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# Magnetic field influence on spectrum rearrangement and spin transformation of coupled quantum dots

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## Abstract

Two-electron systems consisting of two laterally or vertically coupled quantum dots (QDs) are considered. Their behaviour in external magnetic field is studied. Ground state energies and energy spectra were obtained taking into account interelectron interaction for a wide range of values of confining potential steepness ( $\alpha$ ), distance between QDs ( $d$ ), and external magnetic field ( $B$ ). The spontaneous magnetization and the singlet–triplet transformation of the QD molecule ground state controlled by the magnetic field are studied.

## 1. Introduction

Quantum dots (QDs), QD molecules and QD arrays are very interesting low-dimensional objects with high potential of applications in opto- and nanoelectronics, and as model objects for basic studies [1–5].

The modern progress of nanotechnology gives the possibility to produce QDs with controllable parameters, such as the form and steepness of the confining potential, the number of charge carriers, and characteristic size of their localization region. The form of the confining potential is determined by the method employed to prepare the QDs. The hard-wall and parabolic confining potentials are used most frequently. The lateral parabolic-potential model was supported by self-consistent calculations and is applicable to QDs obtained by various methods. Thus, if a single QD is an analogue of an atom (a quantum mechanical analogue of the Thomson atom), then several closely spaced, interacting QDs may be regarded as an artificial giant molecule.

We discuss closely spaced QDs representing giant analogues of molecules (we shall call them horizontal QD molecules) and systems with spatially separated carriers in vertically coupled QDs, and in coupled and double QDs (we call such a system a vertical QD molecule).

Spin states as well as Coulomb interaction between electrons in coupled QD [4, 5] can be used for quantum computation. As a rule, spin states have substantially greater decoherence

times in comparison with other states [6–8]. This is important for quantum calculations and more generally for spintronics.

In this connection we discuss the dependence of the spectra and spin transformation of the QD molecule ground state on all control parameters of the system. The control parameters are the confining potential steepness, interdot distance and tunnel barrier (depending on the interdot distance, etc). The magnetic field influence on these systems is also investigated. We analyse the possibility to control the system by a normal and also a parallel magnetic field, transforming strongly coupled quantum dots with common charge carriers to separate QDs.

We study the possibility of controlling spin states for coupled quantum dots by the external magnetic field as well as by the steepness of the confining potential. The last can be changed by the gate voltage and by a parallel magnetic field. We have analysed the *singlet–triplet transition in coupled quantum dots in the absence of magnetic field* controlled by interdot coupling. (The last is connected with confining the potential steepness dependent gate voltage and interdot distance.) This transition can be controlled by a normal and a parallel magnetic field.

## 2. Horizontal QD molecule

We consider the system of two adjacent QDs taking into account interelectron interaction for a wide region of confining potential parameters, distances between QD centres, and magnetic fields.

We use the following scales for the length, energy and parameter of the confining potential:  $r_0 = \hbar^2 \varepsilon / (2m^* e^2)$ ,  $E_0 = 2m^* e^4 / (\hbar^2 \varepsilon^2)$ ,  $\alpha_0 = E_0 / r_0^2$ , where  $m^*$  is the effective electron mass,  $\varepsilon$  is the dielectric permeability,  $\alpha$  is the steepness confining potential parameter;  $r_0$  and  $E_0$  are the radius and binding energy of the two-dimensional exciton.

If the distance between QD centres  $d$  significantly exceeds the characteristic length  $r_{\text{char}}$  of the electron wavefunction ( $d > kr_{\text{char}}$ ,  $k \sim 3$ ), the QDs are separated and the Heitler–London approximation is applicable. When  $d < r_{\text{char}}$ , the QDs merge into a potential well of complicated form and the molecular orbital approximation is suitable. In the region  $d \sim r_{\text{char}}$  variational methods are optimal [5].

In the Heitler–London approximation we consider two electrons, with each of them confined in its potential well of the form  $U = \alpha r_i^2$ , ( $i = 1, 2$ ), (parabolic lateral potential), where  $r_1$  and  $r_2$  are measured from the closely lying well centres.

