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Two-electron states in symmetric and asymmetric double quantum dots in a magnetic field

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Abstract. We studied, theoretically, the two-electron energy levels for double quantum dots, both symmetric and asymmetric, in the presence of a homogeneous magnetic field. Within the effective-mass approach, we expanded the two-electron wave function, in an orthogonal basis formed by the products of each electron wave function in growth direction z , and one-particle solutions of the magnetic Hamiltonian in the x - y plane. We applied our method to the case of $\text{Al}_x\text{Ga}_{1-x}\text{As}$, for which we showed how the wave functions vary, and how the basis functions are mixed in a nontrivial way by the effect of the Coulomb potential.

1. Introduction

In double quantum dots [1] each electron wave function can be localized either in the same dot, or in different dots, or in both. In the presence of the Coulomb interaction each electron repels each other, minimizing the total energy of the system. Coupled quantum dots with a small number of electrons [2, 3] are excellent candidate subjects for studying the Coulomb blockade effect [4–8] and tunnelling between quantum dots.

In 1993 Bryant [9] studied the energy spectra, charge densities, and correlation functions for interacting two-electron systems in coupled dots as functions of the applied bias. Bryant was interested in charging energies and Coulomb blockade effects in systems with a small number of electrons, and considered the external barriers to be infinite, and no magnetic field. Bryant reduced the six-dimensional Coulomb integral to a three-dimensional integral that was solved numerically. The Coulomb matrix elements were only calculated at zero applied bias to reduce the computer time required for these calculations by several orders of magnitude.

In 1996 Oh *et al* [10] studied the electronic structure in coupled quantum dots with one or two electrons in magnetic fields. They were interested in the spin transitions of the ground state and the optical transitions between the energy levels. They studied a symmetric system of two coupled quantum dots as a function of the magnetic field with no external electric field.

Recently, Kaputkina and Lozovik [11] studied the energy spectra for interacting two-electron systems in horizontal and vertical coupled quantum dots as functions of quantum dot separation, lateral confinement, and magnetic field. They considered each dot as a strictly two-dimensional system.

In this work, we studied the two-electron energy levels in symmetric and asymmetric vertical double quantum dots in the presence of a magnetic field, as a function of the inter-dot barrier and vertical dot widths, the magnetic field strength, and the lateral dot confinement. Within the effective-mass approach we expanded the two-electron wave function

in an orthogonal basis formed by products of the individual electron wave functions in the growth direction z , and one-particle solutions of the magnetic Hamiltonian in the x - y plane. The Coulomb potential between electrons produces off-diagonal terms by mixing our basis states. The resulting six-dimensional Coulomb integral was reduced analytically to a one-dimensional integral; this was done numerically. We obtained the energies and wave functions by diagonalizing the two-electron Hamiltonian in a truncated basis. Our basis set is orthogonal, and we do not use a variational method. We applied our method to study the first eight two-electron states in GaAs-Al_xGa_{1-x}As heterostructures, using barrier heights given by the band-gap discontinuity.

A recent discussion of the most commonly used methods of calculation for the electronic states in quantum dots can be found in reference [12].

2. Formalism

The effective-mass Hamiltonian for two electrons in a double quantum dot, in the presence of a magnetic field B pointing along z , can be written as

$$H = H_1^{xy} + H_2^{xy} + H_1^z(z_1) + H_2^z(z_2) + V_{\text{coul}}(r, |z_1 - z_2|). \quad (1)$$

H_1^{xy} and H_2^{xy} are the x - y Hamiltonians for electrons 1 and 2 in a parabolic potential,

$$H_i^{xy} = \frac{(\mathbf{p}_i - q\mathbf{A}_i)^2}{2m} + \frac{1}{2}m\omega_0^2 r_i^2. \quad (2)$$

$H_1^z(z_1)$ and $H_2^z(z_2)$ are the one-dimensional Hamiltonians for electrons,

$$H_i^z(z_i) = p_{z,i}^2/2m + V_e(z_i). \quad (3)$$

$V_e(z_1)$ and $V_e(z_2)$ are the potentials that define the confinement for electrons in the five regions of z , shown in figure 1. $V_{\text{coul}}(r, |z_1 - z_2|)$ is the Coulomb potential between electrons, including an effective dielectric constant for the system.

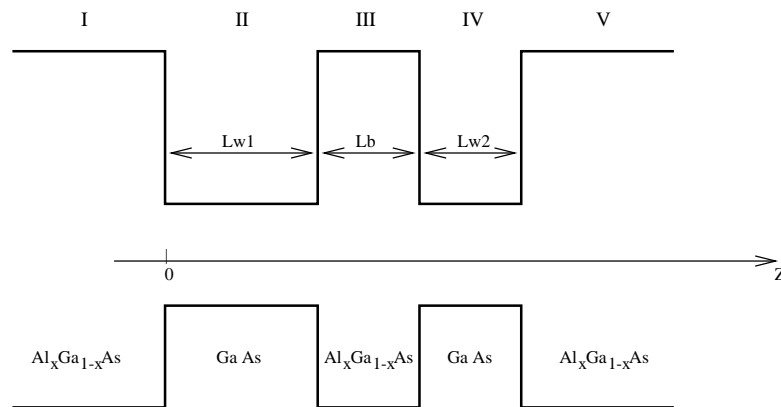


Figure 1. The potential profile in the z -direction for electrons.

