclotron frequencies, respectively.

3 Results and discussion

Introducing new dimensionless variables $r_0\gamma = 1/\overline{\gamma}$ and $r_0\beta = 2/\overline{\beta}$, and converting the sum in equation (12) into an integral over 2D volume in the usual way, while changing the variable $q/4\gamma = x$, the bipolaron ground state energy in units of $\hbar\omega_0$ can be rewritten as;

$$\begin{aligned}\overline{E} = {} & \frac{2}{\overline{\gamma}^2} + \frac{1}{8}\overline{\omega}^2\overline{\gamma}^2 + \frac{2\alpha}{1-\eta}\frac{\sqrt{\pi}}{\overline{\gamma}} + \frac{2}{\overline{\beta}^2} + \frac{1}{8}\overline{\omega}^2\overline{\beta}^2 \\ & - \frac{16\alpha}{\overline{\gamma}}\int_0^\infty \frac{1}{1+8\lambda^2x^2/\overline{\gamma}^2} \\ & \times \left[F(x^2)\right]^2\left[F\left((1-\lambda)^2x^2\overline{\beta}^2/\overline{\gamma}^2\right)\right]^2 dx \\ & - \frac{16\alpha}{\overline{\gamma}}\lambda_1\int_0^\infty \frac{1}{1+16\lambda_2x^2/\overline{\gamma}^2}\Big\{\frac{1}{2}\left[1+F(4x^2)\right] \\ & - \left[F(x^2)\right]^2\Big\}F((1-\lambda)^2x^2\overline{\beta}^2/\overline{\gamma}^2)dx \\ & + \frac{4\alpha}{\overline{\gamma}}\lambda_1^2\int_0^\infty \frac{1}{\left(1+16\lambda_2x^2/\overline{\gamma}^2\right)^2}\Big\{\frac{1}{2}\left[1+F(4x^2)\right] \\ & + \frac{8}{\overline{\gamma}^2}\left[x^2 + \frac{1}{2}\left[\left(\lambda^2-1\right)x^2\left[1+F(4x^2)\right]\right]\right] \\ & - \left(1+\frac{8\lambda^2}{\overline{\gamma}^2}x^2\right)\left[F(x^2)\right]^2\Big\}dx, \end{aligned} \tag{13}$$

where $F(x^2)$ represents the confluent hypergeometric function ${}_1F_1(1,1;x^2)$.

In calculating the bipolaron binding energy, $W = 2E^{SP} - E^{BP}$, one has to take into account the free polaron energy E^{SP}. As pointed out in the Introduction, this is the main problem with bipolaron theory since, to the very least, it must be calculated within the same technique and the same accuracy as done for the bipolaron. Using our approximation scheme, we can extract the free polaron energy in a self consistent way from the bipolaron energy without referring to other approaches. After obtaining the energies with the same accuracies, we are able to thoroughly analyze the stability region of the 2D magnetobipolarons, defined by the criteria $W \geq 0$. In order to see this, it is useful to look at limiting cases with special values of variational parameters.

Firstly, by choosing $\lambda = \lambda_1 = 0$, $\overline{\gamma} = \overline{\beta}$, $\eta = 0$ and taking the related integrals appearing in equation (13), we can easily obtain

$$\overline{E}^{2SP} = \frac{4}{\overline{\gamma}^2} + \frac{1}{4}\overline{\omega}^2\overline{\gamma}^2 - 2\alpha\sqrt{\pi}\frac{1}{\overline{\gamma}}, \tag{14}$$

