Time-dependent atomistic simulations of spin-valley transitions in carbon nanotube quantum dots

Edyta N. Osika, Alina Mreńca and Bartłomiej Szafran

AGH University of Science and Technology,
Faculty of Physics and Applied Computer Science,
al. Mickiewicza 30, 30-059 Kraków, Poland

Carbon nanotubes (CNTs) are considered attractive for quantum information processing using carrier spins due to the absence of the nuclear spin field that is the main source of spin decoherence in nanostructures. In contrast to flat graphene, the semiconducting CNTs can be used to confine charge carriers within electrostatically defined quantum dots. As a graphene-based material, CNTs possess a valley degree of freedom, which is similar to the electron spin and originate from the presence of two non-equivalent valleys in the Brillouin zone. Due to folding of graphene plane, CNTs exhibit a significant spin-orbit coupling [1], which enables electrical control of the carrier spins. The spin-orbit interaction couples the spin and valley degrees of freedom splitting the four-fold degenerate ground state into Kramers doublets, which are further split by external magnetic field. Transitions between the spin-valley states in carbon nanotube quantum dots have been recently observed in experiment [2], as induced by an external periodically changing electric field.

We report on simulations of the spin-valley transitions driven by external AC electric field. We use the tight-binding approach to describe the states localized within a quantum dot taking into account the curvature-induced spin-orbit interaction and external fields. We select the states localized in quantum dot as the basis for the solution of the time-dependent Schrödinger equation. We discuss the spin-, as well as the valley-transitions and their rates, the selection rules and their lifting by atomic disorder, the bend of the tube and electric field component perpendicular to the axis of the CNT. We discuss the effects driving the spin-flips with a particular focus on the lattice imperfections and the electric field component that is perpendicular to the axis of the CNT. We demonstrate that the disorder not only allows for the valley transitions but also drive the spin-flips. Besides the first order transitions we find also fractional resonances.

[1] T. Ando, *J. Phys. Soc. Jpn.* **69**, 1757 (2000); D.V. Bulaev, B. Trauzettel, and D. Loss, *Phys. Rev. B* **77**, 235301 (2008); M. del Valle, M. Margańska, and M. Grifoni, *Phys. Rev. B* **84**, 165427 (2011).
[2] E.A. Laird, F. Pei, and L.P. Kouwenhoven, *Nature Nano.* **8**, 565 (2013).