Quantum entanglement in lateral GaAs/AlGaAs quantum dot molecules

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Abstract. We calculate the excitonic structure of pairs of GaAs/AlGaAs quantum dots forming lateral molecules and obtain the entanglement of exciton states. The following advantages of the lateral geometry over the vertical one are found: (1) The energy structures of the dots forming a molecule can be in principle identical. (2) Comparable tunneling of electrons and holes ensures a high entanglement of antisymmetric excitons. A drawback of existing structures are very low tunneling energies, which make the entanglement vulnerable against differences in the sizes and shapes of both dots.

1. Introduction
Peculiar properties of the quantum computing allow to design algorithms superior to classic ones. A prominent example is Shor’s algorithm factoring large numbers with a polynomial time complexity. Quantum algorithms rely on two-state quantum systems – qubits, and devices coherently manipulating qubits – quantum gates. They might be realized in various physical systems, among which semiconductor quantum dots (QDs) offer several advantages such as easy integration with existing electronic devices. The representation of the qubit by a charge confined in a vertical quantum dot molecule (QDM), with the position in the lower/upper dot representing the 0/1 state, has been proposed [1]. The proposal has been later criticized as based on non-realistic assumptions [2]. In particular, inevitable differences between the electronic structures of the individual dots lower the entanglement significantly. Another drawback is the difference between the tunneling energies for electrons and holes, which further reduces the entanglement of optically dark excitons.

Recent progress in the growth technology makes it possible to prepare lateral QDMs. The interaction between the laterally closely spaced dots has been reported for the InAs/GaAs system [3]. There are also GaAs/AlGaAs quantum dot pairs in which a mutual interaction is expected [4]. The main advantage of the lateral topology is that there is no a-priori obstruction in making both dots identical from the point of view of their electronic structure. In contrast, in the vertical arrangement the strain field in the lower dot and in the upper dot differs. By manipulating the dot sizes, we can put into resonance either the electron levels or the hole levels, but not both at the same time. No such restriction applies to the lateral topology. Lateral QDMs also have the advantage of comparable tunneling energies of electrons and holes [5].
In this paper we present calculations of the excitonic structure of lateral QDMs consisting of two overlapping cones and of the related entanglement. We briefly discuss the characteristic energies of QDMs and their impact on the entanglement: Coulomb attraction, tunneling, and detuning. Realistic calculations follow, which combine the eight-band $\mathbf{k} \cdot \mathbf{p}$ method for single particle states with the configuration interaction method; the typical shape and dimensions of the dots are taken from Refs. [4, 6].

### 2. Entanglement: Effect of characteristic energies

A quantum system consisting of two particles $A$ and $B$ in states $|\phi_A\rangle$ and $|\phi_B\rangle$ is described by the product state $|\phi_{AB}\rangle = |\phi_A\rangle |\phi_B\rangle$, e.g., $|0_A 0_B\rangle$. Applying the principle of superposition to the product states we can construct also states which cannot be expressed as products of individual particle states, a prominent example being $|0_A 1_B\rangle + |1_A 0_B\rangle$. These are so called entangled states. If the system is in an entangled state, the properties of the components are correlated. Here the composed system is an exciton and the components are an electron and a hole.

The entanglement of an exciton in a QDM can be explained in terms of an interplay of three characteristic mechanisms: Coulomb attraction, tunneling, and detuning. To study this effect we employ a simple tight binding (TB) model of a QDM [1, 2]. Let $|e_0\rangle$, $|e_1\rangle$ denote the states of electrons in individual dots labelled as 0 and 1 (representing the 0 and 1 of a qubit), $|h_0\rangle$, $|h_1\rangle$ denote the corresponding hole states. In the basis $|e_0 h_0\rangle$, $|e_0 h_1\rangle$, $|e_1 h_0\rangle$, $|e_1 h_1\rangle$, the Hamiltonian reads

$$
\begin{bmatrix}
E_0 - H_0 - U_{00} & -t_H & -t_E & 0 \\
-t_H & E_0 - H_1 - U_{01} & 0 & -t_E \\
-t_E & 0 & E_1 - H_0 - U_{10} & -t_H \\
0 & -t_E & -t_H & E_1 - H_1 - U_{11}
\end{bmatrix}
$$

Here $E_i$ and $H_i$ are energies of electrons and holes in dot $i$, $t_E$ and $t_H$ are the tunneling matrix elements and $-U_{ij}$ are the Coulomb energies.