Transforming the in-plane coordinates r_1 and r_2 for each electron towards relative coordinates r and centre-of-mass coordinates R , the Hamiltonian (1) transforms to

$$H = \frac{P^2}{2M} + \frac{e^2 B^2}{2M} R^2 + \frac{M\omega_0^2}{2} R^2 + \frac{eB}{M} L_z + \frac{p^2}{2\mu} + \frac{\mu}{8} (\omega_c^2 + 4\omega_0^2) r^2 + \frac{\omega_c}{2} L_z + H_1(z_1) + H_2(z_2) + V_{\text{coul}}(r, |z_1 - z_2|) \quad (4)$$

where p and P are the momentum operators for the coordinates r and R respectively, μ is the reduced mass ($m/2$), M is the total mass ($2m$), ω_c is the cyclotronic frequency (eB/m), ω_0 is a frequency characterizing the quantum dot confinement in the plane x - y , L_z is the angular momentum operator in relative coordinates, and L_z is the angular momentum operator in centre-of-mass coordinates.

The first line of (4) represents a two-dimensional harmonic oscillator, and involves only centre-of-mass coordinates which are not coupled to the others terms, and so can be solved separately. We expanded the solution of the other terms in the Hamiltonian (4), as a linear combination of products of eigenfunctions of the magnetic Hamiltonian in the x - y plane (the second line of (4)), and eigenfunctions of the electron Hamiltonians in the z -direction ($H_1(z_1)$ and $H_2(z_2)$):

$$\Psi_n^{\text{exc}} = \sum_{v_r, v_{e1}, v_{e2}} C_{v_r, v_{e1}, v_{e2}}^n \psi_{v_r}(r, \phi) \psi_{v_{e1}}(z_1) \psi_{v_{e2}}(z_2) \quad (5)$$

in which, in the symmetric gauge,

$$\psi_{v_r, l} = \frac{1}{2\pi} \left(\frac{2(n-l/2 - |l|/2) g_B^{|l|+1}}{(|l|/2 + n - l/2)!} \right)^{1/2} e^{il\phi} \left(\frac{r}{i} \right)^{|l|} e^{-g_B r^2/2} L_{n-l/2-|l|/2}^{|l|}(g_B r^2) \quad (6)$$

where

$$g_B = m\omega/2\hbar \quad \omega = \sqrt{\omega_c^2 + 4\omega_0^2}.$$

The electron wave functions defined in the five regions of z , shown in figure 1, are given by

$$\psi_{v_e}(z_e) = \begin{cases} a_1 e^{k_1(z_e - z_1)} \\ a_2 \cos(k_2(z_e - z_1)) + a_3 \sin(k_2(z_e - z_1)) \\ a_4 e^{k_3(z_e - z_2)} + a_5 e^{-k_3(z_e - z_2)} \\ a_6 \cos(k_4(z_e - z_3)) + a_7 \sin(k_4(z_e - z_3)) \\ a_8 e^{-k_5(z_e - z_4)}. \end{cases} \quad (7)$$

The Coulomb interaction produces off-diagonal terms by mixing our basis states. In order to obtain the system of equations for the coefficients in expansion (5), we need to evaluate the Coulomb integral

$$\int d\phi dr dz_1 dz_2 \psi_{v_r}^* \psi_{v_{e1}} \psi_{v_{e2}} V_{\text{coul}}(r, |z_{e1} - z_{e2}|) \psi_{v_r} \psi_{v_{e1}} \psi_{v_{e2}}. \quad (8)$$

The ϕ -integral is trivial, because of l_z -conservation. Using the explicit expansion for the Laguerre polynomials (L_n) in ψ_{v_r} and ψ_{v_r} (equation (6)), the remaining of integral (8) can be written as a sum of terms of the form

$$\int dz_1 dz_2 \psi_{v_{e1}} \psi_{v_{e2}} \psi_{v_{e1}} \psi_{v_{e2}} \int_0^\infty r dr \frac{r^{2w} e^{-g_B r^2}}{\sqrt{r^2 + (z_1 - z_2)^2}} \quad (9)$$

where w is an integer. On using

$$\frac{1}{\sqrt{r^2 + (z_1 - z_2)^2}} = \int_0^\infty J_0(r\alpha) e^{-|z_1 - z_2|\alpha} d\alpha \quad (10)$$

and after solving the r -integral, this yields

$$\int_0^\infty d\alpha \left(\frac{\alpha^2}{4g_B} \right)^m \exp\left(\frac{-\alpha^2}{4g_B} \right) \int dz_1 dz_2 \psi_{v'e_1} \psi_{v'e_2} e^{-|z_1 - z_2|\alpha} \psi_{v_e1} \psi_{v_e2}. \quad (11)$$

The z_1 - and z_2 -integrals can be solved analytically. The evaluation of these integrals is cumbersome due to the large number of terms resulting from the five different regions of the potential. The z_1 - and z_2 -integrals contain both decoupled terms in which the z_1 - and z_2 -integrals are independent of each other and coupled terms where the integration limits of the z_2 -integral contain z_1 . The remaining α -integral must be calculated numerically.

