Oscillating properties of a two-electron quantum dot in the presence of a magnetic field

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Abstract

We study the system consisted of two electrons in a quantum dot with a three-dimensional harmonic confinement potential under the effect of a magnetic field. Specifically, two different confinement conditions are considered, one isotropic three-dimensional and the other anisotropic quasi-two-dimensional. Singlet and triplet lowest states properties as the energy, the exchange coupling, the two-electron density function and the spatial spreading of the two electrons in terms of the variance along the x-direction are analyzed. In this study we employ the full configuration interaction method with Cartesian anisotropic Gaussian-type orbitals as the basis set. These functions allow us to explore the confining characteristics of a potential due to their flexibility of using different exponents for each direction in space. The convergence of the results, depending on the size of the set of basis functions, is examined and the oscillations of different physical quantities, concerning the singlet and triplet states, as a function of the magnetic field are discussed.

Keywords: two-electron quantum dot, de Haas–van Alpheneffect, de Haas–van Alphen oscillation

(Some figures may appear in colour only in the online journal)

1. Introduction

In the last three decades the area of nanostructures, an overlapping field of new materials and solid state physics, has experienced a huge development. The advance of semiconductor structure technology at the nanoscale [1, 2] has increased interest in studying the properties of confined quantum systems [3]. In this context, one finds that few-electron quantum dots (QDs) play an important role [4, 5]. The usefulness of QDs appears in a wide range of scientific areas spreading from quantum information [6–8] to biology and medicine [9]. In late 90s one has noticed that the physical properties of QDs are directly connected with their geometry, i.e. their size and form [10, 11], and since early 00s an ordinary approach to treating this issue has been in terms of the profile and strength of the confinement potential [12, 13].

The influence of external fields in the QDs properties was also studied by that time; for instance the behavior of the exchange coupling \( J \), as well as the double occupation of a dot by the two electrons of a two-electron double QD was studied as a function of a static magnetic field and the potential barrier height. The latter being controlled via effective mass with a laser field [14]. In the same vein, the dependence of the ground state of one and two electrons, as well as of the exchange energy \( J \) (two electrons case), was also investigated for a double QD as a function of an external magnetic field.
and of the potential barrier between the dots [15]. It is worth mentioning that two-electron double QD still remains as a promising hardware to implement quantum computation [6–8].

We have recently developed a numerical code in order to study confined quantum systems, more specifically, electrons in QDs. In order to test our computational code we have studied the behavior of two electrons within a QD, whose confining potential was a 3D anisotropic parabolic one [16]. In sequence, by making use of our computational tools we have addressed the issue of a two-electron double QD under the effect of a laser field [17], a subject previously seen in reference [14]. However, we have not considered the presence of a static magnetic field, for this leads to a modification in the Hamiltonian that demands a change in the computational code that we have left to treat later. In fact this was the motivation of the present article; to take into account the effect of an external magnetic field. Thus, in order to accomplish this purpose, we have done the corresponding modification in the computational code that, in few words, consisted in using complex coefficients in the linear combination of the basis functions.

Although our focus is to study two-electron double QDs under effect of external influence, we have decided to turn back to a known problem—two electrons in a single QD described by 3D parabolic anisotropic confining potential—as a strategy to deal with the modification done in our code. By doing so, an unexpected behavior of some physical quantities have arisen naturally from our computations; they present an oscillatory comportment as function of the magnetic field which drew our attention. It was then we became aware of work of de Haas and van Alphen [18]. In their work they investigated the diamagnetism of metals by analyzing the dependence of the susceptibility of metals under a magnetic field. They argued that to correctly understand the phenomenon of diamagnetism one must admit that the conduction electrons are not completely free; they must be in some extension bond in the material, under the influence of neighboring atoms. Therefore, in a certain sense the conduction electrons must be confined in the material sites. Besides, they were the first to observe experimentally an oscillatory behavior of the susceptibility as function of the magnetic field which is known in the literature as the de Haas–van Alphen (dHvA) effect.