We next write the singlet-state wavefunction in the Heitler–London approximation

$$\Psi = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) + \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\xi_A(s_1, s_2) \quad (1)$$

where  $\xi_A(s_1, s_2)$  is an antisymmetric spin function, and  $\psi_a(\mathbf{r})$  and  $\psi_b(\mathbf{r})$  are the unperturbed wavefunctions of a single one-electron QD.

The triplet-state wavefunction in the Heitler–London approximation has the following form:

$$\Psi = A[\psi_a(\mathbf{r}_1)\psi_b(\mathbf{r}_2) - \psi_a(\mathbf{r}_2)\psi_b(\mathbf{r}_1)]\xi_S(s_1, s_2) \quad (2)$$

where  $\xi_S(s_1, s_2)$  is a symmetric spin function, and  $\psi_a(\mathbf{r})$  and  $\psi_b(\mathbf{r})$  are the unperturbed wavefunctions of a single one-electron QD.

The energy of the singlet state in the Heitler–London (HL) approximation is

$$W_{\text{sing}} = 4\sqrt{\alpha} + \frac{1}{(1 + e^{-\sqrt{\alpha}d^2})} (Q_k + J_k), \quad (3)$$

where

$$Q_k = \frac{\sqrt{\alpha}}{\pi} \int \int \frac{e^{-\sqrt{\alpha}(r_{1a}^2+r_{2b}^2)/2}}{r_{12}} d\tau_1 d\tau_2;$$

$$J_k = \frac{\sqrt{\alpha}}{\pi} \int \int \frac{e^{-\sqrt{\alpha}/2(r_{1a}^2+r_{2b}^2+r_{1b}^2+r_{2a}^2)/2}}{r_{12}} d\tau_1 d\tau_2 = \sqrt{(\pi/2)}\alpha^{1/4}e^{-\sqrt{\alpha}d^2}.$$

The integral  $Q_k$  is computed numerically.

The energy of the triplet state is

$$W_{\text{tripl}} = 4\sqrt{\alpha} + \frac{1}{(1 - e^{-\sqrt{\alpha}d^2})}(Q_k - J_k). \quad (4)$$

The triplet state becomes the ground state at the condition

$$\delta E_{\text{tripl}} - \delta E_{\text{singl}} = 2 \frac{Q_k e^{-\sqrt{\alpha}d^2} - J_k}{(1 - e^{-2\sqrt{\alpha}d^2})} < 0. \quad (5)$$

Thus *spontaneous magnetization, singlet–triplet transformation* is possible even in the absence of external magnetic field for some critical values of the control parameters—confining potential steepness, interdot distance and tunnel barrier characteristics.

A transverse magnetic field increases the effective confining potential steepness  $\beta^2 = \alpha + (\frac{\omega_c}{4})^2$  ( $\omega_c$  is the cyclotronic frequency) and therefore localizes the electrons and diminishes the overlap of electron wavefunctions and exchange interaction. The effective steepness of the confining potential  $\beta$  in a magnetic field and the distance between QD centres  $d$  are control parameters of the problem.

Two ‘merged’ QDs can be ‘separated’ by a magnetic field as well as by an increase of the distance between the centres.

With increase of the transverse magnetic field, the triplet state becomes the ground state of the QD system. There are two contributions connected with the magnetic field: (1) rise of the effective steepness of the confining potential leading to diminishing of the interdot coupling; (2) interaction of spins with the magnetic field.

Thus it is possible to control the spin state of a QD molecule by normal and parallel magnetic fields.

