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Electron-Electron Interactions in Optical Properties of Graphene Quantum Dots

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In this thesis, I present a theory of electron-electron interactions in optical properties of graphene and transition metal dichalcogenides (TMDCs), two dimensional nanostructures with a hexagonal lattice.

We start our discussion with electron-electron interactions in artificial rings for which the strength of interactions can be varied and exact results can be obtained. The artificial rings are described by the extended Hubbard model and solved using an exact diagonalization method in real and Fourier space of configurations. Exact and analytical results for charged rings are obtained in the limit of very strong interactions. For the quadruple quantum dot ring and the artificial benzene ring, we find that chirality leads to the appearance of a topological phase and an effective gauge field that determines the ground state character with varied interaction strength. For the charged artificial benzene ring, our numerical results show a transition from a degenerate to a non degenerate ground state with increasing strength of Coulomb interactions. We show that the artificial gauge and the transition in the ground state can be detected as changes in the optical absorption spectrum.

In the second part of the thesis, the electronic and optical properties of colloidal graphene quantum dots (CGQD) consisting of many benzene rings are determined. The CGQDs are described by the combination of tight binding, mean field Hartree Fock (HF) and Configuration Interaction methods. The single particle properties are described through the tight binding method based on the pz carbon orbitals. Screened Coulomb interactions between electrons, including direct, exchange, and scattering matrix elements, are calculated using Slater pz orbitals. HF ground states corresponding to semiconductor, Mott-insulator, and spin-polarized phases are obtained as a function of the strength of the screened interaction versus the tunnelling matrix element. The many-body ground and excited states in the semiconducting phase are constructed as a linear combination of a finite number of electron-hole pair excitations from the HF ground state (GS). The Hamiltonian is constructed in the subspace of multi-pair HF excitations to obtain the low energy, many body states by exact diagonalization using the Lanczos method. The degeneracy of the valence- and conduction-band edges of 3-fold rotationally symmetric CGQDs is shown to lead to a characteristic exciton and bi-exciton spectrum. The low-energy exciton spectrum is predicted to consist of two bright-singlet exciton states corresponding to two circular polarizations of light and a lower-energy band of dark singlets and dark triplets. The robustness of the bright degenerate singlet pair against correlations in the many-body state is demonstrated as well as the breaking of the degeneracy by the lowering of symmetry of the CGQD. Band edge biexciton energies and binding energies are predicted, and two degenerate exciton (X) states and a corresponding biexciton (XX) state are identified for the generation of an XX-X cascade. The Auger coupling of XX and excited X states is determined and our theoretical results are compared with experimental absorption and non-linear transient absorption spectra.

In the third and final part of the thesis, we replace the two non-equivalent carbon atoms of the graphene hexagonal lattice with a heavy transition-metal atom M, (e.g. Mo or W) and a dimer X2 (e.g. S). The band-structure of a monolayer MX2 is calculated using density functional theory (DFT). It is shown that a direct gap opens up at all K points of the Brillouin zone and strong spin orbit coupling leads to spin splitting of the valence and conduction bands and emergence of valley dependent optical selection rules. Finally, the magnetoluminescence experiments on a monolayer WS2 emitting circularly polarized light upon its excitation by unpolarized light are described. The emission of polarized light in zero magnetic field is explained by the possibility of formation of a valley polarized 2D electron gas in unintentionally doped WS2.

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