Diagonalizing the system of equations resulting for the coefficients in expansion (5), in a truncated basis, we obtained the energies and wave functions for the two-electron states.

3. Results

We calculated the two-electron energy levels for symmetric and asymmetric GaAs double quantum dots, coupled by $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers ($x = 0.3$). The band gap used in our calculations is given by $E_g(x) = 1.52 + 1.36x + 0.22x^2$. The band-gap offset considered was 60% for the conduction band and 40% for the valence band. We used the same electronic mass for all five regions in the double quantum dot. We used an electron mass $m = 0.067m_e$, and a dielectric constant $\epsilon = 12.5\epsilon_0$. In our calculations we used a truncated basis set composed of twelve Landau-like wave functions, and four wave functions for each electron.

3.1. Energies as a function of well and barrier widths

In this section we present our results for the two-electron energy levels in double quantum dots as a function of well and barrier widths, ranging from zero to large values, in a 10 T magnetic field, and for lateral confinement $\hbar\omega_0 = 4$ meV.

Figure 2 shows the first eight energy levels for a symmetrically coupled double quantum dot, where both dots have widths of 100 Å in the z -direction, and the middle barrier ranges from 0 to 50 Å. For zero barrier width, our basis states $\psi_v(z)$ given by equation (7) correspond to the states for a single 200 Å quantum well. For nonzero barrier, the energies for the first two basis states approach each other. For wide barriers these states approach a single energy value that corresponds to the first level for each independent 100 Å well. This behaviour for the first two basis states (7) for each electron explains the general behaviour for the first set of states in this figure as follows: the first basis state for each electron combines forming the ground two-electron state **11**; the first basis state for one electron combines with the second basis state for the second electron forming the states **12** – **21** and **12** + **21**, which in the absence of Coulomb interaction have the same energy as seen in figure 2 (left); finally the second basis states for each electron combine forming the state **22**. The second more energetic set of states, which can clearly be distinguished from the first set of states for barriers greater than 15 Å, corresponds to Landau-like states for the states in the first set, and originates from the lateral dot confinement and magnetic confinement. For 10 Å barriers the energy for the **22** state approaches the energy for the first Landau-like state **11**, causing an interaction between these states as clearly seen in figure 2 (right). The big Coulomb interaction between these two levels is caused by the strong overlap for the two-electron wave functions for these states. For wide

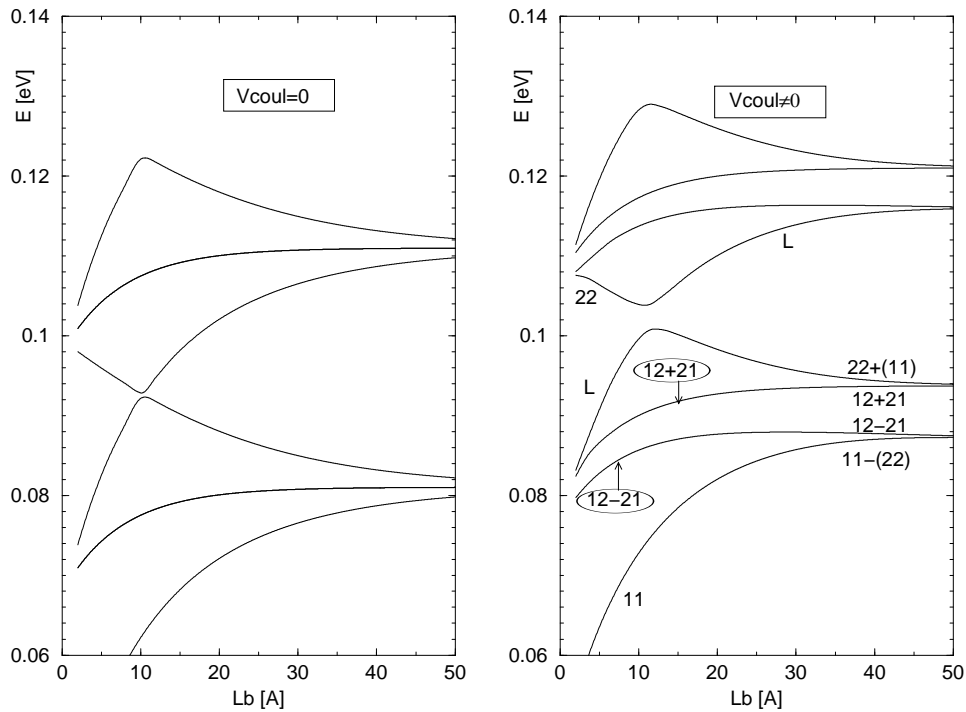


Figure 2. Two-electron ($l = 0$) energy levels for a symmetric double quantum dot as a function of the barrier width, for dots of 100 \AA , with $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$. Numbers close to some curves show the main composition for the two-electron wave function, in terms of DQW basis states. Numbers enclosed in parentheses indicate a small contribution from these states to the total wave function.