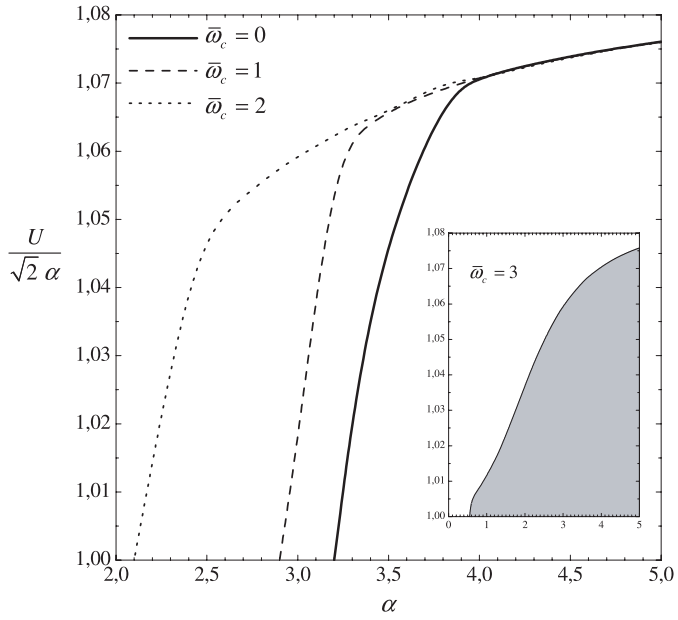
where $\overline{E}^{2SP}$ denotes the two single polaron energy. We should emphasize here that, as also stated in reference [13] for the 2D and 3D bipolaron problem, choosing $\overline{\gamma}$ equal to $\overline{\beta}$ corresponds to taking a trial wave function without any correlation, since from the definition, $\overline{\gamma} = \overline{\beta}$ corresponds to taking $2\gamma = \beta$ in equation (10), and this choice leads to a cancellation of terms $\mathbf{r}_1 \cdot \mathbf{r}_2$, and therefore discards the angular correlations between the particles. Minimization with respect to $\overline{\gamma}$ yields a fourth order equation in $\overline{\gamma}$, as such $\overline{\omega}^2\overline{\gamma}^4 + 4\alpha\sqrt{\pi}\overline{\gamma} - 16 = 0$. An analytical solution to this equation is also possible as indicated in reference [45]. However, for simplicity, in order to get qualitative results, it is sufficient to analyze its limiting values. In the case of strong electron-phonon interaction and weak spatial confinement with or without a magnetic field, $\alpha \gg \overline{\omega}$, one finds $\overline{\gamma} = 4/\sqrt{\pi}\alpha$, and hence the result $\overline{E}^{2SP} = -\pi\alpha^2/4$. This is the well-known two non-interacting polaron ground-state energy in the strong coupling limit in 2D. Another limiting case is $\alpha \ll \overline{\omega}$, and gives $\overline{\gamma} = 2/\sqrt{\overline{\omega}}$. In this case, one finds $\overline{E}^{2SP} = 2\overline{\omega} - \alpha\sqrt{\pi\overline{\omega}}$, which reduces to the results of reference [47] in the absence of a confinement potential, that is, in the case of $\overline{\omega} = \overline{\omega}_c/2$.

Secondly, by choosing $\lambda = 1$, $\overline{\omega} \to 0$, $\overline{\gamma} \to \infty$ ($\gamma \to 0$), $\eta = 0$ and $\overline{\omega}\,\overline{\gamma} \to 0$ in equation (13), that is, in the absence of both magnetic field and spatial confinement, we find

$$\overline{E}^{2SP} = \pi\alpha\left[-\frac{\lambda_1}{\lambda_3} + \frac{\lambda_1^2}{8\lambda_3^3} + \frac{\lambda_1^2}{8\lambda_3}\right], \tag{15}$$

where its minimization with respect to λ_1 and λ_3 yields $\lambda_1 = 2$ and $\lambda_3 = 1$. With these values, equation (15) results in $\overline{E}^{2SP} = -\pi\alpha$, which is the well-known result for the self energy of two non-interacting polarons in the intermediate region [48]. So, one can use equation (13) to obtain single polaron energies in a self consistent way.

