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Spontaneous polarization of the two-dimensional electron gas in WS_2

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Tungsten disulfide represents a class of 2D materials, transition metal dichalcogenides (TMDC), which exist as layers of atomic thickness with atoms organized in a honeycomb lattice. Similarly to graphene, in TMDCs the minimum of the conduction band and the maximum of the valence band are found at the K and K'points in the Brillouin zone. Unlike graphene, these systems exhibit (i) a large direct bandgap, and (ii) strong spin-orbit interaction, which locks the spin and valley degrees of freedom of quasielectrons and quasiholes. The two-dimensional character of TMDCs results in a significant enhancement of Coulomb interactions. In Hartree-Fock (HF) approximation, this leads to a spontaneous valley polarization of the two-dimensional electron gas (2DEG) driven by electron-electron exchange. The valley polarization translates into spontaneously circularly polarized emission recently detected in magnetooptical measurements [1].
We present here a microscopic theory of the two-dimensional electron gas in WS_2 . We develop an atomistic tight-binding (tb) model for single-quasielectron and quasihole states accounting for the spectral content of the subbands in terms of linear combinations of atomistic orbitals. The tb parameters are obtained from ab-initio calculations. The spin-orbit coupling and resulting reversal of the spin order of the conduction band are treated phenomenologically. This allows to formulate the optical selection rules and calculate Coulomb interaction matrix elements atomistically. Using these elements, we calculate the HF phase diagram of the system of N interacting electrons in doped WS_2 and demonstrate the formation of a valley polarized 2DEG state for low enough electronic densities, and a valley-singlet state for larger densities. The effect of correlation and Q minima are also included. The effect of a magnetic field is discussed in terms of Landau levels of interacting massive Dirac Fermions. Finally, we relate the formation of the valley polarized state with magnetooptical experiments.

[1] T. Scrace, Y. Tsai, B. Barman, L. Schweidenback, A. Petrou, G. Kioseoglou, I. Ozfidan, M. Korkusinski, and P. Hawrylak, Nature Nanotechnology 10, 603 (2015).

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