The number of parameters can be further reduced by the following assumptions. We introduce the detuning energy $\Delta$ due to the difference in the dot dimensions: $E_0 = E_1 + \Delta/2$, $H_0 = H_1 - \Delta/2$. We assume that $U_{00} = U_{11} = U_D$, $U_{01} = U_{10} = U_I$; $U = U_D - U_I$ is the Coulomb energy favoring the direct configurations over the indirect. Denoting $E_g = E_1 - H_1 - U_I$ we rewrite the Hamiltonian as

$$
\begin{bmatrix}
E_g + \Delta - U & -t_H & -t_E & 0 \\
-t_H & E_g + \Delta/2 & 0 & -t_E \\
-t_E & 0 & E_g + \Delta/2 & -t_H \\
0 & -t_E & -t_H & E_g - U
\end{bmatrix}
$$

Following [1, 2], we classify the eigenstates according to the following fully entangled states: $|a\rangle = (|e_0 h_0\rangle + |e_1 h_1\rangle)/\sqrt{2}$ (direct, symmetric), $|b\rangle = (|e_0 h_1\rangle + |e_1 h_0\rangle)/\sqrt{2}$ (indirect, symmetric), $|c\rangle = (|e_0 h_1\rangle - |e_1 h_0\rangle)/\sqrt{2}$ (indirect, antisymmetric), $|d\rangle = (|e_0 h_0\rangle - |e_1 h_1\rangle)/\sqrt{2}$ (direct, antisymmetric). The degree of entanglement can be quantified via the entropy of entanglement $S = -\text{Tr} \rho_A \log_2 \rho_A$ with $\rho_A = \text{Tr}_B \rho$, where $\rho$ is the density matrix of the exciton, $\rho_A$ is the reduced density matrix of one component (e.g., electron), $\text{Tr}_B$ is the partial trace over the other component (e.g., hole). The maximal value of the entropy of entanglement for the considered system is 1.

Figure 1 shows the entanglement of the two lowest excitonic states $|a\rangle$ (with the dominant component $|a\rangle$) and $|d\rangle$ (with the dominant component $|d\rangle$) calculated for $U = 10$ meV, $\Delta = 1$ meV and variable $t_E$ and $t_H$. We consider either $t_E = t_H$ (the ideal case) or $t_E = 3t_H$ (the largest difference found in our realistic model of lateral QDMs, see Fig. 2). For $|a\rangle$ there exists an optimal tunneling for which the entanglement is the largest. For lower tunneling, the
detuning prevents the formation of symmetric and antisymmetric orbitals and only one direct configuration dominates the state. For higher tunneling, the Coulomb term looses its importance and the contribution of indirect terms increases. The state $|\delta\rangle$ exhibits similar behavior with a slightly enhanced entanglement if $t_{E}$ and $t_{H}$ differ. However, if $t_{E} = t_{H}$, then entanglement of this state increases as tunneling increases and is fairly large.

The strategies to obtain a large degree of entanglement have to aim at $\Delta \ll t \ll U$. Exploiting of $|\delta\rangle$ is recommendable because of the larger entanglement as compared to $|\alpha\rangle$.

3. Realistic lateral molecules
The realistic calculations consist of two steps. First, we employ the eight band $\vec{k} \cdot \vec{p}$ method to obtain the single particle states. Second, these states are used as basis states for the configuration interaction method yielding the excitons. The values of the material parameters are taken from [7].

