Tight-binding calculations of two-electron energy spectra in carbon nanotube n-p quantum dots

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Semiconducting carbon nanotubes (CNTs) provide a good environment for carrier confinement in electrostatically defined quantum dots (QDs). This feature is particularly relevant in context of spin manipulation of individual electrons, which is a prerequisite for quantum information processing devices. Recently, a few experiments have been conducted which focused on spin manipulation in ambipolar carbon nanotube quantum dots [1-2], with results that remain partially unexplained. The attempts for description of the experimental data assumed that the ambipolar and unipolar dots have similar electron properties. A comprehensive description of unipolar QDs in CNT is available in the literature. No similar description has been provided so far for ambipolar QDs.

We consider ambipolar n-p double quantum dot with one electron localized in n dot and three holes localized in p dot - system investigated experimentally in context of the valley and/or spin blockade of the current flow through a double QD [1]. We solve the problem of a confined electron pair using an exact diagonalization method within the tight-binding approach. In the model we take into account curvature-induced spin-orbit interaction [3], external fields, the electron-electron interaction and the intervalley scattering mediated by the atomic defects.

We demonstrate that the electronic structure of the double n-p dot differs from the n-n dot in a few elementary aspect [4]. The energy splitting due to exchange interaction is found only for specific two-electron states and for limited range of external magnetic field, while in n-n unipolar dots well defined singlet- and triplet-like states are formed with exchange interaction independent of the magnetic field. Also, in contrast to n-n system, the two-electron ground state in ambipolar DQD is fourfold degenerate. We indicate that observed differences for n-n and n-p systems are an effect of opposite electron circulation in the conductance and valence bands for a given valley. We discuss universality of our results for CNTs of various chirality and quantum dots sizes.

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[3] T. Ando, *J. Phys. Soc. Jpn.* **69**, 1757 (2000).
[4] E. N. Osika and B. Szafran, *Phys. Rev. B* **91**, 085312 (2015).