Numerical simulation of quantum transport phenomena

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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 numericalccalculations 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 phyisical 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 Schröinger 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 Brilluin-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 $\hat{H}_{\mathrm{at}}$ the Hamiltonian of a single, isolated atom, and its ith energy-eigenfunction $\varphi_i(\alpha, \mathbf{r})$. Here, α represents all the internal degrees of freedom e.g. spin, atomic orbital, etc. These functions are solutions to the single-atom Schrödinger-equation

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

These atomic orbitals are considered orthonormal i.e.:

$$\int \mathrm{d}\mathbf{r}\varphi_i^*(\alpha, \mathbf{r})\varphi_j(\alpha, \mathbf{r}+\mathbf{R}) = \left\{ \begin{array}{l} 1, \text{ if } i = j \text{ and } \mathbf{R} = 0 \\ 0, \text{ otherwise} \end{array} \right.$$

The full Hamiltonian can be written as

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

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 neigboring 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 $\mathbf{r}_j, j \in \{1, ..., N\}$. 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: $|\Psi\rangle \equiv |n_1, n_2, ..., n_N\rangle$. The ground state (vacuum state) is $|0\rangle = |0, ..., 0\rangle$. Given this, we can define creation and annihilation operators. For bosonic particles, the creation operator $b_j^\dagger$ creates a boson at $\mathbf{r}_j$:

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

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

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

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

$$[b_l, b_m^\dagger] = \delta_{lm}$$
$$[b_l^\dagger, b_m^\dagger] = [b_l, b_m] = 0,$$

Fermionic creation and annihilation operators are slightly different:

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

$$c_j |n_1, ..., n_j, ..., n_N\rangle =$$
$$= (-1)^{\sum_{k=1}^{j-1} n_k} \sqrt{n_j} |n_1, ..., n_j - 1, ..., n_N\rangle$$

If we include spin states σ, the operators $c_{i\sigma}^\dagger$, $c_{j\sigma'}$ satisfy the anticommutation relations:

$$\{c_{i\sigma}, c_{j\sigma'}^\dagger\} = \delta_{ij}\delta_{\sigma\sigma'}$$
$$\{c_{i\sigma}, c_{j\sigma'}\} = \{c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger\} = 0$$

We can also define momentum-space creation and annihilation operators $c_{\mathbf{k}\sigma}^\dagger, c_{\mathbf{k}\sigma'}$:

$$c_{\mathbf{k}}^\dagger |0\rangle = |\mathbf{k}\rangle$$
$$c_{\mathbf{k}} |\mathbf{k}\rangle = |0\rangle$$

They can be transformed back to real space

$$c_j^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_j} c_{\mathbf{k}}^\dagger$$
$$c_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_j} c_{\mathbf{k}}$$

and vice versa:

$$c_{\mathbf{k}}^\dagger = \frac{1}{\sqrt{N}} \sum_{j} e^{i\mathbf{k}\mathbf{r}_j} c_j^\dagger$$
$$c_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j} e^{-i\mathbf{k}\mathbf{r}_j} c_j$$

In second quantization formalism, single-particle operators (operators which involve a sum of single particles) can be written as

$$\hat{F} = \sum_{l,l'} \langle l|\hat{f}|l'\rangle a_l^\dagger a_{l'}$$

where,

$$\langle l|\hat{f}|l'\rangle = \int d^3\mathbf{r}\, \phi_l^*(\mathbf{r}) \hat{f}(\mathbf{r}, \mathbf{p}) \phi_{l'}(\mathbf{r})$$

Using these equations, we can write the second-quantized Hamiltonian for free electrons in momentum-space and position-space as follows:

$$\hat{\mathcal{H}}_{\text{free}} = \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}^{\text{free}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}$$

$$= \frac{1}{N} \sum_{i,j,\sigma} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}}^{\text{free}} e^{i\mathbf{k}(\mathbf{r}_i - \mathbf{r}_j)} c_{i\sigma}^\dagger c_{j\sigma}$$

where,

$$\epsilon_{\mathbf{k}}^{\text{free}} = \frac{\hbar^2 k^2}{2m}.$$

The second-quantized form of the tight binding Hamiltonian is

$$\hat{\mathcal{H}} = -t \sum_{<i,j>,\sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma})$$
$$= \sum_{\mathbf{k},\sigma} \epsilon_{\mathbf{k}}^{\text{tb}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$$

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

In kwant, it is easy to define a two-dimensional tight binding system using the `Builder` class. I created a simple quantum point contact shown in figure 1.
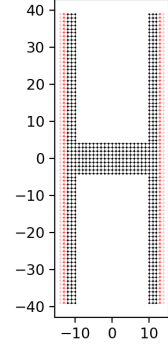

Figure 1: Plot of a square lattice quantum point contact of width $W = 5$ and length $L = 10$ defined in kwant.