The model dots studied here correspond to two realistic systems which use GaAs as the dot material and AlGaAs as the host material: “molecules” [4] and “single dots” [6]. As described in Refs. [4, 6], the dots consist of pure GaAs, the bottom barrier consists of Al$_{0.45}$Ga$_{0.55}$As and the top barrier of Al$_{0.35}$Ga$_{0.65}$As. The shape and dimensions of the structures are obtained with a rather good accuracy from atomic force micrographs. The dots forming the molecule are not completely separate (see Fig. 18 of Ref. [4] and inset of Fig. 2). “Molecules” are modeled as two reverted cones with the characteristic height $h$ of 4 nm, the characteristic radius $r$ of 30 nm, and the distance between the centers of the cones $d$ of 32 nm. For “single dots” structure the values of the parameters are $h = 4$ nm, $r = 14$ nm, $d = 20$ nm; further, the tips of both cones are connected with a mound, which turns the hypothetic molecule into a single dot. However, there is still a lateral narrowing between the tips. In our study we adopted the shape of two reverted cones (we do not consider the connecting mound in “single dots”). We also allow $d$ to vary in order to explore possibilities of improving the existing structures.

For very low values of $d$ the QDM behaves as a single QD. Since the proposal of the qubit under consideration requires that the position of individual particles in one of the dots is well defined, we set the following criterion: The system of two cones forms a molecule if the probability density of the ground state in the area separating the cones is below 25% of its maximum value. This criterion is fulfilled if $d > 14$ nm for $r = 14$ nm and $d > 21$ nm for $r = 30$ nm. To validate that such structures are molecules, we have calculated the effect of an electric field on them (not shown here). In a molecule it is possible to localize the charge carrier in one of the dots by adding a proper detuning (represented by the electric field), different from single dots. The molecular behavior of our structures was confirmed. Modifying the above mentioned criterion to 1% leads to $d > 20$ nm for $r = 14$ nm and $d > 29$ nm for $r = 30$ nm, resulting in an extremely weak coupling between the dots. Therefore we have to accept a large probability density in the separation area as a drawback of considered lateral QDMs. The reason for this undesirable behavior is the shallow barrier between the dots, realized as the narrowing of the dot material only. This point should be considered in improving the growth technology.
Figure 2 shows $t_E$, $t_H$ and $U$ as functions of $d$ for $h = 4$ nm and $r = 14$ nm (the results for $r = 30$ nm are not shown). The electron tunneling for $d$ corresponding to existing structures (32 and 20 nm for $r$ of 30 and 14 nm, respectively) is below 0.15 meV, yielding a negligible entanglement for a realistic detuning. At the molecular limit, however, it increases towards 2.2 meV ($r = 14$ nm) and 1.5 meV ($r = 30$ nm). The $t_E/t_H$ ratio varies between 2 and 3. This is a considerable improvement compared to vertical QDMs, where values above 10 are predicted [2]. The Coulomb energy $U$ is around 20 meV for the distances $d$ yielding a reasonable tunneling. Using the TB model and assuming a detuning $\Delta = 1$ meV, we obtain the maximum entanglement for $t_E$ around 3 meV, a slightly larger value than that we obtained for simulated QDMs. We also calculated the expected detuning by varying the radius of a model dot. The distribution of $r$ with a standard deviation of 0.25 nm (1 nm) yielded a detuning up to 1 meV (5 meV). For the molecule with $h = 4$ nm, $r_1 = 13.9$ nm, $r_2 = 14.1$ nm, $d = 14$ nm we obtained the entropy of entanglement $S = 0.17$ for $|\alpha\rangle$ and $S = 0.20$ for $|\delta\rangle$, while for zero detuning it was $S = 0.94$ for $|\alpha\rangle$ and $S = 0.99$ for $|\delta\rangle$. The minimization of the detuning is therefore essential.

4. Conclusion

In conclusion, existing lateral QDMs presented in Ref. [4] suffer from low tunneling energies (below 0.15 meV). Nevertheless, sufficiently large values (up to 2 meV) can be obtained for the dots brought closer to each other. The ratio $t_E/t_H$ is considerably smaller than in vertical QDMs. The strategy to enhance the entanglement should consist of the following steps: (1) Reducing the distance between QDs in a QDM. (2) Reducing the lateral dimension of QDs and improving the barrier properties, resulting in a full separation of the QDs. (3) Minimization of the detuning by improving the homogeneity of QDs.

Acknowledgments

The work was supported by the Institutional research program MSM 0021622410, the GACR grant GA202/09/0676, and the DFG (FOR730).

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