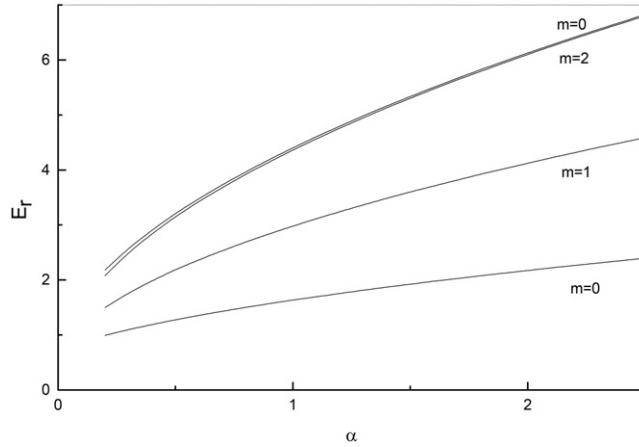
The energy  $W$  increases with  $\beta$  and is asymptotically proportional to  $\beta$  for large  $\beta$ . With increasing magnetic field the effective steepness of the confining potential grows and the exchange interaction goes to zero, and only direct Coulomb interaction survives.

The comparative interdot interaction contribution decreases with growth of the parameters  $\beta$  and  $d$ . For large values of  $\beta$  and  $d$ , the distance between QD centres is much greater than the region of electron localization. As a result the interdot interaction energy becomes only a small correction for isolated QD energy. For intermediate values of the parameters  $\beta$  and  $d$ , the interdot interaction contribution is essential.

When both the control parameters (the effective steepness  $\beta^2$  of the confining potential in the magnetic field and the distance  $d$  between QD centres) are sufficiently small, the Heitler–London approximation overestimates the ‘molecule’ ground state energy. In that case we use the molecular orbital method.

### 3. Vertical QD molecule

Another class of QD molecules is vertical molecules consisting of two vertically coupled (or double) two-dimensional QDs with two electrons, separated by a barrier layer. Each of the QDs can be described by a parabolic confining potential. Axial symmetry of the problem remains in this case even in the presence of a transverse magnetic field.



**Figure 1.** The dependences of the low-lying levels of the relative motion energy  $E_r$  versus confining potential steepness  $\alpha$  at interlayer distance  $d = 0.5$ . Values are scaled in arbitrary units (see section 2).

It is possible to separate the centre-of-mass motion and electron relative motion in the parabolic confining potential. The energy spectrum and wavefunctions corresponding to centre-of-mass motion can be obtained analytically (they are similar to those for a harmonic oscillator). The ground state energies in the absence of magnetic field in the HL approximation are equal to

$$W_{\text{tripl}} = W_{\text{sing}} = 4\sqrt{\alpha} + 2^{3/2}\pi^{1/2}\alpha^{1/4} \exp \sqrt{\alpha}d^2/2\text{erfc}(\alpha^{1/4}d/2^{1/2}). \quad (6)$$

The equation for relative motion  $E_r$  differs from that for the centre-of-mass motion in the inclusion of electron–electron interaction. The energy spectrum and wavefunctions corresponding to electron relative motion are obtained by numerical diagonalization of the total Hamiltonian on the one-particle basis. The eigenvalues of the energy are obtained from the equation

$$\det\{V_{nn'}^m + \delta_{n,n'}(\varepsilon_{nm} - E_r)\} = 0, \quad (7)$$

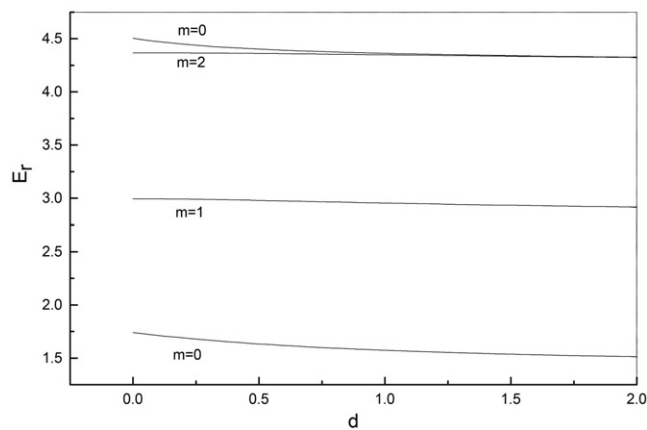
$$\varepsilon_{nm} = 4\sqrt{\alpha/2} \left( n + \frac{|m| + 1}{2} \right) \quad (8)$$

