Electronic structure, magneto-excitons and valley-polarized electron gas in 2D crystals

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We discuss here the electronic and optical properties of monolayer 2D hexagonal crystals, graphene and transition metal dichalcogenites (TMDC) MoS_2 and WS_2. The *ab-initio* calculations [1–4] establish TMDCs as direct-gap single-monolayer semiconductors with valley-selective optical transitions. In order to develop a better understanding of the electronic properties a tight binding model involving Mo and W metal *d*-orbitals and sulfur dimer S_2 *p*-orbitals is developed based on input from *ab-initio* calculations. The roles of *d*- and *p*-orbitals, as well as nearest and next-nearest neighbor hopping, is clarified. The effective tight-binding model is further reduced to the massive Dirac fermion model, which allows the introduction of a magnetic field. The Landé and Zeeman valley effects and the effect of electron-electron interactions and topology in the magneto-exciton and trion spectra are discussed [3–5]. In the discussion of the exciton spectrum we draw analogies with graphene quantum dots with degenerate valence and conduction band extrema, for which the multi-exciton spectrum based on extensive exact diagonalization has already been reported [6]. Finally, we discuss the possibility of broken symmetry ground states of the electron gas, in particular the existence of a valley-polarized electron gas (VPEG), as a ground state of *n*-type WS_2. The valley-polarized state leads to spontaneous circular polarization of the emitted light, an effect which has been recently observed [3].

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