barriers the basis states are better approximated as basis states for the left well (**L**) and for the right well (**R**). For wide barriers our state **11** approach the state **11 – 22** (which in terms of **L** and **R** states can be expressed as **LR + RL**), our state **12 – 21** (or **LR – RL**) gets close to the **11 – 22** state, and the state **12 + 21** (or **LL – RR**) approaches the same energy as the state **22 + 11** (or **LL + RR**).

Figure 3 shows the first eight energy levels for an asymmetrically coupled double quantum dot, where the inter-dot barrier has a width of 25 \AA , the right dot has a width of 100 \AA , and the left dot width ranges from 0 to 100 \AA . The figure on the left shows the two-electron energies obtained without considering the Coulomb interaction between electrons. The figure on the right takes into account the Coulomb interaction, which has the effect of shifting the energies towards higher values and removing some degeneracy. The **11** state corresponds to both electrons being localized in the right (wider) dot, and it is almost uninfluenced by the changes in the left dot size. This state lowers its energy when the size of the left dot approaches that of the right dot, because in this symmetric situation each electron wave function in our basis is spread over both two dots. The **12 – 21** and **12 + 21** states (which have the same energy in the absence of the Coulomb interaction) are strongly influenced by changing the width of the left dot. This behaviour originates from the energy dependency of the second basis state **2** (which is localized in the left dot) on the dot width. The **22** state corresponds to both electrons being localized in the left (varying) dot; the energy of this state is much more influenced by varying the left dot width, because both of the constituent basis states are mainly

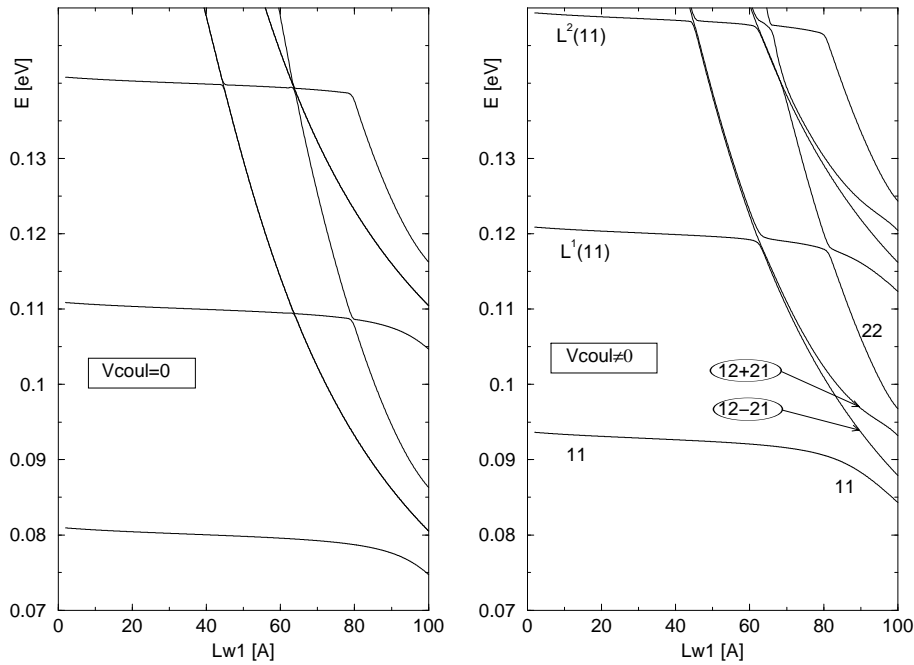


Figure 3. Two-electron ($l = 0$) energy levels for an asymmetric double quantum dot as a function of the left dot width, for a barrier of 25 \AA , a right dot width of 100 \AA , $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$.

localized in this dot. In this figure there are several regions where the energy of a Landau-like state gets close to those of other states, causing an interaction between these states. The small Coulomb interaction between these levels is caused by the small overlap for the two-electron wave functions for these states.

Figure 4 shows the first eight energy levels for a symmetrically coupled double quantum dot, where the inter-dot barrier has a width of 25 \AA and the left and right dot widths are varied simultaneously from 0 to 100 \AA . The figure on the left shows the two-electron energies obtained without considering the Coulomb interaction between electrons. Because the energies depend so strongly on dot widths, we subtracted the energy from the first state obtained without Coulomb interaction shown in the inset of the figure on the left. The figure on the right takes into account the Coulomb interaction. The composition of the states in terms of the constituent basis states is similar to those in previous cases. The maxima present for some states, for dot widths near 15 \AA , can be explained by noting that when the second basis-state energy is close to the higher permissible energy in the finite double quantum well (caused by the confinement in the z -direction), this state does not change its energy at the same rate as the first state does when the dot width decreases.