The subject of electrons under a magnetic field has been of interest for a long time and several authors have theoretically addressed this issue [19–23]. In all these treatments the medium has been described as a bunch of free electrons. In particular, in references [22, 23] despite the authors were concerned with the dHvA effect they were unable to carry out the assumption suggested by de Haas and van Alphen that the conducting electrons are not entirely free. More recently, in the framework of QDs, the electron–electron interaction as well as a confining potential have been theoretically taken into account and an oscillatory behavior in certain physical quantities has been reported [24, 25]. These oscillatory behaviors are clearly a manifestation of a dHvA effect type. Since then several authors have been reporting such phenomenon in different systems [26–29]. In the following we intend to discuss this subject further.

Therefore, in this article we study the system consisted of two electrons in a single QD with a 3D anisotropic parabolic confining potential under the effect of a magnetic field B. We analyze the behavior of some physical quantities as function of B: the singlet and triplet energies, $E_S$ and $E_T$, respectively; the corresponding exchange coupling $J = E_T - E_S$; the two-electron density function; and the spatial spreading of the two electrons in terms of the variance along the x-direction.

The present paper is organized as follows. In section 2 our theoretical approach is presented. In section 3, we apply our model for two regimes of confinement and, in particular, for a quasi-2D regime where the effects of the magnetic field are shown in different properties of the system. Finally, in section 4, we summarize our conclusions. Throughout the paper we use atomic units.

2. Theoretical approach

We want to solve the time independent Schrödinger equation for a system of N electrons submitted to an arbitrary potential $\hat{V}(x, y, z)$ whose Hamiltonian is written as:

$$\hat{H} = \sum_{j}^{N} \hat{O}_1(\vec{r}_j) + \sum_{j}^{N} \sum_{\kappa<j}^{N} \hat{O}_2(\vec{r}_j, \vec{r}_\kappa),$$

where

$$\hat{O}_1(\vec{r}_j) = \frac{1}{2m_c} \left( \vec{p}_j + \vec{A}(\vec{r}_j) \right)^2 + g\mu_B \vec{S}_j \cdot \vec{B}_j + \hat{\mathcal{V}}(\vec{r}_j),$$

$$\hat{O}_2(\vec{r}_j, \vec{r}_\kappa) = \frac{1}{\kappa|\vec{r}_j - \vec{r}_\kappa|},$$

$m_c$ is the effective electronic mass, $e$ is the absolute value of the electron’s charge, $g$ is the effective gyromagnetic factor, whose value is $-0.44$ for GaAs, $\mu_B = 1/2$ is the Bohr’s magneton and $\kappa$ is the relative permittivity or dielectric constant of the QD. It is convenient to choose the gauge

$$\vec{\nabla} \cdot \vec{A} = 0 \quad (3)$$

which, in the case of a constant magnetic field

$$\vec{B} = B\hat{z},$$

yields

$$\vec{A}(\vec{r}) = -\frac{1}{2} \vec{r} \times \vec{B} = \frac{1}{2} (-y\hat{x} + x\hat{y}) B. \quad (4)$$

Detailing the first term of $\hat{O}_1(\vec{r}_j)$, one gets

$$\frac{1}{2m_c} \left( \vec{p}_j + e\vec{A}(\vec{r}_j) \right)^2 = \frac{\nabla^2_j}{2m_c} - \frac{i\vec{A} \cdot \nabla_j}{m_c} + \frac{\vec{A}^2_j}{2m_c},$$

where we have used equation (3).

According to equation (4) one has

$$-\frac{i}{m_c} \vec{A} \cdot \nabla = \frac{1}{2m_c} \vec{B} \cdot \vec{L}. \quad (6)$$
and 
\[ \frac{\Lambda^2}{2mc} = \frac{B^2}{8m_c}(x^2 + y^2). \] (7)

The potential represents the resulting interaction felt by each of the two electrons with all the other particles—electrons and atomic nuclei—that constitute the QD. In the present work we are interested in studying the electronic structure of a system composed of two electrons confined in an anisotropic 3D harmonic QD, whose potential is expressed as
\[ V(x, y, z) = \frac{m_c}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right). \] (8)

The electronic properties of confined systems, such as electrons in a QD, can be obtained due to the flexibility of our program which can take into account the anisotropy of the potential on the basis employed. In addition, one can modify the mass of the electron by means of effective electronic mass \( m \) and/or change the environment in which they evolve via the dielectric constant \( \kappa \) (see reference [14]).

