# Spin-Spin Interaction In Artificial Molecules With In-Plane Magnetic Field 

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Coupled quantum dots, also called Artificial Molecules (AM), extend to the molecular realm the similarity between Quantum Dots (QDs) and artificial atoms ${ }^{1}$; inter-dot tunneling introduces an energy scale which may be comparable to other energy scales in the system, namely, single-particle confinement energies, carrier-carrier interaction, and magnetic energy. In AMs carriers sitting on either dot are not only electrostatically coupled, but also have their spin interlaced when tunneling is allowed ${ }^{2}$. One convenient way to control inter-dot tunneling, and, hence, effective spin-spin interaction, is by applying a magnetic field with a finite component perpendicular to the tunneling direction, $B \|$. This is particularly important in vertically coupled QDs, where otherwise tunneling in a given sample is fixed by sample parameters. This possibility extends the use of a vertical field, $B_{\perp}$, to drive the system from a low correlation (low field) regime to a high correlation (high field) one. In addition to the vertical component of the field, therefore, the in-plane magnetic field can be used to fully control the spin-spin interaction and, therefore, the spin character of the ground state of few-electron systems.

In this work we study theoretically the few-electron phase diagram, with particular respect to the spin ordering, in vertically coupled QDs in the ( $B_{\perp}, B_{n}$ ) plane. Our numerical approach is based on a real-space description of single-particle states which fully includes the complexity of typical samples, i.e., layer width, finite band-offsets etc. We include carrier-carrier Coulomb interaction, represented in a Slater determinant basis, by exact diagonalization methods.

Figure 1 shows (a) the single particle levels and (b) the two-electron energies at $B_{\perp}=0$ for a typical AM sample as a function of the in-plane field. The geometry is sketched in the inset. Single-particle levels come in symmetric (S) / antisymmetric (AS) multiplets which are degenerate at zero field due to cylindrical symmetry. At finite field, the multiplets split since the field removes the symmetry. Increasing the in-plane field further, however, suppresses the tunneling, and S and AS levels become degenerate.

As shown in Fig. 1(b), the two-electron ground state (GS) is a spin singlet at low field, but spin-spin interaction is suppressed with field due to the reduction of the tunneling probability, and singlet and triplet states become degenerate. Correspondingly, the GS evolves from a nearly pure S-like state $|\uparrow \downarrow\rangle_{S}$ to a fully entangled state $|\uparrow \downarrow\rangle_{S}+\exp \left[i \vartheta\left(B_{\|}\right)\right]|\uparrow \downarrow\rangle_{A S}$. At very large fields, Zeeman energy prevails and favors triplet ordering.


FIG. 1. AM energy levels $\left(B_{\perp}=0\right)$ with two identical quantum wells 10 nm wide, a 3 nm barrier, and parabolic lateral confinement (10 meV). (a) Single-particle levels. (b) Two-electron levels. Insets: main components of the wavefunctions in terms of $S$ (left boxes) and $A S$ (right boxes) states.

Next we consider the effect of a finite $B_{\|}$in the high $B_{\perp}$ regime. Top figure 2 shows one example of how the usual picture of Fock-Darwin states $^{3}$, i.e., the states of a 2 D parabolic confinement with a strictly vertical field, can be modified when the field is tilted from the vertical direction $(\theta=0)$ of the AM , as shown by the arrow. The main effect here is that, while $B_{\perp}$ decreases, tunneling is suppressed by the increasing $B_{\mathrm{n}}$ and S and AS states come close to each other. The effect is larger for the highest, more delocalized states. A finite $B_{n}$, breaking the axial symmetry of the AM with vertical field, may also remove the degeneracies between S/AS Fock-Darwin states with angular momentum differing by $\pm 1$ [not shown in top Fig. 2].

Bottom figure 2 shows the two-particle levels when the field is rotated from the vertical direction. In the moderate field regime shown here, not sufficient to induce the singlet-triplet transition ${ }^{4}$, the lowest energy levels are nearly unaffected by the rotation except for the shift due to the reduction of the tunneling energy, with the single state being the lowest. However, as the in-plane field increases, the two-electron wavefunction evolves into an entangled state occupying both S and AS levels.

At sufficiently high vertical field one or more (depending on the sample parameter) singlet-triplet transitions take place at given threshold fields, with the triplet state eventually being the stable one. Since a finite $B_{\|}$affects the tunneling and, therefore, the exchange energy, the threshold fields will also be affected ${ }^{5}$. The full single-triplet phase diagram will discussed in the paper. Implications of in-plane fields in the localization regime (Wigner crystallization) will also be


FIG. 2. Energy levels for a AM with two identical quantum wells 10 nm wide, a 3 nm barrier, and parabolic lateral confinement ( 10 meV ) at $B=8 \mathrm{~T}$ as a function of the tilting angle. (Top) Calculated single-particle levels (dots) and corresponding Fock-Darwin states for $B_{n}=0$ (solid and broken lines). (Bottom) Two-electron levels. Insets: main components of the wavefunctions in terms of $S$ (left boxes) and $A S$ (right boxes) states. discussed.

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