Valley qubit in gated MoS_2 monolayer quantum dot

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The aim of presented research is to construct quantitative models describing quantum information carriers, single electrons confined in dwo-dimensional crystals of transition metal dichalcogenides (TMDC) [1]. Then design of nanodevices based on TMDC monolayer, performing operations on properly defined qubits. Such monolayers have a number of interesting properties. Unlike graphene, they have direct band gap and relatively high value of spin-orbit coupling. Moreover, they possess the ability of using valley pseudospin, in addition to spin, as quantum bit. Thus, they are important materials for spintronics and recently introduced valleytronics.

The proposed nanodevice consists of TMDC monolayer flake with nearby gates. Appropriate voltages applied to the gates crate electric fields within the monolayer. The electrostatic quantum dots within the flake, induced by the local gating, confines single electrons. A qubit is encoded in the electron valley degree of freedom. The valley transitions are induced by the confinement potential oscillatory modulations, and allow to perform operations on the valley-qubit confined in the nanodevice. The proposed manipulation scheme is all-electrically controlled by voltages applied to the local gates.

We use the three-band tight-binding approach [2] to model TMDC monolayer flakes. We describe exact potential of the nanodevice taking into account proper boundary conditions on the electrodes by solving the Poisson equation. The time-evolution of the system is supported by realistic self consistent Poisson-Schrödinger tight-binding calculations. The tight-binding calculations are further confirmed by simulations within the continuum model [3]. We are developing previously used [4] precise realistic simulations of the time evolution of semiconductor nanodevices. Now introduced for new and attractive materials with the interesting properties.

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