By making use of equations (2), (4)–(7) one can write the operator \( \hat{O}_1(\vec{r}) \) as
\[ \hat{O}_1(\vec{r}) = -\frac{\nabla^2}{2m_c} + \frac{m_c}{2} \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right) + \frac{B^2}{8m_c}(x_j^2 + y_j^2) + \mu_B \left( \frac{1}{m_c}L_{ij} + gS_{ij} \right) B \]
\[ = -\frac{\nabla^2}{2m_c} + \frac{m_c}{2} \left( \Omega_{1L}^2 x_j^2 + \Omega_{2L}^2 y_j^2 + \omega_z^2 c_j^2 \right) + \mu_B \left( \frac{1}{m_c}L_{ij} + gS_{ij} \right) B, \] (9)

where \( \Omega_{1L}^2 = (\omega_x^2 + \omega_y^2) \) and \( \omega_1 = B/2m_c \) is the Larmor frequency. With all these considerations equation (1) yields
\[ \hat{H} = \sum_j \left[ -\frac{\nabla_j^2}{2m_c} + \frac{m_c}{2} \left( \Omega_{1L}^2 x_j^2 + \Omega_{2L}^2 y_j^2 \right) + \omega_z^2 c_j^2 \right] + \mu_B \sqrt{\frac{2}{m_c}} \omega L_{jF} + \mu_B B gS_z + \sum_{n<j}^{N} \frac{1}{|\vec{r}_{j} - \vec{r}_{n}|}. \] (10)

The basis employed within the framework of the full configuration interaction (full-CI) method is similar to the one used in our previous works [16, 17], i.e. the functions of the basis are Cartesian anisotropic Gaussian-type orbitals (c-amiGTO):
\[ g^{\text{cart}}(\vec{r}) = x^n y^m z^p \exp(-\zeta x^2 - \zeta y^2 - \zeta z^2), \] (11)

whose exponent \( \zeta_i \) \((i = x, y, z)\) are given by
\[ \zeta_i^{(k)} = \frac{m_c \omega_i}{2} \left( \frac{3}{2} \right)^{k-1} \quad (k = 1, 2), \] (12)

where \( \zeta_i^{(1)} = m_c \omega_i / 2 \) when \( k = 1 \) and \( \zeta_i^{(2)} = 3m_c \omega_i / 4 \) when \( k = 2 \). In the present case \( \omega_i \) is replaced by \( \Omega_{1L} \) for \( i = x, y \).

We have employed three different bases: 2s2p2d, consisting of 20 functions, with 210 (190) CSFs and 400 (190) determinants for the singlet (triplet) states; 2s2p2d2f, consisting of 40 functions, with 820 (780) CSFs and 1600 (780) determinants for the singlet (triplet) states; and 2s2p2d2f1g, consisting of 55 functions, with 1485 (1485) CSFs and 2916 (1485) determinants for the singlet (triplet) states. For the sake of simplicity, from now on we shall refer them as 20f, 40f, and 55f, respectively.

Therefore, the solution of the Schrödinger equation \( \hat{H}\Phi = E\Phi \) is written as a linear combination of configuration state functions (CSFs),
\[ \Phi = \sum_{n=1}^{N_{\text{CSF}}} C_{n}^{\text{CSF}} \Psi_{n}^{\text{CSF}}, \] (13)

where \( N_{\text{CSF}} \) is the number of CSFs, \( \Psi_{n}^{\text{CSF}} \) is the \( n \)th CSF, and \( C_{n}^{\text{CSF}} \) is its corresponding coefficient. On the other hand, a CSF is constituted of Slater determinants, i.e.
\[ \Psi_{n}^{\text{CSF}} = \sum_{m=1}^{N_{\text{det}}} \epsilon_{m|n}^{\text{det}} \text{det}_{\omega,m}, \] (14)

where \( \text{det}_{\omega,m} \) is the \( m \)th determinant of the \( n \)th CSF.

In appendix A we show the expressions of the angular momentum integrals that were implemented in our numerical code. They depend only of the overlap integrals which have already been used in our previous works.

