Electronic and Optical Properties of 2D Electron Gas in Transition Metal Dichalcogenide Crystals in High Magnetic Fields

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Single layers of transition metal dichalcogenides (TMDCs) are two-dimensional (2D) semiconductors enabling exploration of many physical phenomena [1]. These include massive Dirac fermions, strong electron-electron interactions leading to excitons with binding energies ~500 meV, valley degrees of freedom allowing for selective excitation with circularly polarized light, nontrivial topology resulting in a valley Zeeman effect, and valley- and spin-polarized broken symmetry states [2-6].

In this work we describe the electronic and optical properties of 2D electron gas in TMDC monolayers in high magnetic fields. We start with determining the electronic structure of TMDC monolayers from first principles. We then perform the analysis of Kohn-Sham wavefunctions allowing us to describe the microscopic details of spin and orbital contributions. In the next step, we describe the TMDC monolayer using the *ab initio*-based massive Dirac fermion (MDF) model [4,6]. Subsequently, we discuss the Landau level structure of MDFs for two spins in the two non-equivalent valleys, and the resulting spin and valley Zeeman splitting. Finally, we study the evolution of optical properties as a function of the electronic density. Following on our earlier work [6-8], we determine the emission and absorption spectra of an exciton, a trion and filled integer Landau levels in the two non-equivalent valleys. We describe the effect of electron gas of MDFs on the magneto-exciton spectrum using exact diagonalization tools. We focus on the effect of the zero Landau level in conduction band on the emission spectrum and discuss its potential signature in experiments [9,10].

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