The quantum point contacts have a specific, quantized conductance in function of energy [9]. I calculated the transmission coefficients of the structure shown in figure 1, and plotted against the energy. The results (shown in fig. 2.) reflect the transmission quantization presented in [9].
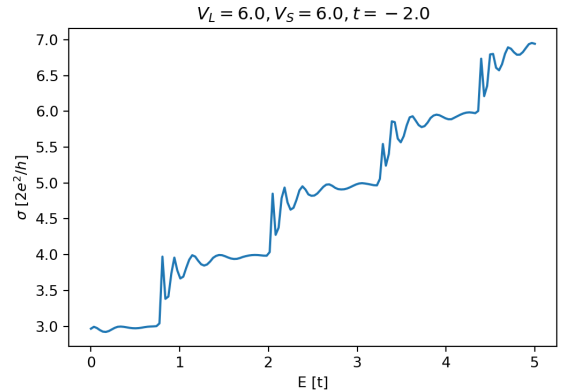

Figure 2: Transmission coefficients calculated using the system shown in figure 1. The potential in the scattering region and in leads is $V_L = V_S = 6$eV, while the hopping energy is $t = -2$eV.

Using kwants built-in function `kwant.physics.two_terminal_shotnoise`, I was able to easily calculate the shot-noise [8] between leads. I created the structure shown on figure 1, then calculated the two-terminal shot-noise between leads. The results are shown on figure 3.
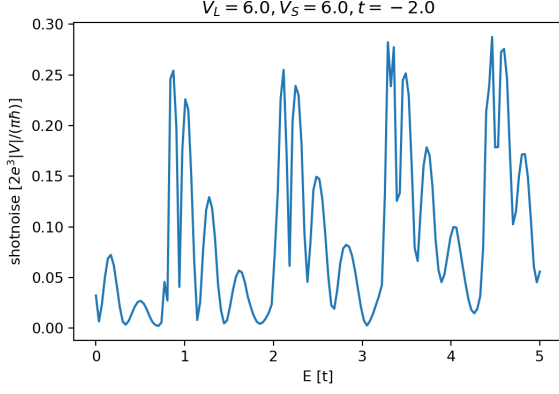
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Figure 3: Shot noise in function of the electron energy.

Figure 5: Transmission coefficient of a quantum point contact as a function of the external magnetic flux.

If a tight-binding system is placed in magnetic field, this can be taken into account by using Peierls' substitution:

$$t_{ij} \rightarrow t_{ij} \times \exp\left(i\frac{e}{\hbar}\int_{\mathbf{x}_j}^{\mathbf{x}_i}\mathbf{A}(\mathbf{x})d\mathbf{s}\right)$$

For 2D square lattices this can be rewritten as

$$\exp\left(i\,2\pi\frac{\phi}{\phi_0}\frac{(y_i+y_j)(x_i-x_j)}{2a^2}\right)$$

where $\phi = Ba^2$ is the flux through a unit cell in the square lattice, and $\phi_0 = h/e$ is the magnetic flux quantum. To study the effect of magnetic field in case of 2D square lattices, I defined a quantum point contact in kwant. This structure is shown on figure 4.

Graphene minimal conductivity

topological Anderson Insulators

$$\mathcal{H} = \sum_i V_{\text{dis}}\,|i\rangle\langle i| + \sum_{<i,j>} t_{ij}\,|i\rangle\langle j|$$

$$V_{\text{dis}} = \sum_i W_i\,|i\rangle\langle i|$$

$$t_{ij} = \exp\left(i\,2\pi\frac{\phi}{\phi_0}\frac{(y_i+y_j)(x_i-x_j)}{2a^2}\right)$$

Figure 4: A quantum point contact of width $W = 5$ and length $L = 15$ defined and plotted using kwant.

Figure 6:

Using kwant's built-in functions, I calculated the transmission coefficients between leads 0 and 1, for a range of magnetic field strengths. Th results are plotted on figure 5.
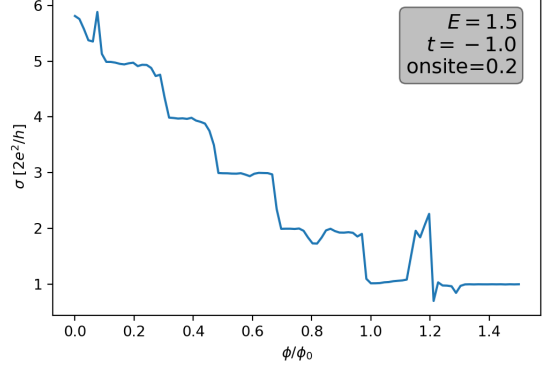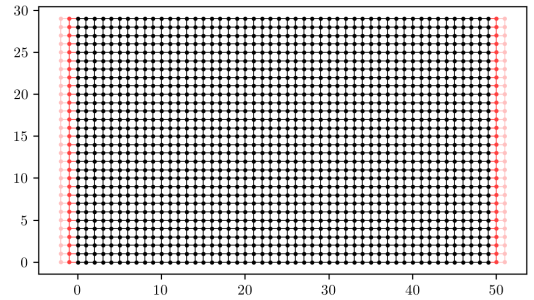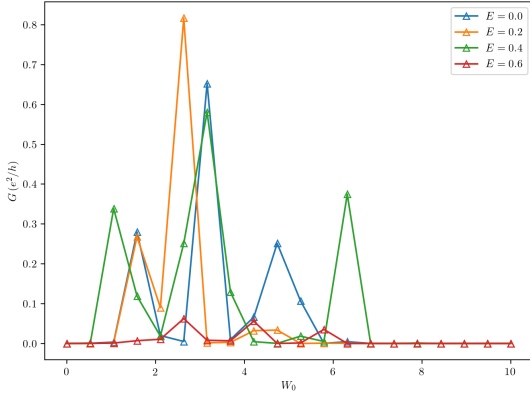
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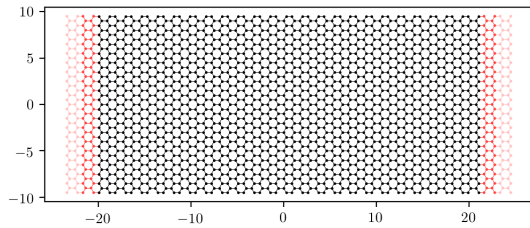
Figure 7:

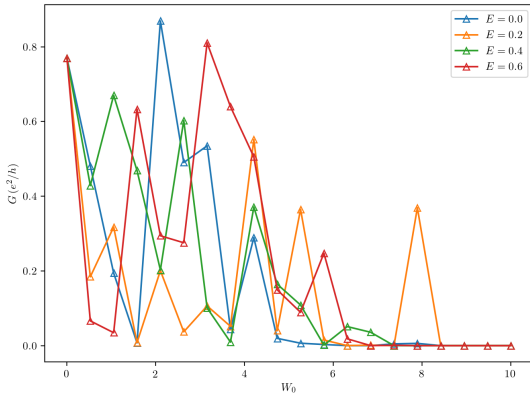Figure 8:

Figure 9:
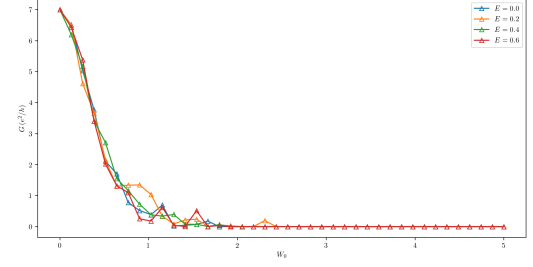
Figure 10:
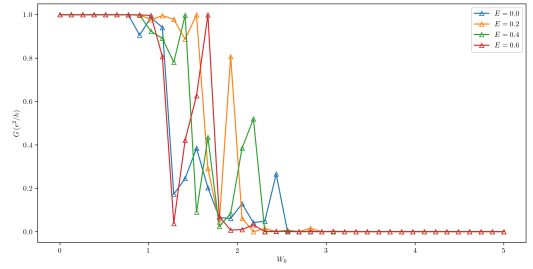
Figure 11:

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.

[5] Hua Jiang, Lei Wang, Qing-Feng Sun, and X. C. Xie. Numerical study of the topological Anderson insulator in HgTe/CdTe quantum wells. *Physical Review B*, 80(16):165316, Oct 2009.

[6] Jian Li, Rui-Lin Chu, J. K. Jain, and Shun-Qing Shen. Topological Anderson Insulator. , 102(13):136806, Apr 2009.

[7] Thibaud Louvet, Pierre Delplace, Andrei A. Fedorenko, and David Carpentier. On the origin of

minimal conductivity at a band crossing. *Physical Review B*, 92(15):155116, Oct 2015.

[8] J. Tworzydło, B. Trauzettel, M. Titov, A. Rycerz, and C. W. J. Beenakker. Sub-Poissonian Shot Noise in Graphene. , 96(24):246802, Jun 2006.

[9] H. van Houten and C. W. J. Beenakker. Quantum Point Contacts. *arXiv e-prints*, pages cond–mat/0512609, Dec 2005.

A Some appendix

A.1 Some subsection