3. Results and discussion

For a proper parameterization of our problem, we shall express the magnetic field in terms of a characteristic magnetic field \( B_c = 2m_c \omega_z \), as well as the energy in terms of \( \omega_z \). In all calculations, we consider \( \omega_z = \omega_z = 0.000111 \), while we assume the values 0.000111 and 1.11 for \( \omega_z \). For \( \omega_z = 0.000111 \) one has an energy of 3 meV and \( B_c \approx 1.49 \times 10^{-5} \approx 3.5 \text{ T} \). In what follows, we shall consider \( \omega_z = 0 \).

In order to emphasize the importance of the electronic correlation in this study, we show in figure 1 the singlet and triplet energies obtained from Hartree–Fock (HF) and FCI computations. The electronic correlation in the HF method is partially taken into account, since it considers only the correlation between electrons with the same spin, whereas FCI has no such restriction. Hence, in figure 1 it is displayed the energies as function of the normalized field \( b \) \((b = B/B_c)\) for \( \omega_z = 0.000111 \) using the basis set 55f. At first, one observes that the effect of electronic correlation presents in the FCI computation is more relevant in the case of the singlet than in the triplet one. Nevertheless, in the case of the triplet, the accuracy of the FCI method in comparison with HF becomes evident from values of \( b \) higher than 3. Another important aspect is that HF method predict only a single crossing between singlet and triplet states at \( b \approx 0.75 \). On the other hand, FCI leads to an oscillation between the singlet and triplet energies that are not so evident in a energy representation as the one depicted in figure 1. In order to highlight these crossings we make use of the exchange coupling \( J \) which plays an important role in
Figure 1. It is displayed the singlet and triplet energies as function of the magnetic field \( b \) for \( \omega_z = 0.000111 \) using the basis set 55f. (a) The top panel shows the energies obtained by using the HF method. The solid (open) squares correspond to the singlet (triplet) energies. (b) The bottom panel displays the same HF energies (the solid and open squares) together with the ones obtained by using the FCI method: the solid (open) triangles stand for the singlet (triplet) energies. The vertical scale is the same of the top panel, only its size is stretched to facilitate the visualization of the points.

Figure 2. \( J_{\text{norm}} \times b \) for confinement conditions given by \( \omega_z = \omega_x = \omega_y = 0.000111 \) (see the text for details). As highlighted in the legend the open triangles correspond to the results obtained with the basis 20f, whereas the solid circles and squares to the basis 40f and 55f, respectively.

Observe that Wagner et al [25] studied the issue of two electrons confined by a 2D harmonic potential, where the center-of-mass and the relative motions could be separated and the solution of the latter being solved numerically [31]. This problem can be seen as a limit of the present 3D case when \( \omega_z \rightarrow \infty \). In particular, the authors showed that, with the increase of the magnetic field, there is no crossing between the singlet and triplet states when the electron–electron interaction is disregarded. On the other hand, our results displayed in figure 1 indicate that the HF method, which includes electron–electron interaction within an independent particle model, is capable of recovering the first intersection between singlet and triplet states, but fails for higher values of the magnetic field. Figure 1 refers to \( \omega_z = 0.000111 \), but we observe the same behavior with \( \omega_z = 1.11 \). The oscillation between singlet and triplet as the state with the lowest energy is only obtained when all electronic correlation is taken into account. This is accomplished using the FCI method. It is worth noting that the computational code that we have been developing [16, 17] is easily extended to a larger number of electrons, while the methodology employed in reference [25] is restricted to the problem of two electrons.

In figures 2 and 3 we display the behavior of \( J_{\text{norm}} \) as function of the normalized field \( b = \frac{B}{B_c} \) for \( \omega_z = 0.000111 \) and \( \omega_z = 1.11 \), respectively. The first thing we notice in the behavior of \( J_{\text{norm}} \) is its oscillatory comportment around zero, meaning a successive change of the groundstate between the lowest singlet (\( J_{\text{norm}} > 0 \)) and the lowest triplet states (\( J_{\text{norm}} < 0 \)). As it is well known, the accuracy of the results depends largely on the atomic basis used.

