Quantum transport of excitons in lateral TMDs heterostructures

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ABSTRACT

We theoretically investigate exciton transport in lateral TMD's heterostructures within the Non-Equilibrium Green's Function (NEGF) formalism. An original self-energy is developed to describe the crucial exciton-phonon interactions.

INTRODUCTION

Excitonic devices, which are based on carriers made of bound electron-hole pairs, are very promising for energy-efficient operation. In that context, 2D materials transition metal dichalcogenides (TMDs), in which binding energy of excitons is much larger than in common semiconductors (few hundreds of meV), represent a great opportunity to develop that kind of devices operating at room temperature. However, most of the theoretical transport studies reported so far rely on classical physics: they are mainly based on fluid mechanics or empirical models [1].

MODEL AND DISCUSSIONS

We develop a NEGF quantum transport approach for the bosonic nature of excitons to investigate the dynamics of excitons in the TMDs lateral heterostructure shown in Fig. 1. Excitons are generated by a laser in the left reservoir, and we calculate the number of excitons collected in the right reservoir in which they recombined. The left reservoir boson statistics is estimated from the laser power.

Based on the tight-binding triangular lattice exciton model proposed in Ref. [2], we calculate the electronic band structure which reproduces the main features of typical transition metal dichalcogenides for the valence (v) and conduction (c) band (see Fig. 2 in the case of WSe_2).
The exciton bands are then obtained including the Coulomb interaction between the electron and the hole (Fig. 3a)). Typical binding energies of the first four optical excitons are between 100 and 500 meV. The corresponding square modulus of their wave-function is shown on Fig. 4 for the first four states. We also observe that simple effective mass scheme remains very accurate to determine the energy band of the first exciton state. The extracted effective masses of the first excitonic state at Γ point for the two TMDs are given in Fig. 3b).

Using those effective masses, we computed the transport properties of the first excitonic state of the TMD heterostructure shown in Fig. 1. Two incident laser powers have been considered. At low laser power (*i.e.* 3 mW), the resulting chemical potential μ is located at 0.11 eV below the excitonic band, leading a Boltzman character of the exciton distribution. As shown in Fig. 5, the exciton density is very close to the one obtained with a Fermi-Dirac distribution for electrons. However, at higher laser power (*i.e.* 10 mW), μ rises up to 0.017 eV below the bottom of the band. The Bose-Einstein character becomes now crucial to describe the exciton transport (see Fig. 6).

Exciton-phonon coupling is negligible in a given exciton state. It becomes however predominant when considering multiple bands (see Fig. 3). Based on the work of Antonius and Louie [3], we have developed a real-space exciton-phonon self-energy with a similar expression as the one of the electron-phonon coupling. Impact on TMDs heterostructures will be discussed.

REFERENCES

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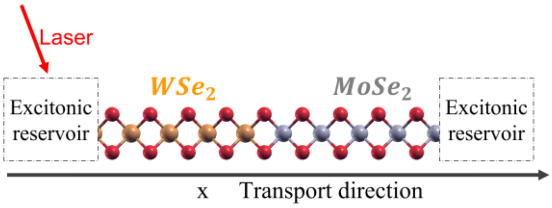


Figure 1. Lateral heterostructure of WSe_2-$MoSe_2$. Excitons are generated by an incident laser in the left reservoir.

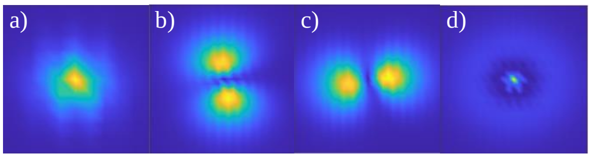


Figure 4. Probability of presence of the fourth exciton states at Γ: a) $E_1 = -0.4935$ eV, b) $E_2 = -0.1050$ eV, c) $E_3 = -0.1050$ eV, and d) $E_4 = -0.0847$ eV. For the first and fourth states (spin up), the central location between hole and electron emphasizes tightly bound exciton states.

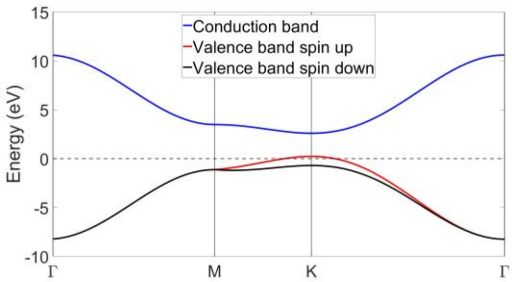


Figure 2. WSe_2 band structure without Coulomb interaction. The two spin channels are degenerate for the conduction band, while for the valence band, there is a splitting of the up and down spins due to spin-orbit coupling.

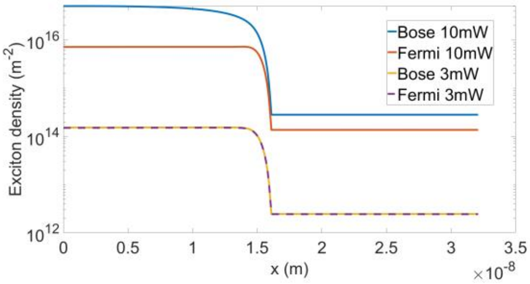
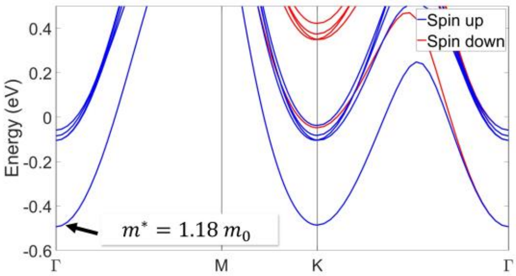


Figure 5. Exciton densities along the TMD heterostructure of Figure 1 for two incident laser powers applied in the left contact: P_{low}= 3 mW, P_{high}= 10 mW, and two assumed distributions (Fermi-Dirac and Bose-Einstein).

a)



b)

	WSe_2	$MoSe_2$
Effective mass (m^*)	$1.18m_0$	$1.63m_0$

Figure 3. a) WSe_2 exciton band structure with Coulomb interaction for the different spin states. b) Effective mass estimated from the exciton band structure obtained using the triangular model of Ref. [2].

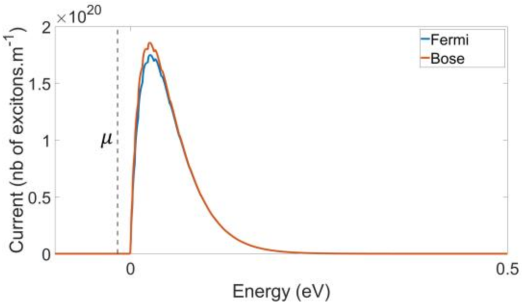


Figure 6. Exciton current spectra of the TMD heterostructure under a high incident laser power (10 mW) assuming Bosonic (red line) and Fermionic (blue line) transport.