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Double-occupancy probability and entanglement of two holes in double Ge/Si quantum dots

A. I. Yakimov[1], *A. A. Bloshkin, A. V. Dvurechenskii*

Rzhanov Institute of Semiconductor Physics, Siberian Branch RAS
630090 Novosibirsk, Russia

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We have calculated the exchange energy, double occupation probability of the lowest singlet state, and degree of entanglement of two holes in vertically coupled double Ge/Si quantum dots. We determined the conditions on which the exchange coupling is large enough for a fast swap operation in quantum computation and the double-occupancy probability is still low, thus maximizing the entanglement for a small computation error. We found that both the degree of entanglement and double-occupancy probability for quantum dots with different dot size collapse onto universal, size independent curves when plotted as a function of singlet-triplet splitting.

The systems of two coupled quantum dots (QDs) represent the basic elementary gates for a solid-state quantum computer, with the electron spins in the dots serving as quantum bits (qubits) [1 – 3]. Loss and DiVincenzo [1] suggested a scheme in which the two-qubit operations are performed on the physical qubits by controlling the exchange interaction between two electrons in neighboring quantum dots as a function of time. In a simplified model, the two spin have Heisenberg coupling with the effective exchange interaction being the difference between the spin-triplet and spin-singlet states J_{ST}. For successful quantum gate operations, it is necessary to have both a vanishing double-occupancy probability during the swap operation for a small computation error and a sizable exchange coupling for a fast gating. To obtain swap time in a femptosecond range the singlet-triplet splitting should be on the order of 10 meV. The laterally coupled QDs might not be a good candidate for this purpose because of the small exchange energy (typically, < 1 meV) owing to the large interdot separation [2, 4 – 6]. However, J_{ST} may be enlarged up to ~ 100 meV in vertically stacked self-assembled QDs [7 – 9].

Theoretical analysis of two-electron states in vertically aligned InAs/GaAs QDs has been performed in ref. [7] and [8]. It has been demonstrated that the requirements for quantum computation are best met at interdot distance of 6-8 nm, where the double-occupancy probability is kept less than 0.1 and the exchange energy is not vanishingly small (1-5 meV). The key requirement is that the lifetime of the spin is long compared with the time required for the operation of logic gates. It has become now clear that spatially inhomogeneous coupling of nuclei via the hyperfine interaction to the electron spin results in rapid spin dephasing (see, ref. [10], and references therein). Because the valence band couples more weakly to the nuclear spins, hole spin dynamics can be extremely slow [11]. Moreover, as shown recently [12], the problem of coherent manipulation of hole spin can be circumvented by making use of electric-dipole spin resonance technique instead of standard electron spin resonance for electrons. Therefore, the case of two holes confined in a pair of coupled QDs deserves special attention. In this work we have calculated the exchange energy, double occupation probability, and degree of entanglement of two holes in vertically coupled double Ge/Si quantum dots. Here the term "spin" is rather an index for two Kramers degenerate states. In the two-particle electron problem, where spin-orbit interaction is negligible, the two-electron wave functions can be systematized as either spin singlet or triplet since the spatial and spin part separate. In the case of two holes, however, such a separation is in general no longer possible. Nevertheless one can consider the projection of the total angular momentum as an analog of electron spin for hole states (i.e., the effective spin) and classify the two-hole states as the effective spin singlet or triplet.

We consider two identical vertically aligned pyramidal Ge nanoclusters with four {105}-oriented facets and a (001) base embedded into the Si matrix as shown in Fig.1. Each pyramid lies on a 4 ML Ge wetting layer. The nanoclusters are separated by a Si barrier of thickness d measured from wetting layer to wetting layer. The pyramid base length l is varied from 10 nm to 20 nm in different calculations; the pyramid aspect ratio h/l is fixed and equal to 0.1. The shape and size for our dot molecules are inspired from the experimental studies of self-assembled Ge/Si QDs [13].