For the isotropic (spherically symmetric) case, one observes from figure 2 that, until \( b \approx 3 \), the result obtained with the basis 20f is in good accordance with the ones obtained with the bases 40f and 55f. Beyond this value, it diverges from the two others. Therefore, one can see that the basis 20f describes well the first oscillation of \( J_{\text{norm}} \) which occurs in the range of \( b \) from 0 to approximately 3. In addition, the results for \( J_{\text{norm}} \) predicted by the computation with the bases 40f and 55f remain in good accordance until \( b \approx 4 \), where they split, but yet remaining close till larger values of \( b \) (\( \approx 6 \)). Hence, the introduction of functions with \( l = 3 \) in the basis set, what happens when one passes from basis 20f to 40f, allows one to describe well the first part of the second oscillation which occurs approximately in the interval of \( b \) from 3 to 4. But the second part of it, from \( b = 4 \) to 6, the basis 40f is not sufficiently accurate to describe it.

It is worth saying that we can be confident of a result when it is obtained with different basis sets. This is what happens in the case of \( J_{\text{norm}} \) with \( b \) from 0 to \( \approx 4 \). Observe that all results agree with each other until the beginning of the second half
period. In the final part of it the result of basis 20f differs from the ones of bases 40f and 55f, showing the limit of confidence of this basis set. In the same manner the results of 40f and 55f agree until the middle of the third half period. From this general behavior of the concordance of the result of these basis sets, we recognize a pattern of improvement in the basis used necessary to describe each half period of the oscillatory motion of $J_{\text{norm}}$ as function of $b$. Therefore we believe the basis 55f should describe properly this oscillation until the beginning of the fourth half period, $b \approx 5$.

In figure 3 we observe a similar behavior to that seen in the previous figure. In this case, however, the confining potential is no longer spherically symmetric, as happens in the former. Now, the confinement strength in the $z$-axis is much stronger than in the other two directions ($\omega_z \gg \omega_x = \omega_y$) and, thus, one can consider it as a quasi-2D case. Therefore, although $J_{\text{norm}}$ presents a similar behavior, one can notice that it oscillates faster as a function of $b$. Besides, the concordance between the results obtained with different basis sets become worse; the results of the three sets of bases agree only up to $b \approx 1.5$ and the concordance between bases 40f and 55f remains just up to $b \approx 2.5$.

The results from figures 2 and 3 show the need of having atomic basis functions with high $l$ in the CI calculation to properly describe the oscillations between singlet and triplet states. Additionally, they indicate that the fundamental state of a two-electron QD alternates between singlet and triplet states, more precisely between states with $l = 0$ (singlet), $l = 1$ (triplet), $l = 2$ (singlet), $l = 3$ (triplet), and so on, in accordance with previous results in the literature [25, 32, 33]. Other interesting observation is that the $J_{\text{norm}}$ oscillations occur for larger $b$ values in the 3D case ($\omega_z = 0.000111$) than in the quasi-2D one ($\omega_z = 1.11$). This behavior is also observed in the study of the chemical potential and the addition energy at reference [34].

From now on we shall focus our attention in the quasi-2D case ($\omega_z = 1.11$). All physical quantities, that can be experimentally observed, are connected with the electrons' spatial distribution. Thus, let us turn our attention to the behavior of the localization of an electron along an axis, say the $x$-axis, expressed in terms of its root-mean-square position ($\sigma_x = \sqrt{\langle x^2 \rangle}$). Hence, one has

$$\langle x^2 \rangle = \int dx_1dx_2 \rho(x_1, x_2) x_1^2,$$

(15)

where

$$\rho(x_1, x_2) = \int d\beta_1 d\beta_2 dy_1dy_2 dz_1dz_2 |\Phi|^2,$$

(16)

is the two-electron localization distribution along the $x$-axis, $\Phi = \Phi(\vec{r}_1, \vec{r}_2, \beta_1, \beta_2)$ is the solution of equation (10), $\beta_1$ and $\beta_2$ stand for the spin coordinates of the two electrons, and $\vec{r}_1 = (x_1, y_1, z_1)$ and $\vec{r}_2 = (x_2, y_2, z_2)$ their spatial coordinates. In order to compute equation (16) we have adopted the following approximation: in the expansion of $\Phi$, equation (13), we have only taken into account the CSFs, whose coefficient has modulus greater than 0.09.