Figure 5 shows the first eight energy levels for a symmetrically coupled double quantum dot, where the inter-dot barrier has a width of 25 \AA , and the left and right dot widths are varied simultaneously from 0 to 100 \AA . This figure shows the energy levels for two-electron states with angular momentum $l = 1$. In this figure we subtracted the energy from the first state obtained without considering Coulomb interaction shown in the inset of the figure on the left. The behaviour of the energy levels is similar to that in the previous case for $l = 0$, but here the energies are higher as can be seen clearly in the inset.

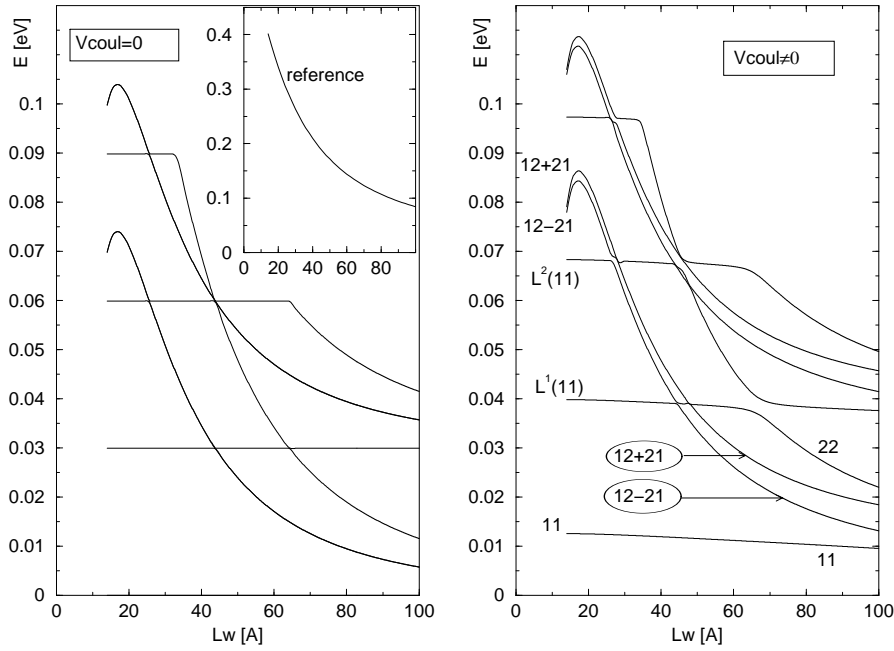


Figure 4. Two-electron ($l = 0$) energy levels for a symmetric double quantum dot as a function of dot width, for a barrier of 25 \AA , $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$. We subtracted the energy from the first state obtained without considering Coulomb interaction shown in the inset of the figure on the left.

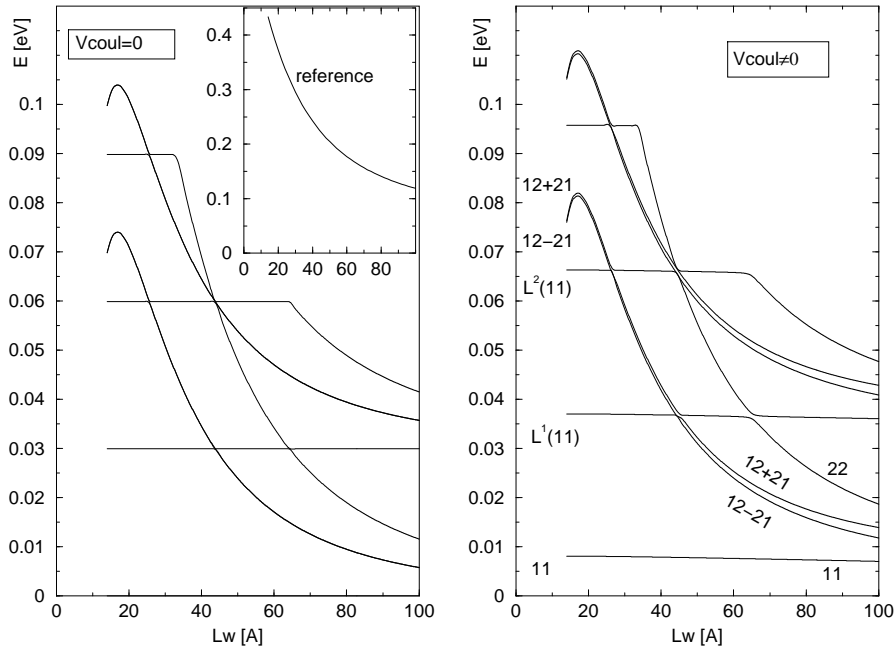


Figure 5. Two-electron energy levels, with angular momentum $l = 1$, for a symmetric double quantum dot as a function of dot width, for a barrier of 25 \AA , $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$. We subtracted the energy from the first state obtained without considering Coulomb interaction shown in the inset of the figure on the left.