[1]e-mail: yakimov@isp.nsc.ru

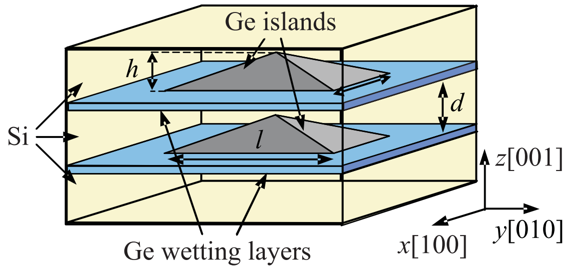

Fig.1. Schematic picture of a Ge/Si double QD used for simulation of hole states

We study a realistic situation when both Si matrix and Ge nanoclusters are inhomogeneously strained due to the $\sim$ 4% lattice mismatch between Si and Ge. The finite element calculations of three-dimensional spatial distribution of strain components $\varepsilon_{\alpha\beta}$ are performed using the package COMSOL MULTIPHYSICS with the approach described in [14]. The strain tensor elements are subsequently used as input to a single-particle strain-dependent Hamiltonian. The single-particle energies and wave functions are obtained using a six-band $\mathbf{k}\cdot\mathbf{p}$ approximation, based on the method of Bir and Pikus [15], which includes spin-orbit and strain effects. The resulting hole eigenstates are six-component spinors with an admixture of two HH states, two LH, and two SO states. The detailed form of the single-particle Hamiltonian terms was given in [16]. In what follows we restrict ourselves to the two lowest hole states, σ_g and σ_u, made of symmetric and antisymmetric combination of the s-like single-dot orbitals.

Based on single-particle molecular orbitals obtained above, a configuration-interaction (CI) calculation can then be built. The CI method includes the effects of direct Coulomb interaction among charge carriers, exchange, and correlation due to interconfiguration coupling. As compared to single-configuration approaches such as Hartree-Fock [17, 18] and local spin density [19], the CI treatment will lead to a more faithful and accurate description of the actual two-particle wave functions in the double-dot system [2, 7, 8, 20]. The many-body Hamiltonian can be written as

$$H = \sum_{i\sigma} E_i \psi^\dagger_{i\sigma}\psi_{i\sigma} + \frac{1}{2}\sum_{ijkl}\sum_{\sigma,\sigma'}\Gamma^{ij}_{kl}\psi^\dagger_{i\sigma}\psi^\dagger_{j\sigma'}\psi_{k\sigma'}\psi_{l\sigma}, \quad (1)$$

where E_i, $\psi_i = \sigma_g$ or σ_u are the single-particle hole energy levels and corresponding molecular orbitals, respectively, σ, σ' are the indices of effective spin,

$$\Gamma^{ij}_{kl} = \int\int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\psi^*_i(\mathbf{r}_1)\psi^*_j(\mathbf{r}_2)\psi_k(\mathbf{r}_2)\psi_l(\mathbf{r}_1)}{\epsilon(\mathbf{r}_1,\mathbf{r}_2)|\mathbf{r}_1-\mathbf{r}_2|}, \quad (2)$$

$\epsilon(\mathbf{r}_1,\mathbf{r}_2)$ is the position-dependent dielectric function. Here $V_{ij} = \Gamma^{ij}_{ji}$ and $K_{ij} = \Gamma^{ij}_{ij}$ represent diagonal Coulomb and exchange integrals, respectively, while the remaining terms are scattering terms. The configuration interaction approach consists of directly diagonalizing the Hamiltonian represented on a basis of Slater determinants which are the product of single-particle molecular states. The degree of entanglement for indistinguishable fermions is calculated as [8]

$$D = -\sum_i \gamma_i^2 \log_2 \gamma_i^2, \quad (3)$$

where γ_i are Slater decomposition coefficients.

