Electronic structure, magnetoexcitons and valley polarized electron gas in 2D crystals

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We discuss the electronic and optical properties of monolayer 2D hexagonal crystals, graphene and transition metal dichalcogenites (TMDCs), MoS2 and WS2. The ab-initio calculations [1-3] establish TMDCs as direct gap, single monolayer, semiconductors with valley selective optical transitions. In order to develop a better understanding of the electronic properties and their response to external magnetic field a tight binding model involving Mo and W metal d-orbitals and sulfur dimer S2 p orbitals is developed based on input from ab-initio calculations. The role of d- and p-orbitals and nearest and next nearest neighbor hopping is clarified. The effective tight binding model is further reduced to the massive Dirac Fermion model which allows introduction of the magnetic field. The Lande and Zeeman Valley effects and the effect of e-e interactions in the magneto-exciton spectrum are discussed [4]. In the discussion of the exciton spectrum we draw analogies with graphene quantum dots with degenerate top of the valence and bottom of conduction band for which multi-exciton spectrum based on extensive exact diagonalization is known [5]. 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 WS2. 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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