3.2. Energies as a function of magnetic field and dot confinement

Increasing the magnetic field in a symmetric or asymmetric double quantum dot produces a shift in the two-electron energy levels towards higher energies and an increase in the interaction energy. The increase in the energy of interaction between electrons is a consequence of two effects. First, the wave-function confinement in the x - y plane produces a stronger interaction in the z -axis, as the electron wave functions penetrate into the barrier. Second, the repulsion between electrons in the plane increases, because their wave functions are confined to a smaller region.

The large interaction between electrons obtained when increasing the applied magnetic field is similar to the effect of a change in the barrier and dot widths. This can be used to study these systems in regions of interest, without the need for the growth of many different samples.

Figure 6 shows the magnetic field effects on the two-electron energy levels for an asymmetric double quantum dot, where the inter-dot barrier has a width of 25 \AA , the right dot has a width of 100 \AA , the left dot has a width of 80 \AA , and the lateral confinement corresponds to $\hbar\omega_0 = 4 \text{ meV}$. The figure on the left shows the two-electron energies obtained without considering the Coulomb interaction between electrons. The figure on the right takes into account the Coulomb interaction. The first set of two-electron states corresponds to states defined by the confinement in the z -direction. The second more energetic set of states, which can be clearly distinguished from the first set of states for magnetic fields greater than 12 T , corresponds to Landau-like states for the states in the first set. The bigger slope for the **11** and **22** state when the Coulomb interaction is included is caused by the stronger interaction between electrons localized in the same dot when the in-plane localization increases. The

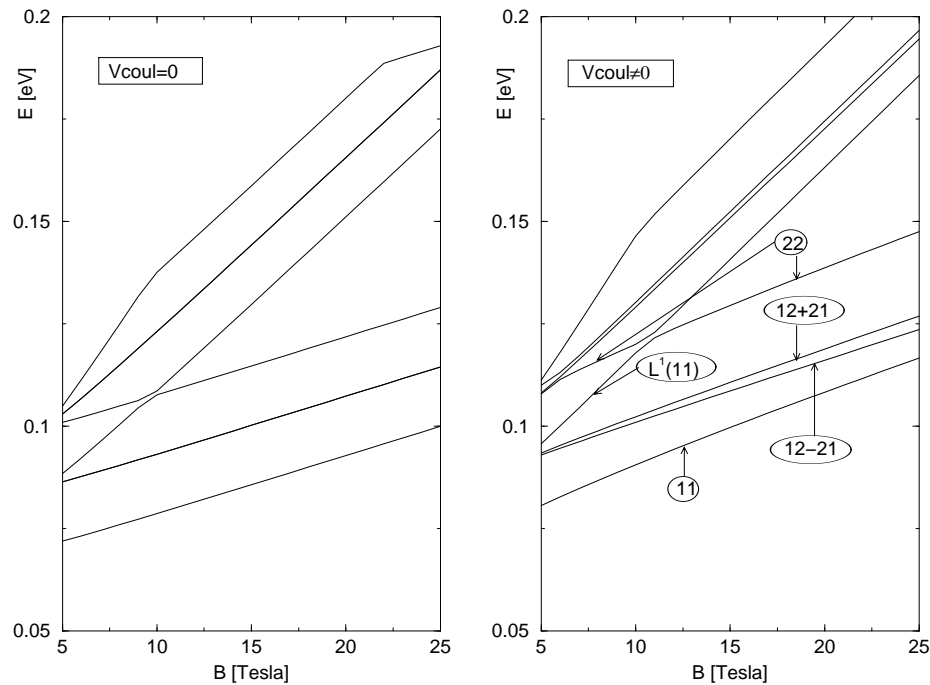


Figure 6. Two-electron ($l = 0$) energy levels for an asymmetric double quantum dot as a function of the external magnetic field, for a left dot width of 80 \AA , a right dot width of 100 \AA , a barrier of 25 \AA , and $\hbar\omega_0 = 4 \text{ meV}$.

slope for the $12 - 21$ and $12 + 21$ states is a consequence of the different dot localization for the electrons involved in these states.

Figure 7 shows the lateral dot confinement effects on the two-electron energy levels for a symmetric double quantum dot in a 10 T magnetic field, where the inter-dot barrier has a width of 25 Å, and the right and left dot each have a width of 100 Å. The figure on the left shows the two-electron energies obtained without considering the Coulomb interaction between electrons. The figure on the right takes into account the Coulomb interaction, which has the effect of shifting the energies towards higher values and removing the degeneracy in the $12 - 21$ and $12 + 21$ states. It is clear from this figure that for a lateral dot confinement ($\hbar\omega_0$) below 4 meV the effective confinement is dominated by the magnetic confinement, and that for confinement over 4 meV it is dominated by the lateral geometrical confinement. The first set of two-electron states corresponds to states defined by the confinement in the z -direction. The second more energetic set of states, corresponds to Landau-like states for the states in the first set.

