CORRELATION IN TWO-ELECTRON SYSTEMS IN COUPLED QUANTUM DOTS*

S. Bednarek, T. Chwiej, J. Adamowski and B. Szafran

Faculty of Physics and Nuclear Techniques
University of Mining and Metallurgy
Al. Mickiewicza 30, 30-059 Kraków, Poland

A theoretical study of correlation has been performed for an electron pair confined in a vertically coupled double quantum dot by a method, which transforms the three-dimensional two-electron problem into the effective one-dimensional two-electron problem. We have found that the electron correlation cannot be neglected at any interdot distance and becomes strong at large interdot distances.

PACS numbers: 73.21.–b

A quantum dot (QD) is a physical object of the nanoscale size, in which we can manipulate with the electronic properties. The electron–electron correlation is an example of such effect, which can be artificially changed by changing the QD parameters, *e.g.*, the dot size and interdot separation. The present paper is devoted to a theoretical study of the correlation in the two-electron system confined in the coupled QD's.

We consider the vertically coupled double QD in the nanodevice [1] with a cylindrical shape, which consists of GaAs, AlGaAs, and InGaAs layers. The two QD's are created within the InGaAs layers. The corresponding quantum wells of 12 nm height and 300 meV depth are separated by by the barrier with the varying thickness b. In our previous paper [2], we have determined the confinement potential by solving the Poisson equation for the single vertical QD [3]. Based on the results of Ref. [2], we approximate the lateral confinement potential in the QD by the harmonic potential $V(r) = \alpha r^2$, where $\alpha = m\omega^2/2 = 0.05$ meV/nm^2. The total confinement potential is the sum of the double-well (triple-barrier) rectangular potential in the z direction (cylinder axis) and the harmonic potential in the transverse (x, y)

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directions. Thus, the one-electron wave function can be separated as follows: $\Psi(x, y, z) = \psi(x, y)\varphi(z)$, where $\varphi(z)$ is the solution of the one-dimensional eigenproblem in the z direction and

$$\psi(x, y) = (2\beta/\pi)^{1/2} \exp[-\beta(x^2 + y^2)] \tag{1}$$

is the solution of the eigenproblem in the $x - y$ plane, where $\beta = m\omega/2\hbar$. If the two potential wells are separated by a sufficiently thick barrier, $i.e.$, the tunnel coupling between the QD's is weak, the electrons can be found with a high probability in different QD's. Therefore, the x, y-dependent part of the wave function is only slightly perturbed by the electron–electron interaction and the two-electron wave function takes on the approximate form $\Psi(x_1, y_1, z_1, x_2, y_2, z_2) = \psi(x_1, y_1)\psi(x_2, y_2)\chi(z_1, z_2)$, where $\chi(z_1, z_2)$ is the the eigenfunction of the effective one-dimensional Hamiltonian

$$H(z_1, z_2) = T + V(z_1) + V(z_2) + U(z_1 - z_2) + 2\hbar\omega, \tag{2}$$

where T is the kinetic-energy operator for the motion of two electrons in the z direction and $V(z)$ is the double-well confinement potential. We have found a useful one-dimensional approximation for the Coulomb interaction between the electrons. For this purpose, the effective potential energy $U(z_1 - z_2)$ has been calculated as the average value of the three-dimensional Coulomb potential with the use of wave function (1) and integration over the x, y coordinates. The resulting effective electron–electron interaction potential energy

$$U(z) = (e^2/4\pi\varepsilon_0\varepsilon_{\rm s})(\pi\beta)^{1/2} \exp(\beta z^2) \mathrm{erfc}(\beta^{1/2}|z|) \tag{3}$$

does not possess any singularity. In Eq. (3), $\varepsilon_{\rm s}$ is the static dielectric constant.

The eigenproblem of Hamiltonian (2) depends on the two variables only; therefore, we can obtain its numerical solution with an arbitrary precision [4]. We will call this solution "exact". The correlation energy, calculated as the difference between the "exact" ground-state energy and the corresponding energy estimate obtained by the restricted Hartree–Fock (RHF) method, is displayed in Fig. 1(a) for the two lowest energy levels (singlet and triplet). Fig. 1(a) shows that for the small barrier thickness ($b < 2$ nm) the correlation effect is small. If, however, b exceeds 2 nm, the absolute value of the correlation energy considerably increases and for the distinctly separated QDs the confined electron system becomes strongly correlated. This strong correlation results from the interelectron interaction induced breakdown of the two-electron wave function parity symmetry in the external confinement potential.