In Fig.2, we show the calculated values of singlet-triplet splitting for double QDs of different size l as

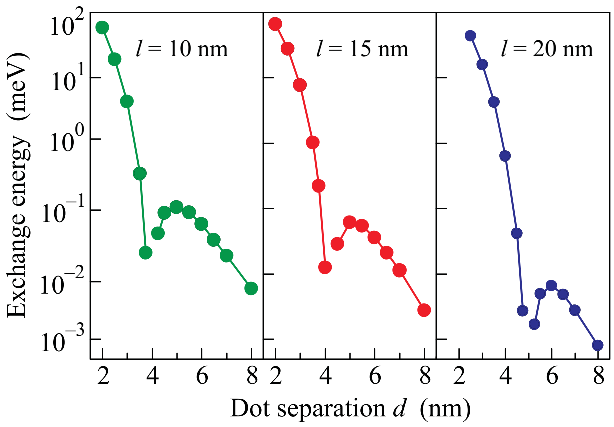

Fig.2. The singlet-triplet splitting plotted in semilogarithmic scale as a function of dot separation d and dot base length l

a function of dot separation d. At large d, the exchange energy is strongly reduced as the dot size increases due to the deepening of hole levels and suppression of the quantum-mechanical coupling with increasing l. The dips around $d \approx 4-5$ nm show the single-particle crossing and many-particle anticrossing points originated from the asymmetry-induced localization of single-particle hole wave functions on different dots. These phenomena have been discussed in detail in ref. [9].

Entanglement of two singlet holes is shown in Fig.3. At a fixed interdot spacing d, D decreases with increasing l (see inset of Fig.3). However, being plotted as a function of exchange energy, the degree of entanglement for quantum dots with different dot sizes collapses onto a single curve which can be fitted as $D = \exp(-J_{ST}/J_0)$ with $J_0 = 6.5 \pm 0.5$ meV.

Further we analyze also the dot double occupancy which is the probability of two holes occupying the dot $\eta = T$ (top) or B (bottom) at the same time. To obtain the bihole localization parameters, we solve the CI problem in the dot-centered Wannier basis ϕ_η and find the

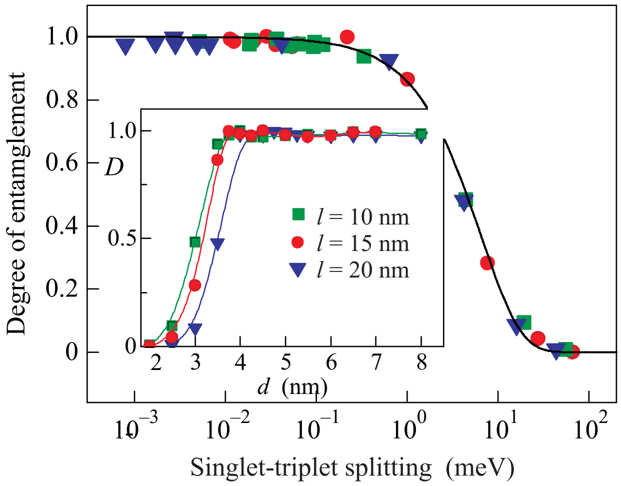

Fig.3. The degree of entanglement D for the two-hole ground-singlet state as a function of singlet-triplet splitting. The solid line is the fit to the data with the exponential function $D = \exp(-J_{ST}/J_0)$ with $J_0 = 6.5 \pm 0.5$ meV. The lateral dot size l is indicated. Inset: D vs the dot separation d

probability of two holes simultaneously occupying the top or bottom dots as the weight of the respective configuration in the many-particle wave function [7]. The dot-centered basis ϕ_η can be obtained from a unitary rotation of molecular orbitals ψ_i, i.e.

