

# Numerical simulation of quantum transport phenomena

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April 11, 2019

## Abstract

*In recent years electronic transport properties of a variety of low dimensional electron systems, such as carbon based novel materials like carbon nanotubes or graphene, boron nitride, dichalcogenides, a selection of intriguing molecules and the surface states of topological insulators has captured the imagination of the solid-state community. These systems have several interesting properties that make them not only interesting for theoretical investigations but could also lead to revolutionary applications from wearable electronics to quantum computers. To take control of these peculiar features a comprehensive and detailed theoretical study is needed. During my work, I used Kwant to investigate these systems by numerical calculations. Kwant is a free and open source, powerful, and easy to use Python package for numerical calculations on tight-binding models with a strong focus on quantum transport.*

## Introduction

### The tight binding approximation

One of the main goals of solid-state physics is to explain physical properties of crystals, such as band structure, conductance, etc. based on their geometry. The electronic properties of crystals depend on their band structure. The band structure describes the range of energies that an electron within the solid may have (bands) and ranges of energy that it may not have (band gaps). To calculate the band structure of a solid within the tight binding model, the following approximations are made: we consider a single electron inside a static potential; we consider an infinite-size system; and we assume that the system is lattice-periodic. The band structure then can be calculated by finding the allowed energy levels of the electron. These energy eigenstates of the electron can be found by solving the time-independent Schrödinger equation:

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi_{n\mathbf{k}}(\mathbf{r}) = E_{n\mathbf{k}} \Psi_{n\mathbf{k}}(\mathbf{r}),$$

where  $n$  is the band index and  $\mathbf{k}$  is a wavevector in the first Brillouin-zone. Solving this equation is very hard in general, but thanks to the lattice-periodic structure of crystals, several approximate calculations can be made. One of these approximations is the so-called tight binding approximation, which is often used in solid-state physics.

The tight binding approximation assumes, that electrons are tightly bound to atoms to which they belong, and the effect of the other atoms arises as a perturbation.

First denote  $\hat{H}_{\text{at}}$  the Hamiltonian of a single, isolated atom, and its  $i$ th energy-eigenfunction  $\varphi_i(\alpha, \mathbf{r})$ . Here,  $\alpha$  represents all the internal degrees of freedom e.g. spin, atomic orbital, etc. These functions are solutions to the single-atom Schrödinger-equation

$$\underbrace{\left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{\text{at}}(\mathbf{r}) \right]}_{\hat{H}_{\text{at}}} \varphi_i(\alpha, \mathbf{r}) = \varepsilon_i \varphi_i(\alpha, \mathbf{r}),$$

These atomic orbitals are considered orthonormal i.e.:

$$\int d\mathbf{r} \varphi_i^*(\alpha, \mathbf{r}) \varphi_j(\alpha, \mathbf{r} + \mathbf{R}) = \begin{cases} 1, & \text{if } i = j \text{ and } \mathbf{R} = 0 \\ 0, & \text{otherwise} \end{cases}$$

The full Hamiltonian can be written as

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + \sum_{\mathbf{R}_l} V_{\text{at}}(\mathbf{r} - \mathbf{R}_l)$$

where  $\mathbf{R}_l$  are vectors pointing to the atoms in the lattice. Assuming that the atomic orbitals are decaying fast in function of  $|\mathbf{r}|$ , we can write that

$$\hat{H} \varphi_i(\alpha, \mathbf{r}) = \varepsilon_i \varphi_i(\alpha, \mathbf{r}).$$

According to the Bloch-theorem, the eigenfunctions in a lattice-periodic potential obey the following identity:

$$\Psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\mathbf{R}} \Psi_{n\mathbf{k}}(\mathbf{r}),$$

where  $\mathbf{R}$  is a real-space translation vector.

The idea is to write  $\Psi_{n\mathbf{k}}(\mathbf{r})$  as a linear combination of atomic wavefunctions localized to the neighboring atoms:

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}_l} e^{i\mathbf{k}\mathbf{R}_l} \varphi_n(\alpha, \mathbf{r} - \mathbf{R}_l),$$

where  $N$  is the number of lattice sites in the crystal.

