LSQUANT: Linear Scaling Quantum Transport Methodologies

Jose H. Garcia
Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain
e-mail: josehugo.garcia@icn2.cat

ABSTRACT SUBMISSION

In this session we will present a recently developed linear scaling or order-n computational techniques for quantum transport simulations name LSQUANT. We will be focusing on explaining the general formalism of the Kubo formula, and how in the noninteracting picture it converges in the Kubo-Greenwood for electrical conductivities and Kubo-Bastin for the Hall conductivity. We will also give further highlights regarding the trade-off between computational cost and accuracy of these numerical schemes and will consider also disordered linear chain and graphene to reinforce the content.

INTRODUCTION

The development of materials and devices relies on a balanced triad of experimentation, theory, and numerical simulations. The focus here is electronic devices, with a key focus on understanding the flow of electrons in response to an electric field, a central question in condensed matter physics that links to the performance of a myriad of devices. To accurately simulate electronic transport in complex materials and devices at the length scales observed in experiments, two elements are necessary: a realistic depiction of the structure and electronic properties of the material in question, and an efficient numerical method for simulating electronic transport.

Ab initio methods like density functional theory (DFT) have been successful in describing various properties of a wide range of materials, but their computational cost limits their application to large systems. This is where quasiparticle-based real-space tight-binding (TB) models come in, allowing for efficient numerical simulation.

The review focuses on efficient numerical calculations of the Kubo and Kubo–Bastin formulas for the electrical and Hall conductivities. These have been used in a wide array of realistic models of disordered and two-dimensional materials, multilayer graphene, organic semiconductors, conducting polymers, quasicrystals, silicon nanowires, carbon nanotubes, and three-dimensional models of topological insulators. Charge, spin, and Hall transport coefficients have been numerically computed in different transport regimes. These methods have proven to be a cornerstone for the simulation of quantum transport in complex situations, especially in the presence of weak magnetic fields and for disordered systems containing many millions of atoms.

Here, we will give a comprehensive description of the most efficient linear-scaling algorithms for studying electronic transport in complex forms of disordered materials. It is intended to serve as a valuable resource for future developers and users of such methodologies, which can be applied to a large variety of materials of current interest for fundamental science and advanced technologies.

THE SESSION

In this session we will go through the theory of quantum transport methodologies based on the Kubo formula. We will briefly go into the theory of tight binding Hamiltonians and how to construct inputs for the LSQUANT[1] code. We will provide a tutorial of how to perform quantum transport calculations and what are the key parameters to make realistic simulations. At the end we will discuss scalability and potential extensions of the method.

REFERENCES

[1] Z Fan, JH Garcia, AW Cummings, JE Barrios-Vargas, M Panhans, A Harju, F Ortmann, S Roche. *Linear scaling quantum transport methodologies,* Physics Reports Volume **903**, (2021).

[1]https://www.lsquant.org/