In fact, both quantities, $\sigma_x$ and $\rho(x_1, x_2)$, give interesting information on the behavior of the electrons inside the QD in the presence of the magnetic field and we shall discuss them in next.

Thus, in figure 4 we display the behavior of $\sigma_x$, for the singlet and triplet states, as a function of the magnetic field, computed by using the bases 40f and 55f. The first thing to notice is that the two bases are in good agreement up to $b \approx 3.3$; up to this point $\sigma_x$ develops more than two oscillations, for the singlet state, and, for the triplet, the second oscillation is almost complete. At $b \approx 3.7$ the results for the triplet state obtained by the two bases no longer agree, whereas for the singlet they still remain in accordance. Besides the oscillatory comportment, present in $J_{\text{norm}}$ and also here, we observe another interesting aspect as well. In figure 3 one has the extremes of $J_{\text{norm}}$, its minima and maxima, occurring approximately at $b = 0.75, 1.8, 2.6, 3.7$ if one follows the curve of the 55f result. By observing figure 4 one can see that, at the vicinity of these
Figure 5. Contour map of $\rho(x_1, x_2)$—the spatial distribution of the two electrons along the $x$-axis—for the singlet and triplet states. The left panels (a)–(f) correspond to the singlet state and the right ones (g)–(l) to triplet. The confinement conditions are the same as figure 3 and correspond to a quasi-2D QD. From top (a) and (g) to bottom (f) and (l) $b = 0, 1.11, 1.48, 2.59, 3.70, 5.92$, respectively.
values of $h$, the curves of $\sigma_z$ for the singlet and triplet states cross. At first we expected to see a correlation between the points where $J_{\text{norm}} = 0$ and the ones of the crossing of $\sigma_z$ for the singlet and triplet. However, if there is any type of correlation, it seems to be with $dJ_{\text{norm}}/dh = 0$. This is an issue to be addressed in a future work.

Now, let us analyze the behavior of $\rho(x_1, x_2)$. In figure 5 are displayed the contour maps of $\rho(x_1, x_2)$ for the singlet and triplet states under different values of the magnetic field; the confinement strength conditions are the same of figure 3, i.e. $\omega_z = 1.11$ and $\omega_x = \omega_y = 0.000111$. The contours are plotted in the phase-space $x_1 \times x_2$ that corresponds to the positions of electron 1 and 2, respectively, along the $x$-axis; since the electrons are indistinguishable, one finds a reflection symmetry with respect to the diagonal line $x_2 = x_1$ corresponding to the exchange of the electrons.

The situation depicted by panel (a) shows that the electrons, in the singlet state for $b = 0$, are spread throughout the phase-space, being more concentrated along the line $x_2 = -x_1$ and its surroundings, mainly in the interval $x \in (-200, 200)$. On the other hand, the panel (g) shows the electrons in the triplet state for $b = 0$ concentrated at $x = \pm 300$. From these two figures, one would expect that the interaction energy $1/(\kappa|\vec{r}_1 - \vec{r}_2|)$ between the two electrons would make the singlet energy higher than that of the triplet, leading to $J < 0$. However, figure 3 shows us the opposite; we must remember that the distributions along the other directions, in particular the $y$-direction—since it is a quasi-2D system—, have also to be considered and, in the present case, they are responsible to make $J > 0$, as shown in figure 3. The objective of figure 5 is indeed to give an idea of how the magnetic field affects the spatial distribution of the electrons.