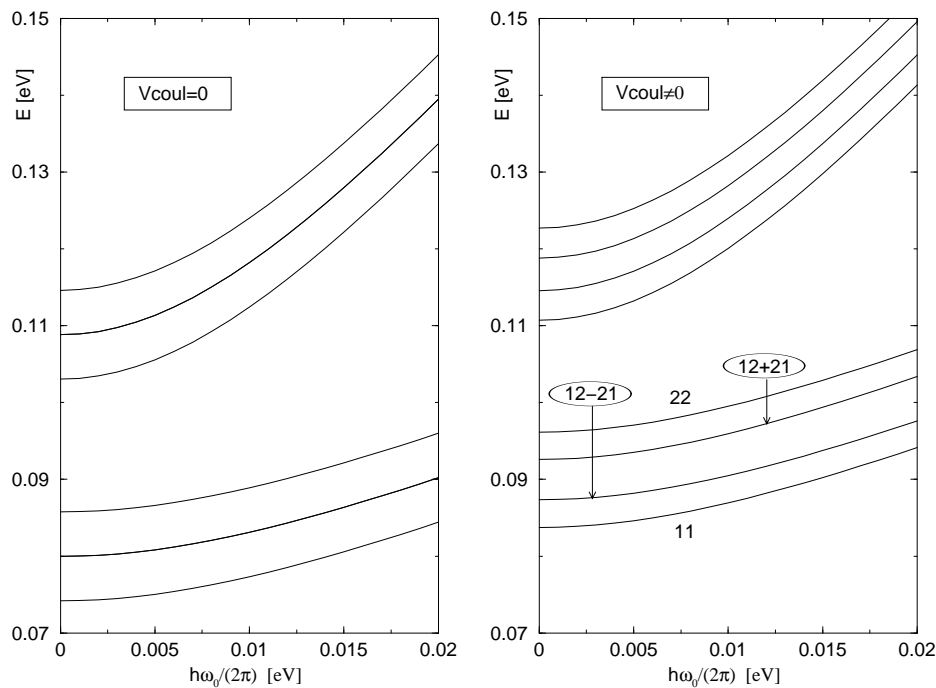


Figure 7. Two-electron ($l = 0$) energy levels for a symmetric double quantum dot as a function of the lateral confinement ($\hbar\omega_0$), for dots of width 100 Å, a barrier of 25 Å, and $B = 10$ T.

3.3. Coulomb energies for different well widths

Using our previous results for two-electron energies in different double-quantum-dot geometries, it is possible to construct for each state the difference between the energies obtained considering and without taking into account the Coulomb interaction. Plotting this energy difference as a function of well width shows the evolution in the Coulomb energy for each state and the transitions between different states.

Figure 8 shows the Coulomb energy as a function of the left dot width for an asymmetric double quantum dot, where the inter-dot barrier has a width of 25 Å, the right dot has a width

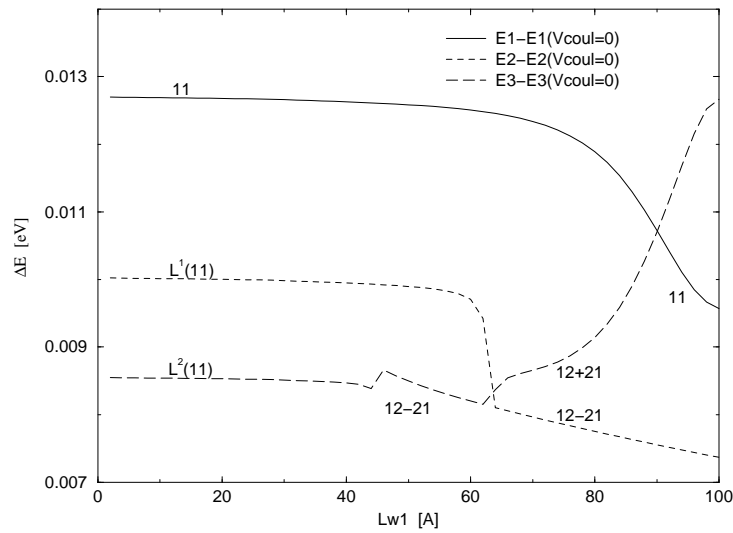


Figure 8. Coulomb energies for the first three two-electron states with $l = 0$, for an asymmetric double quantum dot as a function of the left dot width, for a right dot width of 100 \AA , a barrier of 25 \AA , $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$.