In order to investigate both magnetic field and size dependence of the BPSR, we have solved equation (12) self consistently and shown the numerical results in Figures 1a and 1b. For comparison and clarity, Figure 1a includes only the effect of a magnetic field on the BPSR in the absence of confinement potential, while the other presents the effect of spatial confinement together with a magnetic field. As seen from Figure 1a, a polaron-bipolaron transition appears for $\alpha_c = 3.2$ at $\overline{\omega}_c = 0$ and moves to lower α values with increasing magnetic field. This differs from the well-known path integral result by 10%, which amounts to 2.9. We note from the figure that the critical values of α for $\overline{\omega}_c = 0$, 1 and 2 are in reasonable agreement with those obtained by the authors of references [38,39], in the absence of a spatial confinement potential. They predict $\alpha_c = 2.6$ and 2.4 for $\overline{\omega}_c = 1$ and 2, respectively. The latter differs from our value of 2.1, by 14%, therefore these values are not much different from each other, and are agreement within about 10%. There is, however, a difference with the α-dependence of the curves. By a rough comparison of the behavior of the curves in Figure 1a and in Figures 4 of references [38,39], one can easily see that the BPSR is narrow in references [38,39], while it is relatively wide in



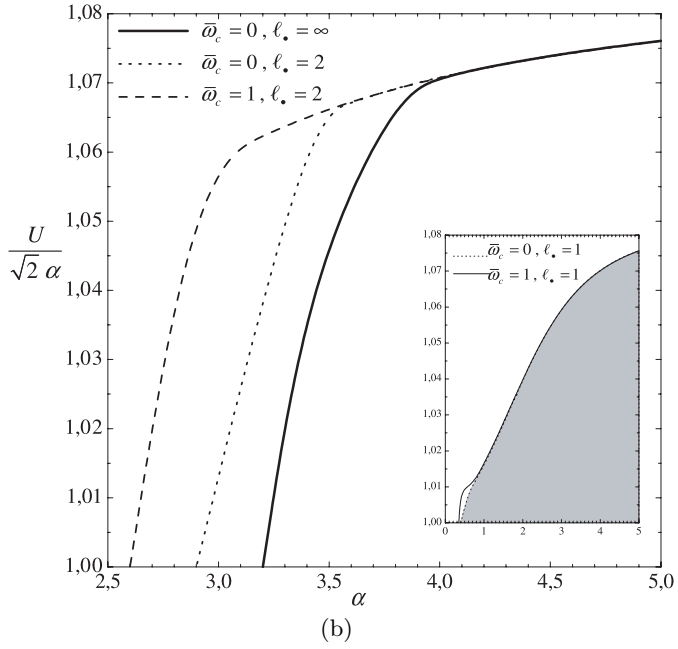


Fig. 1. Phase plane showing the boundaries of 2D BPSR in which the condition $W(\alpha, \eta; \overline{\omega}_c, \overline{\omega}_\bullet) = 0$ is fulfilled, (a) in the absence and (b) presence of a confining potential. $\alpha < \alpha_c$ and $\alpha > \alpha_c$ corresponds to polaronic and bipolaronic regions, respectively. The solid curves show the 2D bulk case. $\ell_\bullet = \sqrt{2/\overline{\omega}_\bullet}$ is the confinement length in units of the polaron radius r_0.

our case, and is broadened considerably as the magnetic field increases. Therefore in our approach, the BPSR is very sensitive to increasing magnetic field. In order to emphasize this point further, and to distinguish the stability regions, we also give a plot for $\overline{\omega}_c = 3$ in the inset. It seems that further increase of magnetic field yields $\alpha_c = 0.6$ and causes an additional enlargement in the BPSR.

In Figure 1b we show the effect of spatial confinement on the BPSR by again plotting the $[U/\sqrt{2}\alpha(= 1/1-\eta), \alpha]$ plane, together with the effect of a magnetic field. According to Figure 1b and its inset, a polaron-bipolaron transition occurs at $\alpha_c = 2.9$ and 0.4 for QDs whose sizes are of the order of two and one polaron radii, respectively, in the absence of a magnetic field. Introducing a magnetic field in such QDs with sizes of the order of two polaron radius, leads to a remarkable increase in the BPSR, i.e. for $\overline{\omega}_c = 1$ one gets a wider BPSR with $\alpha_c = 2.6$. However, for QDs whose sizes are of the order of the polaron radius, there is no apparent change in the decrease of α_c, and therefore an increase in the BPSR with increasing magnetic field, i.e. $\overline{\omega}_c = 1$, except for a tail as shown in the inset of Figure 1b.

