Spin-orbit coupling, quantum dots and magnetoconductance oscillations in monolayer transition metal dichalcogenides

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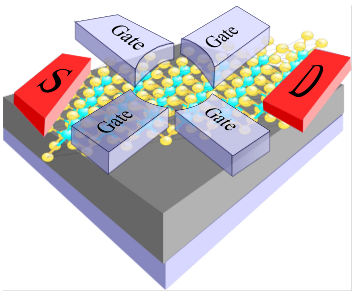
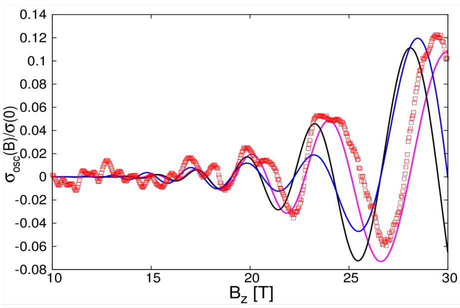
We have developed a **k.p** theory framework (see [1] and a recent review in [2]) to describe the dispersion of the conduction and valence bands at their extrema (the K, Q, Γ and M points of the hexagonal Brillouin zone) in atomic crystals of semiconducting monolayer transition metal dichalcogenides (TMDCs). We parametrized the essential parts of the **k.p** Hamiltonians for MX_2 monolayers (here M={Mo, W} and X={S, Se, Te}) using density functional theory calculations. We use this theory framework to study a variety of problems that are not easy to address by first-principles calculations. We considered the Rashba-type spin-orbit coupling in these materials [3] and found that it consist of two parts. The first one is known from earlier studies on two-dimensional electron gas. In addition, however, there is a second part which is specific of monolayer TMDCs. In contrast to graphene, one can form quantum dots by electrostatic gating in these materials and we have studied the single-particle spectrum of such quantum dots. We found that in external magnetic field they can serve as simultaneous valley and spin filters. Finally, motivated by recent experimental progress [4,5] in the measurement of magnetoconductance properties of TMDCs, we investigate how the spin-orbit coupling and the broken valley degeneracy of the Landau levels (LL) affect the Shubnikov-de Haas oscillations in TMDCs [6]. To this end we first study the Landau level spectrum. We find that in a wide magnetic field regime the valley degeneracy breaking of the LLs is linear in magnetic field. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. We then use the self-consistent Born approximation and the Kubo-formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We point out how the doping level affects the magnetoconductance and compare the results of our theoretical calculations with recent measurements[4] .



Schematic of a quantum dot in a monolayer TMDC [3]



Shubnikov-de Haas oscillations in the magnetoconductance: measurement (squares) and theory (solid lines) [6]

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