Using these results, we can calculate the  $s$ -band ( $n = 1$ ):

$$E(\mathbf{k}) = \int d\mathbf{r} \Psi_{1\mathbf{k}}^*(\mathbf{r}) \hat{H} \Psi_{1\mathbf{k}}(\mathbf{r}) = \varepsilon_s + \sum_{\mathbf{R}_j} e^{i\mathbf{k}\mathbf{R}_j} \gamma(|\mathbf{R}_j|),$$

where

$$\varepsilon_s = \int d\mathbf{r} \varphi_s^*(\mathbf{r}) \hat{H} \varphi_s(\mathbf{r}),$$

and

$$\gamma(|\mathbf{R}_j|) = \int d\mathbf{r} \varphi_s^*(\mathbf{r}) \hat{H} \varphi_s(\mathbf{r} - \mathbf{R}_j).$$

The sum above is over all the neighbors of the atom at positions  $\mathbf{R}_j$ , and the values  $\gamma(|\mathbf{R}_j|)$  are called overlap integrals.

## Second quantization formalism

In the second quantization formalism, we are considering a lattice with  $N$  sites, labeled by the positions  $\mathbf{r}_j, j \in \{1, \dots, N\}$ . The state of the lattice can be expressed in terms of the number of particles at each site. This is called the occupation number representation:  $|\Psi\rangle \equiv |n_1, n_2, \dots, n_N\rangle$ . The ground state (vacuum state) is  $|0\rangle = |0, \dots, 0\rangle$ . Given this, we can define creation and annihilation operators. For bosonic particles, the creation operator  $b_j^\dagger$  creates a boson at  $\mathbf{r}_j$ :

$$b_j^\dagger |n_1, \dots, n_j, \dots, n_N\rangle = \sqrt{n_j + 1} |n_1, \dots, n_j + 1, \dots, n_N\rangle$$

The annihilation operator  $b_j$  destroys a boson at  $\mathbf{r}_j$ :

$$b_j |n_1, \dots, n_j, \dots, n_N\rangle = \sqrt{n_j} |n_1, \dots, n_j - 1, \dots, n_N\rangle$$

From these relations, we can derive the bosonic commutation relations:

$$\begin{aligned} [b_l^\dagger, b_m^\dagger] &= [b_l, b_m] = 0, \\ [b_l, b_m^\dagger] &= \delta_{lm} \end{aligned}$$

Fermionic creation and annihilation operators are slightly different:

$$\begin{aligned} c_j^\dagger |n_1, \dots, n_j, \dots, n_N\rangle &= \\ = (-1)^{\sum_{k=1}^{j-1} n_k} \sqrt{n_j + 1} |n_1, \dots, n_j + 1, \dots, n_N\rangle \end{aligned}$$

## The Kwant package

Kwant is a Python package for numerical quantum transport calculations [4] designed such that the natural concepts of the theory of quantum transport (lattices, symmetries, electrodes, orbital/spin/electron-hole degrees of freedom) are exposed in a simple and transparent way.

Kwant is free software available at <http://kwant-project.org/>. A kwant system consists of a finite scattering region, described with a scattering Hamiltonian  $H_S$  and a number of infinite regions known as leads. The leads are built of unit cells, each unit cell described with a Hamiltonian  $H_L$ . The connections between unit cells of the leads are described with a block-submatrix  $V_L$ , while the hopping from the scattering region to the lead region is described with another block-matrix  $V_{LS}$ . The Hamiltonian of such a system looks like below:

$$H = \begin{pmatrix} \ddots & V_L & & \\ V_L^\dagger & H_L & V_L & \\ & V_L^\dagger & H_L & V_{LS} \\ & & V_{LS}^\dagger & H_S \end{pmatrix}$$

In kwant, designing a tight-binding system is a mapping between the vertices and edges (sites and hoppings) of a graph to the corresponding values of the Hamiltonian. This is done using a **Builder** object. Sites can be often classified by type of atom or the lattice to which they belong [4].

## Quantum point contact

## Graphene minimal conductivity

## References

- [1] The official homepage of the kwant project: <https://kwant-project.org>.
- [2] The official documentation for kwant 1.3.2 <https://kwant-project.org/doc/1/>.
- [3] Supriyo Datta. *Electronic transport in mesoscopic systems*. Cambridge Studies in Semiconductor Physics and Microelectronic Engineering. Cambridge University Press, 1995.
- [4] Christoph W. Groth, Michael Wimmer, Anton R. Akhmerov, and Xavier Waintal. Kwant: a software package for quantum transport. *New Journal of Physics*, 16:063065, Jun 2014.

## A Some appendix

### A.1 Some subsection