As also pointed out in reference [28], the physical picture behind the above discussion of Figure 1 can be explained as follows. In the bipolaron theory, boundaries of the stability region depend sensitively on the region where the screened Coulomb repulsion between electrons is compensated by the phonon mediated attraction. For larger inter-electron distances than the polaron radius, the long-range character of the Coulomb repulsion does not allow the formation of polaron pairing, therefore each electron moves in its own polarization potential well. When the distance between polarons is decreased to the order of a few polaron radii, virtual phonon clouds surrounding each electron start to overlap, and thus attraction suppresses the repulsion. For distances smaller than the polaron radius, again, repulsion dominates due to its divergent nature at the bipolaron center, while the attraction remains finite at the origin. In other words, a stable bipolaron can occur only at intermediate distances, i.e., $|\mathbf{r}_1 - \mathbf{r}_2| \sim r_p$, depending on the values of the material parameters. Therefore, reducing the dimensionality of the system by a spatial confinement and/or a magnetic field can be a favorable feature for bipolaron formation.

4 Conclusion

We have presented a variational scheme based on the use of LLP-H canonical transformations to explain how the stability region of 2D magnetobipolarons confined in a 2D parabolic QD potential depends on the material parameters α and η, the size of the QD, and the strength of magnetic field. In our calculations, to derive both free polaron and bipolaron energies, and hence determine the BPSR, we have used an Ansatz similar to that of Adamowski [11], and we have chosen Gaussian-Gaussian type trial wavefunctions for both center of mass and internal motion, as a consequence of the confined nature of the problem. LLP-H canonical transformations together with these Ansatzs have allowed us to perform a self consistent calculation of both single polaron and bipolaron ground-state energies, which are valid in the entire range of electron-phonon coupling strengths. Here, we should emphasize again that the difference between our Ansatz and that of Adamowski lies only in the treatment of the $\mathbf{r}$ independent term of the variational function. In order to determine this part of the

Ansatz, we have followed a variational procedure to obtain the **q** dependence of this term instead of predicting it. To ensure that our calculation of the bipolaron ground-state energy based on these Ansatzs yields two polaron ground-state energies in a self consistent manner, we have also made a number of checks for various limiting cases, and found the well-known expressions for both strong [47] and intermediate [48] coupling regimes.

Summarizing the important aspects of our work, we have investigated a strong dependence of the BPSR on both magnetic field and spatial confinement, as well as on material parameters, in 2D structures. Our analysis reveals that (i) α_c becomes remarkably small by decreasing the size of QD, and therefore in QDs whose sizes are of order of a few polaron radius it is possible to find bipolaron states even in the case where the electron-phonon coupling strength takes smaller values ($\alpha \sim 1$), (ii) the presence of a magnetic field leads to a significant enhancement of the BPSR in 2D QDs since it brings an additional magnetic confinement in the lateral plane. We have also found that our qualitative results are consistent with those observed by Pokatilov et al. [28,30] in the absence of a magnetic field, and in 3D parabolic QDs. Our results provide further evidence for coexistence of polaron and bipolaron states in nanostructures whose sizes are of the order of the polaron radius.

As for the validity of our approach, it should be noted that, although a comparison with BPSRs calculated within our approach and those of references [38,39] indicates that our approach provides a relatively wider BPSR than those found in references [38,39], ours estimates the critical value of η to be 0.079, whereas it is estimated to be 0.158 [18] by the path integral approach. We should further note two points. Firstly, we have assumed that the QD is formed from a 2D system with zero thickness by means of a 2D parabolic potential, whereas, in reality these systems have finite thickness. Hence, one should remember that the polaron radius has to be greater than the thickness of the 2D layer in order to have a stable bipolaron as demonstrated by Peeters and Devreese [49]. Secondly, we have expressed the energies and lengths used in this work in units of $\hbar\omega_0$ and $r_0 = \sqrt{\hbar/2m\omega_0}$, respectively. One should also note that the latter represents the polaron radius when $\alpha < 1$. As shown by Pokatilov et al. [50], when $\alpha \gg 1$ it is a complicated function of both electron-phonon coupling strength and magnetic field, and thus a new scale should be introduced in coordinate space.