We have also performed the calculations with the use of the unrestricted Hartree–Fock (UHF) method, in which each one-electron orbital is independently optimized for each spin state, which allows for a localization of
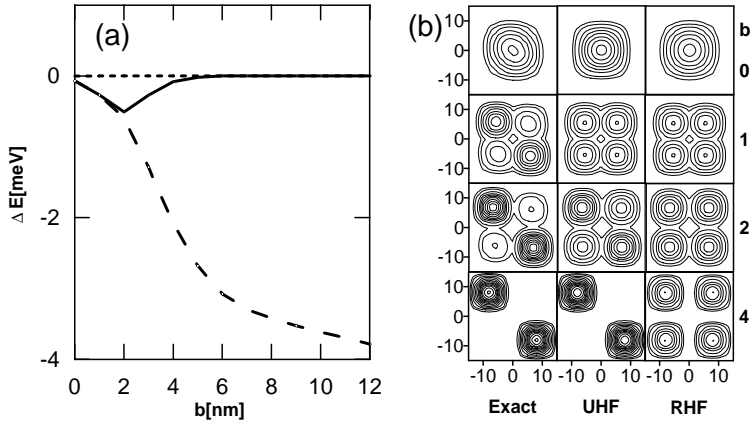
Fig. 1. (a) Energy difference (ΔE) between the "exact" and RHF (dashed curve) [UHF (solid curve)] results for the singlet and triplet states. For the triplet state ΔE calculated by both the methods is almost zero (horizontal line at zero energy). (b) Contours of the two-electron wave function plotted as functions of the electron coordinates z_1 and z_2 (in nm) for the barrier thickness $b = 0, 1, 2$, and 4 nm. The left, central, and right panel display the results obtained by the "exact", UHF, and RHF method, respectively.

electrons in different QD's. We have found that the UHF method leads to the considerable improvement of the energy estimates with respect to the RHF results and reproduces — to a large extent — the correlation effect. Fig. 1(a) shows that the UHF energy estimates are nearly exact both for the small and large interdot separations. Only for $b = 1 \div 4$ nm the error of the UHF method is rather large. We note that — in this intermediate barrier-thickness regime — the external-potential symmetry of the wave function is broken due to the Coulomb interaction.

In order to get more physical insight into the electron correlation in the QD's, we have plotted in Fig. 1(b) the contours of the two-electron wave function for different b. The case $b = 0$ corresponds to the single QD with the two potential wells joined into the one potential well. In this single QD, the maximum of the electron density is located approximately at the dot center. However, due to the Coulomb repulsion the electrons are localized slightly apart. If the interdot barrier is introduced, the electrons prefer to be localized in different QD's. For $b = 4$ nm the probability of finding both the electrons in the same QD vanishes. On the contrary, the RHF wave functions do not allow for this separation [cf. right panel in Fig. 1(b)]. According to the RHF results, both the electrons are spread over the two QD's independently of each other. The RHF wave function is symmetric with

respect to the interchange of electron coordinates z_1 and z_2. This symmetry agrees with the symmetry of the confinement potential, but prohibits the interelectron correlation to be properly included by the RHF method. The breaking of the confinement-potential symmetry by the Coulomb interaction is the source of the strong electron correlation. Fig. 1(b) shows that the wave functions obtained by the UHF method much better reproduce the true electron distribution. We note that — in the UHF method — the localization of the electrons in different QD's appears with some "delay" if b increases. Nevertheless, for large b the UHF wave-function contours are almost indistinguishable from the exact ones.

In summary, we have proposed a method for solving the two-electron eigenproblem in the coupled QD's and found the effective one-dimensional electron–electron interaction potential, which allows us to reduce this problem to the "exactly" soluble one-dimensional problem. We have shown that the electron correlation becomes strong at large interdot distances. We have also found that the UHF method fairly well reproduces the correlation effects. It is interesting that the coupled QD nanostructure can be treated as the correlated electron system, in which the correlation can be tuned by changing the interdot distance.

REFERENCES

[1] M. Pi, A. Emperador, M. Barranco, F. Garcias, K. Muraki, S. Tarucha, D.G. Austing, *Phys. Rev. Lett.* **87**, 66801 (2001).

[2] S. Bednarek, B. Szafran, J. Adamowski, *Phys. Rev.* **B64**, 195303 (2001).

[3] S. Tarucha, D.G. Austing, T. Honda, R.J. van der Hage, L.P. Kouwenhoven, *Phys. Rev. Lett.* **77**, 3613 (1996).

[4] B. Szafran, J. Adamowski, S. Bednarek, *Physica E* **5**, 185 (2000).