Atomistic Non-equilibrium Green's Function Simulation of Graphene Nano-ribbons in the Quantum Hall Regime

nanoHUB online simulation and more — an NCN project

Objective:

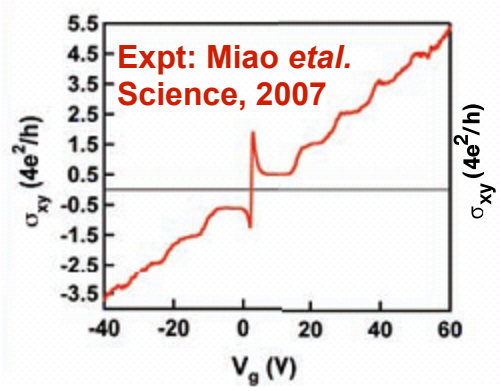
- To simulate Quantum Hall plateaus of Graphene nano-ribbons.

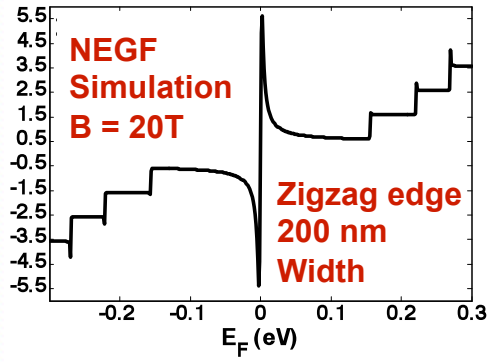
Approach:

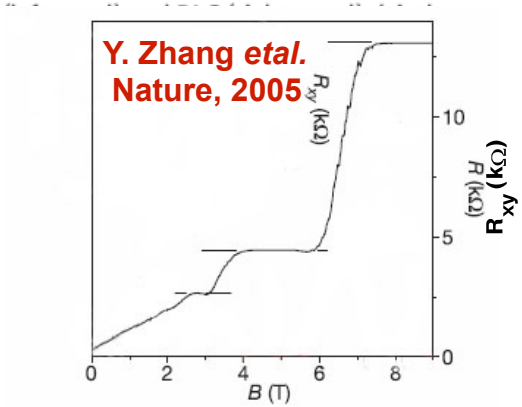
- Ballistic NEGF with nearest neighbor tight-binding model based on p_z orbital basis.
- Magnetic field (B) is included in both contacts and the channel through Peirels substitution.
- Surface green's function was calculated by Sancho-Rubio algorithm.
- Both Zigzag and Armchair edge ribbons were considered.

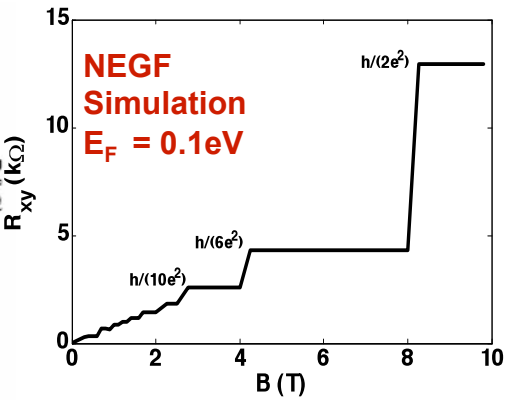
Impact:

- Simulating large dimensions is essential to keep the B-field with in the experimental limit (10-20T).
- Atomistic basis were essential to reproduce exact Quantum Hall plateaus.









Result:

- Hall conductance plateaus are coming at half-integer filling (per spin per valley)
- B-field in the contact self-energies made its effect seamless from the channel to the contacts, there by helped to capture the effect of having large channel length.

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