Polaron-bipolaron transitions can be seen by using optical absorption experiments since calculations on optical and magneto-optical absorption of both polarons [51,52] and bipolarons [53–55] clearly indicate the existence of this transition. We hope that the results presented in this paper will provide further experimental insight in interpreting the optical spectra in QDs.

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References

1. B.S. Kandemir, T. Altanhan, Phys. Rev. B **60**, 4834 (1999); B.S. Kandemir, A. Çetin, Phys. Rev. B **65**, 054303 (2002)
2. N.F. Johnson, J. Phys.: Condens. Matter **7**, 965 (1995); T. Demel, D. Heitmann, P. Grambow, K. Ploog, Phys. Rev. Lett. **64**, 788 (1990); A. Lorke, J.P. Kotthaus, K. Ploog, Phys. Rev. Lett. **64**, 2559 (1990)
3. L. Jacak, P. Hawrylak, A. Wójs, *Quantum Dots* (Springer, Berlin, 1998)
4. S.I. Pekar, *Research on Electron Theory of Crystals* (Gostekh-teorizdat, Moscow and Leningrad, 1951) [in Russian: English translation: US AEC, Washington DC, 1963]
5. V.L. Vinetskii, M.S. Giterman, Zh. Eksp. Teor. Fiz. **33**, 730 (1958); **40**, 1459 (1961) [Sov. Phys.-JETP **13**, 1023 (1961)]
6. D. Emin, T. Holstein, Phys. Rev. Lett. **36**, 323 (1976)
7. S.G. Suprun, B. Ya. Moĭzhes, Fiz. Tverd. Tela (Leningrad) **24**, 1571 (1982) [Sov. Phys. Solid State **24**, 903 (1982)]
8. Y. Takada, Phys. Rev. B **26**, 1223 (1982)
9. M.H. Cohen, E.N. Economou, C.M. Soukouilis, Phys. Rev. B **29**, 4496 (1984)
10. H. Hiramoto, Y. Toyozawa, J. Phys. Soc. Jpn **54**, 245 (1985)
11. J. Adamowski, Phys. Rev. B **39**, 3649 (1989)
12. G. Verbist, F.M. Peeters, J.T. Devreese, Phys. Rev. B **43**, 2712 (1991)
13. F. Bassani, M. Geddo, G. Iadonisi, D. Ninno, Phys. Rev. B **43**, 5296 (1991)
14. G. Verbist, F.M. Peeters, J.T. Devreese, Solid State Commun. **76**, 1005 (1990)
15. J. Adamowski, S. Bednarek, J. Phys.: Condens. Matter **4**, 2845 (1992)
16. G. Verbist, M.A. Smondyrev, F.M. Peeters, J.T. Devreese, Phys. Rev. B **45**, 5262 (1992)
17. D. Emin, Phys. Rev. B **48**, 13 691 (1993).
18. P. Vansant, M.A. Smondyrev, F.M. Peeters, J.T. Devreese, J. Phys. A **27**, 7925 (1994)
19. P. Vansant, F.M. Peeters, M.A. Smondyrev, J.T. Devreese, Phys. Rev. B **50**, 12 524 (1994)
20. V.M. Fomin, M.A. Smondyrev, Phys. Rev. B **49**, 12 748 (1994)
21. A. Chatterjee, S. Sil, Int. J. Mod. Phys. **7**, 4763 (1994)
22. F. Luczak, F. Brosens, J.T. Devreese, Phys. Rev. B **52**, 12 743 (1995)
23. G. Iadonisi, V. Cataudella, G. De Filippis, V. Mukhomorov, Eur. Phys. J. B **18**, 67 (2000); V.K. Mukhomorov, J. Phys.: Condens. Matter **13**, 3683 (2001)
24. M.A. Smondyrev, V.M. Fomin, in *Proceedings in Nonlinear Science on Polarons and Applications*, edited by V.D. Lakhno (J. Wiley, Sons Ltd., Chichester, 1994), p. 13
25. A.S. Alexandrov, N. Mott, *Polarons and Bipolarons* (World Scientific, Singapore, 1995)
26. J.T. Devreese, *Encyclopedia of Applied Physics* (VCH Publishers, Weinheim, 1996), Vol. 14, pp. 383-413
27. S. Mukhopadyay, A. Chatterjee, J. Phys.: Condens. Matter **8**, 4017 (1996)

