Fine Structure of Excitons in Gated 2D TMD’s Heterostructures

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With the development of advanced methods for fabricating 2D material heterostructures, devices based on atomically thin semiconducting transition metal dichalcogenides (TMDs) are emerging as a promising platform in the field of quantum information science. Semiconducting TMDs typically exhibit a direct bandgap at the K-point in the hexagonal Brillouin zone, with optical properties dominated by the physics of excitons and other many-body complexes. They have potential for realizing spin qubits with long coherence time due to spin-valley locking, caused by the strong spin–orbit interaction and the symmetries of their 2D lattice. Various 2D heterostructures also offer possibilities to engineer long-lived optical complexes, such as interlayer excitons. These promising properties motivate our recent efforts to understand these 2D materials [1-6].

In the first part, I will present our theoretical approach to electronic structure of TMD's. Starting from general properties obtained using ab initio methods, I will discuss the construction of the tight-binding models for both mono- and bi-layer structures [1, 2, 3]. Next, I will describe various gate-induced potentials that influence the electronic structure and create confining potentials.

In the second part of the talk, I will review our approach to the exciton problem [4]. In our method, we turn on electron-electron interactions, form a Hartree-Fock ground state, and construct electron-hole excitations. We compute electron-electron interactions and solve the Bethe-Salpeter equation to obtain a highly converged spectrum of exciton states. We disentangle the effects of electron-hole dispersion, details of band structure on Coulomb intra/inter - valley interactions, topology of wavefunctions, screening and dielectric environment. In particular, we discuss the effects of possible total exciton momentum mixing terms induced by electrical means, in the form of terms breaking translational symmetries. By precisely including spin splitting and spin rotations, we establish the splitting between dark and bright exciton species.

[1] M. Bieniek, M. Korkusiński, L. Szulakowska, P. Potasz, I. Ozfidan, P. Hawrylak, „Band nesting, massive Dirac fermions, and valley Landé and Zeeman effects in transition metal dichalcogenides: A tight-binding model”, Phys. Rev. B 97, 085153 (2018),
[2] M. Bieniek, K. Sadecka, L. Szulakowska, P. Hawrylak, „Theory of Excitons in Atomically Thin Semiconductors: Tight-Binding Approach”, Nanomaterials 1582 (2022)
[3] K. Sadecka, M. Bieniek, J. Pawłowski et al, “Electrically tunable valley couplings in MoSe2/WSe2 bilayer semiconductor”, TBA (2024)
[4] M. Bieniek, L. Szulakowska, P. Hawrylak, “Band nesting and exciton spectrum in monolayer MoS2”, PRB 101, 125423 (2020)
[5] J. Pawłowski, D. Miravet, M. Bieniek, M. Korkusiński, J. Boddison-Chouinard, L. Gaudreau, A. Luican-Mayer, P. Hawrylak, "Interacting holes in a gated WSe2 quantum channel: valley correlations and zigzag Wigner crystal", TBA (2024)
[6] D. Miravet, L. Szulakowska, M. Bieniek, M. Korkusiński, P. Hawrylak, “Theory of excitonic complexes in gated WSe2 quantum dots”, TBA (2024)