Now, going ahead on the other panels of figure 5, we observe that for $b = 1.11$ the singlet (panel (b)) has concentrated at $x \approx \pm 250$, whereas the triplet (panel (h)) has their peaks moved from $x = \pm 300$ to $x \approx \pm 175$. For $b = 1.48$ one finds the singlet (panel (c)) and the triplet (panel (i)) with their peaks approximately at the same position, $x \approx \pm 250$ and $x \approx \pm 175$, respectively. However, their electron distributions become narrower; one can see this from the scale displayed on the right of the panels, where the top values in both cases are larger. For $b = 2.59$ the singlet distribution has its peak moved backward from $x \approx \pm 250$ to $x \approx \pm 175$ (panel (d)) and the triplet has its peak distribution moved forward from $x \approx 175$ to $x \approx 225$ (panel (j)). For $b = 3.70$ the singlet peak distribution has gone back from $x \approx \pm 175$ to $x \approx \pm 225$ (panel (e)) and the triplet one has gone further from $x \approx \pm 225$ into $x \approx \pm 250$ (panel (k)). Finally in the last two panels, (f) and (l), corresponding to $b = 5.92$, one can see the singlet peak approximately at the same position, $x \approx \pm 225$ and the triplet peak backward at $x \approx \pm 200$. Therefore, there is a back and forth movement around $x \approx \pm 200$ of the electron distributions in the singlet and triplet states as the magnetic field increases, and this movement is accompanied by a narrowing of the distribution. Observe that these movements of both distributions are not synchronized, leading to a complicated oscillatory behavior of physical quantities, such as $J_{\text{norm}}$, as a function of the magnetic field.

4. Conclusions

In this paper we have studied a two-electron QD in the presence of a magnetic field. Our focus was the properties of the singlet and triplet lowest states, such as their energy, the exchange coupling, etc. We have analyzed their behavior as a function of the magnetic field intensity under two different confinement conditions. In one case we have considered a 3D isotropic confinement potential and the other, a quasi-2D one. In both cases the potential was parabolic along the three axes, but in the latter the strength along the $z$-direction was taken much greater than in the other two directions. Our analysis relied on numerical results obtained by using the full-CI method with Cartesian anisotropic Gaussian-type orbitals as the basis set. The confidence of the results has been discussed in terms of the convergence of the results as a function of the size of the basis set. In addition, we have reported an oscillatory motion of the physical quantities as a function of the magnetic field. This motion obtained from our computation resembles a phenomenon found in the literature known as the dHvA effect. What is quite amazing in this fact is that a semiconductor QD, with more than one electron, seems to satisfy the condition of having its inner electrons partially free, or partially confined, as predicted by de Haas and van Alphen 90 years ago. The understanding of the physics behind the interplay of a confinement potential together with the Coulomb interaction and the quantum requirements fulfilled by the electrons in the presence of a magnetic field is a challenging task; we believe that QDs with more than one electron is a promising system to help to achieve it.

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Appendix A. Angular momentum integrals

The angular momentum integral is given by

$$I_{\mu\nu}^{LZ} = \int_{-\infty}^{\infty} d\vec{r} g_\rho(\vec{r}, \vec{\eta}) \left[ -i \left( -\frac{\partial}{\partial \eta} - \frac{\partial}{\partial \zeta} \right) \right] g_\nu(\vec{r}, \vec{\eta}) .$$

Defining the overlap integral $S_\alpha(n_x, m_x)$ as

$$S_\alpha(n_x, m_x) = \int_{-\infty}^{\infty} d\xi e^{i(n_x + m_x)\xi} e^{-(\zeta + \eta)\xi^2} ,$$

(A.1)

and similarly for $S_\alpha(n_y, m_y) e S_\alpha(n_z, m_z)$, we obtain

$$I_{\mu\nu}^{LZ} = -i S_\alpha(n_y, m_y) \left[ I_\alpha^{LZ}(n_x, m_x) \right] \left[ -2\zeta S_\alpha(n_x + 1, m_x) - 2\eta S_\alpha(n_x, m_x) + m_x S_\alpha(n_x, m_x - 1) \right] - I_\alpha^{LZ}(n_y, m_y) \left[ -2\zeta S_\alpha(n_z + 1, m_z) + m_z S_\alpha(n_z, m_z - 1) \right] - I_\alpha^{LZ}(n_z, m_z) \left[ -2\zeta S_\alpha(n_z + 1, m_z) + m_z S_\alpha(n_z, m_z - 1) \right]$$
\[-2\eta_x S_x (n_x, m_x + 1) + n_x S_x (n_x - 1, m_x) + m_x S_x (n_x, m_x - 1)\]  
which shows that our result depends solely upon the overlap integrals whose values are known (see reference [35]) and similarly for \(I_y^p\).

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