$$V_{nn'}^m = \left( \frac{n!n'}{(n + |m|)!(n' + |m|)!} \right)^{1/2} \sum_{i=0}^n \sum_{j=0}^{n'} \frac{(-1)^{i+j}}{i!j!} \binom{n + |m|}{n - i} \binom{n' + |m|}{n' - j} \\ \times (\alpha/2)^{(|m|+i+j+1)/2} \Gamma(i + j + |m| + 1) d^{2(i+j+|m|+1/2)} \\ \times \Psi(i + j + |m| + 1, i + j + |m| + 3/2; \sqrt{\alpha/2}d^2), \quad (9)$$

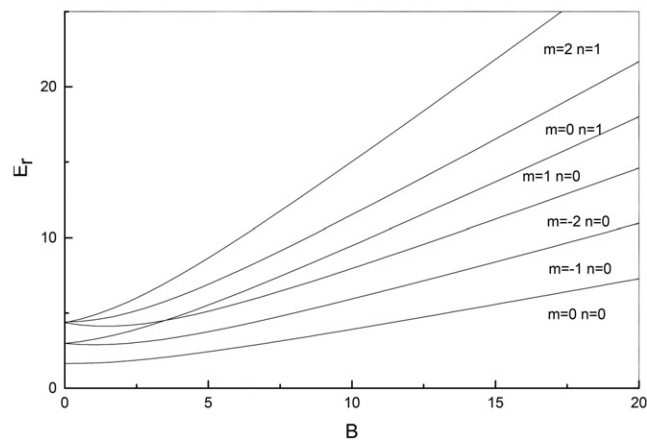
where  $\Gamma$  is the Euler gamma-function, and  $\Psi$  is degenerated hypergeometric Tricomi function.

If a transverse magnetic field is present, one should replace the parameter  $\sqrt{\alpha}$  with the effective confining potential steepness  $\beta$  and the term  $m\omega_c/4$  should be added to the energy. A transverse magnetic field leads to a singlet–triplet transition for vertical molecules.

The dependences of low-lying levels of the relative motion energy  $E_r$  versus parameter  $\alpha$  are presented in figure 1. The energy levels increase monotonically with  $\alpha$ . When  $\alpha$  is large enough (i.e. the confining potential is strong or the interlayer distance is large) the interelectron interaction is small in comparison with other parameters of the problem. As a result the energies of the relative motion are asymptotically equal to the energies of a two-dimensional harmonic



**Figure 2.** The dependences of the low-lying levels of the relative motion energy  $E_r$  versus the confining potential interlayer distance  $d$  when  $\alpha = 1$ .



**Figure 3.** The dependences of the low-lying levels of the relative motion energy  $E_r$  versus the transverse magnetic field  $B$  at  $\alpha = 1$ ,  $d = 1$ .

oscillator, i.e., they are linear on  $\alpha^{1/2}$ . The dependences of the low-lying levels of the relative motion energy  $E_r$  versus interlayer distance  $d$  when the parameter  $\alpha = 1$  are given in figure 2. The Coulomb interaction energy decreases and the energy levels decrease monotonically with  $d$ . The external magnetic field influence on the low-lying energy levels is presented in figure 3. The relative interdot interaction contribution decreases with growth of the parameter  $\beta$  as well as  $d$ .

#### 4. Conclusion

In summary, we analysed controlling of the ground state and spectra of horizontal and vertical QD molecules by gate voltage and external magnetic field or by construction of molecules (interdot distance). We proved that the singlet–triplet transformation of the ground state is controlled by the magnetic field or interdot separation for a QD molecule.

The possibility of controlling the ground state of a coupled QD system can be used for quantum calculations. One qubit can be determined by the spin of excess electrons in QDs.

A two-qubit gate can be created using two coupled QDs. The tunnel barrier between two adjacent QDs can be controlled by the gate voltage or by the external magnetic field.

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