$$\phi_\eta = \sum_i U_{\eta i}\psi_i, \tag{4}$$

where $U_{\eta i}$ is a unitary matrix chosen to maximize the total self-Coulomb energy. The procedure of finding matrices $U_{\eta i}$ is described in [8]. Figure 4 shows the total double-occupancy probability $P_{tot} = P_{BB} + P_{TT}$ of the lowest singlet state. At small d, $P_{tot} \approx 0.5$ as the two holes are delocalized into two dots. At $d \sim 4-5$ nm, the ground-state singlet consists of a single configuration $|\sigma_g^\uparrow\sigma_u^\downarrow\rangle - |\sigma_g^\downarrow\sigma_u^\uparrow\rangle$ with σ_g and σ_u orbitals being entirely localized on different dots. As discussed in [9], for such a configuration both the spatial correlation and strain asymmetry lead to a dramatic drop of the double hole occupation. The local minimum at $d \sim 4-5$ nm is a consequence of this effect.

A remarkable finding is that the $P_{tot}(J_{ST})$ data for QDs with different size also can be scaled onto one curve $P_{tot} = 0.46 \times [1 - \exp(-J_{ST}/J_P)]$ with a single parameter $J_P = 12.5 \pm 0.5$ (solid line in Fig.4). Note that $J_P \simeq 2J_0$ [2)]. This observation indicates that J_0 is an inherent parameter of small-sized Ge/Si quantum dots. It is reasonably to suppose that J_0 can serve as a measure of the exchange coupling for which the double-occupancy probability is small (~ 0.1) and the entanglement is large enough (~ 0.5) when designing the Si-based quantum-dot qubits. The interdot distance, at which $J_{ST} = J_0$, depends on the dot size and lies in the range of 3-4 nm. Note the appropriate dot separation for Ge/Si QDs (3-4 nm) is less than that found for electrons in InAs/GaAs QDs [7] (6-8 nm) due to larger carrier effective mass in Ge/Si heterosystem.

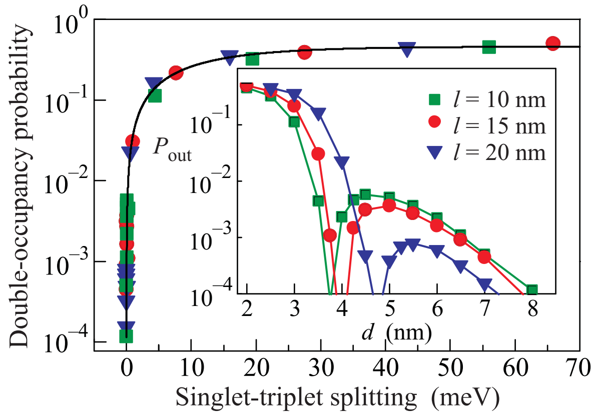

Fig.4. Double-occupancy probability P_{tot} for the lowest singlet state as a function of singlet-triplet splitting. The solid line is the fit to the data with the exponential function $P_{tot} = 0.46 \times [1 - \exp(-J_{ST}/J_P)]$ with $J_P = 12.5 \pm 0.5$ meV. Inset: P_{tot} vs the dot separation d

To conclude, we have calculated the exchange energy J_{ST}, double occupation probability P_{tot} of the ground state, and degree of entanglement D of two-hole system confined in vertically aligned double Ge/Si quantum dots. We have shown that the degree of entanglement and the double-occupancy probability scales with exchange coupling. A single scaling parameter, $J_0 = 6.5 \pm 0.5$ meV, collapses the P_{tot} and D data onto universal curves independent of dot size. When $J_{ST} = J_0$, the double-occupancy probability is small (~ 0.1) and the entanglement is large enough (~ 0.5) to use coupled Ge/Si QDs in two-qubit quantum operations.

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[2)] In fact, no wonder that $J_P = 2J_0$ because D is determined by the Slater decomposition coefficients squared [see eq. (3)], while P_{tot} is the weight of the respective configuration (i.e. the coefficient in a first degree) in the two-hole wave function.

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