of 100 \AA , in a 10 T magnetic field, and the lateral confinement corresponds to $\hbar\omega_0 = 4 \text{ meV}$. In the **11** ground state, both constituent electrons are mainly localized in the right (wider) dot. Because both electrons are localized in the same dot, there is a strong Coulomb interaction almost independent of the left dot size. When the width of the left dot approaches that for the symmetric situation where both dots have a width of 100 \AA , the first basis state for each electron spreads over the two dots. This delocalization in the basis states produces a decreasing Coulomb interaction for the **11** state when the left dot width reaches the symmetric configuration. The second state goes towards the symmetric situation, transforming from a Landau-like state of the **11** state towards the **12 – 21** state. The third state goes towards the symmetric situation, first transforming from a Landau-like state of the **11** state towards the **12 – 21** state, and then transforming towards the **12 + 21** state. The big differences between the Coulomb energies for the **12 + 21** state and the **12 – 21** state can be understood by writing these states in terms of left dot states (**L**) and right dot states (**R**). Although the barrier width it is not too wide, the **12 – 21** state behaves mainly as a **RL – LR** state, and the **12 + 21** state behaves as a **LL – RR** state. This makes it clear that in the **12 – 21** state each electron is mainly localized in a different dot, and in the **12 + 21** state each electron is mainly localized in the same dot.

Figure 9 shows the Coulomb energy as a function of dot width for a symmetric double quantum dot, where the inter-dot barrier has a width of 25 \AA , the left and right dot widths are varied simultaneously from 0 to 100 \AA , in a 10 T magnetic field, and the lateral confinement corresponds to $\hbar\omega_0 = 4 \text{ meV}$. Symmetry forces all our basis states to be equally localized in each dot. With increasing dot widths, our basis states get more delocalized over the two dots. This delocalization in the basis states produces a decreasing Coulomb interaction for all the two-electron states with increasing dot width, provided that these states do not change constitution in terms of basis states. This is exactly what happens for the **11** ground state. The second state goes towards the wider-dot situation, transforming from a Landau-like state of the **11** state towards the **12 – 21** state. The third state goes towards the wider-dot situation,

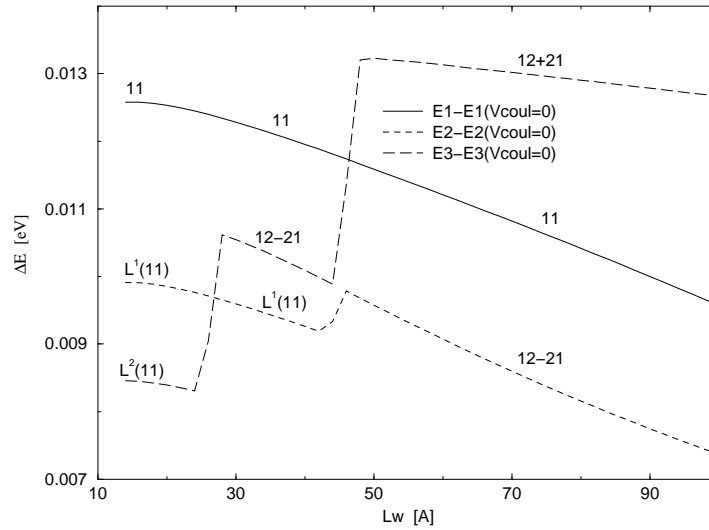


Figure 9. Coulomb energies for the first three two-electron states with $l = 0$, for a symmetric double quantum dot as a function of dot width, for a barrier of 25 \AA , $B = 10 \text{ T}$, and $\hbar\omega_0 = 4 \text{ meV}$.

first transforming from a Landau-like state of the **11** state towards the **12 – 21** state, and then transforming towards the **12 + 21** state. The big differences in the Coulomb energies for the **12 + 21** state and the **12 – 21** state can be explained again by the fact that in the **12 – 21** state each electron is mainly localized in a different dot, and in the **12 + 21** state each electron is mainly localized in the same dot.

4. Conclusions

In this work we studied the energies and wave functions for several two-electron states in double quantum dots, in a magnetic field pointing in the growth direction z . We calculated the energy for symmetric and asymmetric double quantum dots as a function of barrier width, dot (or dots) widths, magnetic field, and lateral dot confinement.

There are some regions of parameters where the mixing of lateral states and vertical states is very strong. In these regions, the widely used approximation of decoupling the lateral and vertical components is not valid.

In our method of calculation we used an orthogonal basis that involves functions of single-particle solutions of the double quantum well in the z -direction, which makes our method appropriate for small-to-medium barrier widths.

In our results we do not include the effect of considering the presence of spin. This effect can be readily included by the addition of a term of the form $g^* \mu_B \vec{B} \cdot \vec{S}/\hbar$, and taking into account the symmetry for the two-electron wave function under interchange of particles. This term can be responsible for transitions of states with angular momentum $l = 1$ towards the ground state [13–16] (this effect appears for wider barriers than those considered in this work, as shown in reference [10]).

All the energies presented in our results were obtained without considering the centre-of-mass energy; if total energies are needed, the energy corresponding to first line of (4) must be added.

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