28. E.P. Pokatilov, V.M. Fomin, J.T. Devreese, S.N. Balaban, S.N. Klimin, J. Phys.: Condens. Matter **11**, 9033 (1999)
29. E.P. Pokatilov, V.M. Fomin, J.T. Devreese, S.N. Balaban, S.N. Klimin, Phys. Rev. B **61**, 2721 (2000)
30. E.P. Pokatilov, M.D. Croitoru, V.M. Fomin, J.T. Devreese, Phys. Stat. Sol. B **237**, 244 (2003)
31. R.T. Senger, A. Erçelebi, Phys. Rev. B **60**, 10 070 (1999)
32. M.A. Smondyrev, E.A. Kochetov, G. Verbist, F.M. Peeters, J.T. Devreese, Europhys. Lett. **19**, 519 (1992)
33. J.T. Devreese, F. Brosens, Phys. Rev. B **45**, 6459 (1992)
34. S. Sil, A. Chatterjee, Solid State Commun. **87**, 917 (1993)
35. V.M. Fomin, J.T. Devreese, Solid State Commun. **96**, 79 (1995)
36. W.B. da Costa, F.M. Peeters, J. Phys.: Condens. Matter **7**, 1293 (1995)
37. F. Brosens, J.T. Devreese, Solid State Commun. **96**, 133 (1995)
38. F. Brosens, J.T. Devreese, Phys. Rev. B **54**, 9792 (1996)
39. J.T. Devreese, F. Brosens, Z. Phys. B **104**, 605 (1997)
40. W.B. da Costa, F.M. Peeters, Phys. Rev. B **57**, 10 569 (1998)
41. B.S. Kandemir, T. Altanhan, Eur. Phys. J. B **27**, 517 (2002)
42. T.D. Lee, F.E. Low, D. Pines, Phys. Rev. B **90**, 297 (1953)
43. W.J. Huybrechts, J. Phys. C **10**, 3761 (1977)
44. K. Takegahara, T. Kasuya, J. Phys. Soc. Jpn **39**, 1292 (1975); J. Pollmann, H. Büttner, Phys. Rev. B **16**, 4480 (1977); M. Wagner, *Unitary Transformations in Solid State Physics* (Elsevier Science Publishers B. V., 1986)
45. B.S. Kandemir, T. Altanhan, Eur. Phys. J. B **33**, 227 (2003)
46. F.M. Peeters, Wu Xiaoguang, J.T. Devreese, Phys. Rev. B **33**, 3926 (1986)
47. Wu Xiaoguang, F.M. Peeters, J.T. Devreese, Phys. Rev. B **32**, 7964 (1985); D.M. Larsen, Phys. Rev. B **32**, 2657 (1985); D. Ninno, G. Iadonisi, Phys. Rev. B **39**, 10963 (1989)
48. F.M. Peeters, J.T. Devreese, Phys. Rev. B **31**, 3689 (1985); D.M. Larsen, Phys. Rev. B **30**, 4087 (1984); S. Das Sarma, Phys. Rev. Lett. **52**, 859 (1984)
49. F.M. Peeters, J.T. Devreese, Phys. Rev. B **31**, 4890 (1985)
50. E.P. Pokatilov, S.I. Beril, V.M. Fomin, G.Yu. Ryabukhin, Phys. Stat. Solidi (b) **169**, 429 (1992)
51. F.M. Peeters, J.T. Devreese, Phys. Rev. B **28**, 6051 (1983)
52. F.M. Peeters, J.T. Devreese, Phys. Rev. B **34**, 7246 (1986)
53. J.T. Devreese, V. Fomin, F. Brosens, Solid State Commun. **96**, 613 (1995)
54. J.T. Devreese, V. Fomin, Phys. Rev. B **54**, 3959 (1996)
55. J.T. Devreese, S.N. Klimin, V. Fomin, Phys. Rev. B **63**, 184307 (2001)