ETH zürich

Master / Semester Thesis

Electron-electron interactions in quantum transport simulations

The Big Picture

Next-generation electronics are made of increasingly shrinking nanostructures, such as nano-sheets and nano-wires. For example, semiconducting monolayers are extensively researched because of their beneficial electronic properties and single-atomic layer thickness. One of these materials is the transition metal dichalcogenide MoS_2, shown in the figures below. However, these new structures pose new challenges for the modeling community due to reduced electronic screening. This enhances the electron-electron interactions, which are intrinsically hard to model, but have a strong impact on device operations.

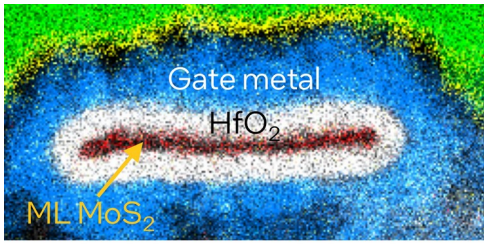

Figure 1: Gate-all-around NMOS device with a monolayer (ML) MoS2 channel. Image from ***W. Mortelmans et al, Intel, Paper #24.3 IEDM 2024.***

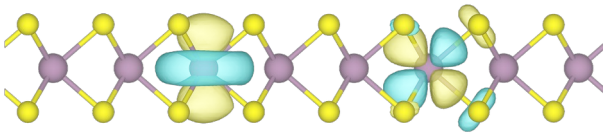

Figure 2: Monolayer MoS2, with two visible Wannier functions. The Wannier functions can be seen as electronic orbitals.

Project Description

In this project, you will study approximations for electron-electron interactions within the non-equilibrium Green's function (NEGF) formalism. The idea is to go beyond mean-field approaches to model dynamics of quasiparticles and electron-electron scattering phenomena, such as impact ionization and Auger recombination. Your work will be implemented in our new quantum transport code. Join us and help us in our quest for faster and more accurate device simulations!

Type of Work

The project will consist of:

- Theoretical investigations of approximations for electron-electron interactions.
- Model implementation and verification in Python.
- Performing simulations and analyzing results.

Prerequisites

We are seeking a highly motivated candidate with a strong interest in nanoelectronics and simulations. Knowledge of quantum mechanics and solid-state physics is required. The candidate should also have some Python programming skills. Naturally, experience with quantum transport is beneficial.

Status: Available

Looking for 1 Master/semester student

Interested candidates please contact: Anders Winka → awinka@iis.ee.ethz.ch
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