Excitons in Gated WSe2 Quantum Dots

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Absorption of a single photon generates a single exciton, comprising an electron and a hole. In this work, we present a theory of single excitons [1, 2] confined in gated WSe2 quantum dots [3]. Gated quantum dots allow for the manipulation of a controlled number of either electrons or holes in a single layer of 2D materials, such as WSe2. However, confining excitons in gated quantum dots presents a nontrivial challenge, as the electron is repelled when the hole is confined in the dot.

Achieving confinement of excitons in gated quantum dots requires a delicate balance between the repulsion of electrons by the gate potential and the attraction by the Coulomb potential of a hole localized within the dot. Once confined, excitons, and hence photons, can be detected via transport experiments. We begin by describing our quantum dot within a computational box containing over a million atoms, utilizing a tight-binding microscopic Hamiltonian [4]. The gated quantum dot is defined by applying gates that result in a Gaussian confining potential, which is attractive for holes and repulsive for electrons. By expanding the quantum dot wavefunction in bulk band states, we obtain quantum dot energy levels and wavefunctions. These wavefunctions capture the effects of confinement potential, size, valley, and spin [5, 6].

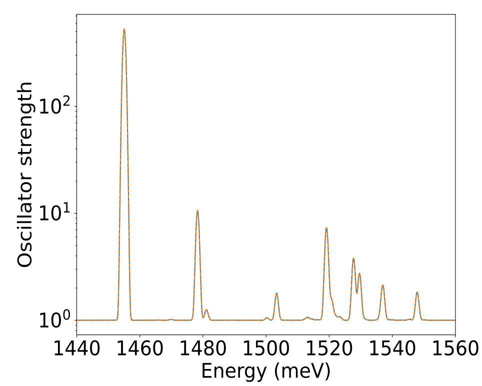

Fig. 1. Excitonic absorption spectra. The absorption spectrum of a $R = 20$ nm WSe2 quantum dot as a function of the photon energy.

Next, we construct the spectrum of electron-hole pairs and expand the exciton wavefunction in terms of these electron-hole pairs. We do so in the basis of an auxiliary quantum dot in which both holes and electrons are confined and electron repulsion by the gate is treated as a perturbation. Using these atomistic wave functions, we calculate Coulomb matrix elements, crucial for determining whether electron-hole pairs are sufficiently attracted to overcome electron repulsion by the confinement potential. Furthermore, we compute the dipole transition between hole and electron states to determine the absorption spectrum (see Fig. 1).

We then solve the Bethe-Salpeter equation to obtain exciton levels in our auxiliary quantum dot. Expanding the potential repelling electron in a quantum dot on the basis of exciton states in the auxiliary quantum dots allows for efficient attraction of the electron to the hole localized in the dot, overcoming the repulsive potential of the gate. Finally, we determine the dot radius, confining potential, and strength/screening of electron-electron interactions for which exciton is confined in a quantum dot and can be detected in transport experiments.

References

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