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Spin-orbit coupling, quantum dots, and qubits in transition metal dichalcogenides ANDOR KORMÁNYOS, University of Konstanz, VIKTOR ZÓLYOMI, NEIL D. DRUMMOND, Lancaster University, GUIDO BURKARD, University of Konstanz — We derive an effective Hamiltonian describing the dynamics of electrons in the conduction band of transition metal dichalcogenides (TMDC) in the presence of perpendicular electric and magnetic fields [1]. We discuss both the intrinsic and Bychkov-Rashba spin-orbit coupling (SOC) induced by an external electric field. We identify a new term in the Hamiltonian of the Bychkov-Rashba SOC which does not exist in III-V semiconductors. Due to the strong intrinsic SOC is an effective out-of-plane g-factor for the electrons which differs from the free-electron g-factor $g \simeq 2$. Using first-principles calculations, we estimate the various parameters appearing in the theory. Finally, we consider quantum dots (QDs) in TMDC materials and derive an effective Hamiltonian allowing us to calculate the magnetic field dependence of the bound states in the QDs. We find that all states are both valley and spin split, which suggests that these QDs could be used as valley-spin filters. We explore the possibility of using spin and valley states in TMDCs as qubits, and conclude that, due to the relatively strong intrinsic SOC in the conduction band, the most realistic option appears to be a combined spin-valley (Kramers) qubit at low B fields.

[1] A. Kormányos et al., arXiv:1310.7720.

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