Numerical simulation of quantum transport phenomena using the kwant package

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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 numericalc 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 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 $\hat{H}_{\text{at}}$ 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

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

These atomic orbitals are considered orthonormal i.e.:

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

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 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 ($n=1$):

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

where

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

and

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

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 annihillation operators. For bosonic particles, the creation operator $b^\dagger_j$ creates a boson at $\mathbf{r}_j$:

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

The annihillation 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:

$$[b_l, b^\dagger_m] = \delta_{lm}$$
$$[b^\dagger_l, b^\dagger_m] = [b_l, b_m] = 0,$$

Fermionic creation and annihillation operators are slightly different:

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

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

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

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

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

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

They can be transformed back to real space

$$c^\dagger_j = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{-i\mathbf{k}\mathbf{r}_j}c^\dagger_{\mathbf{k}}$$
$$c_j = \frac{1}{\sqrt{N}}\sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}_j}c_j$$

and vice versa:

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

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

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

where,

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

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

$$\hat{\mathcal{H}}_{\text{free}} = \sum_{\mathbf{k},\sigma}\epsilon^{\text{free}}_{\mathbf{k}}c^\dagger_{\mathbf{k},\sigma}c_{\mathbf{k},\sigma}$$
$$= \frac{1}{N}\sum_{i,j,\sigma}\sum_{\mathbf{k}}\epsilon^{\text{free}}_{\mathbf{k}}e^{i\mathbf{k}(\mathbf{r}_i-\mathbf{r}_j)}c^\dagger_{i\sigma}c_{j\sigma}$$

where,

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

The second-quantized form of the tight binding Hamiltonian is

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

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]. Kwant has internal solver algorithms, that are optimized, and capable of parallel computing. The task that kwant does, is to solve the eigenvalue problem of the system defined, then construct the scattering matrix, $S_m n$. Then, for example the conductance between leads a and b can be calculated as

$$G_{ab} = \frac{e^2}{h} \sum_{n\in a, m\in b} |S_m n|^2$$

A more detailed description of kwant can be found in the original kwant paper [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.

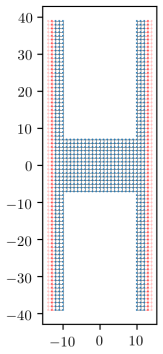

Figure 1: Plot of a square lattice quantum point contact of width $W = 8$ and length $L = 10$ defined in kwant.

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].

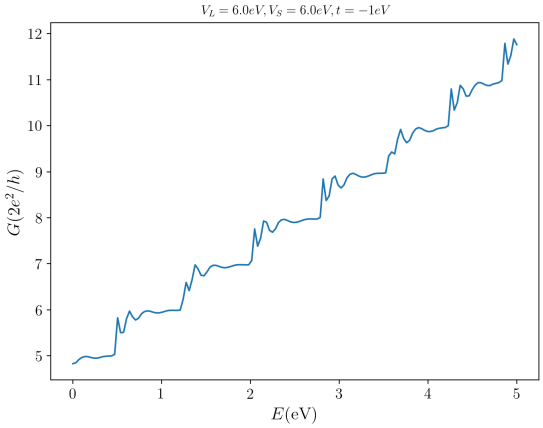

Figure 2: Transmission coefficients calculated using the system shown in figure 1. The potential in the scattering region and in leads is $V_L = V_S = 6$eV, while the hopping energy is $t = -2$eV.

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.

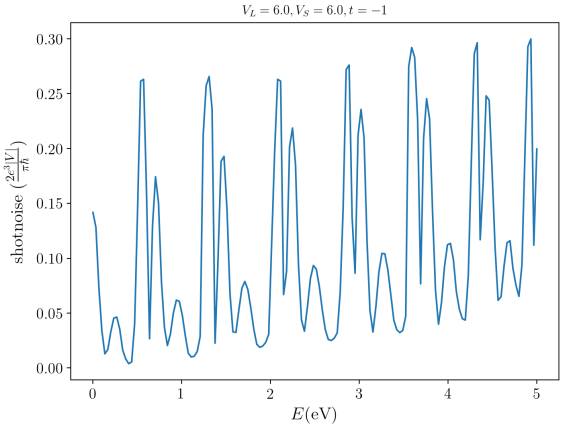

Figure 3: Shot noise in function of the electron energy.

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

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

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.

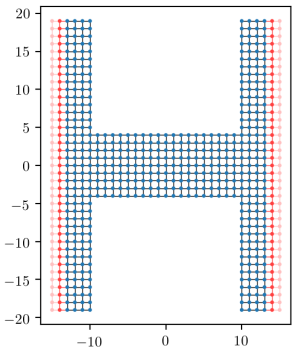

Figure 4: A quantum point contact of width $W = 5$ and length $L = 10$ defined and plotted using kwant.

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.

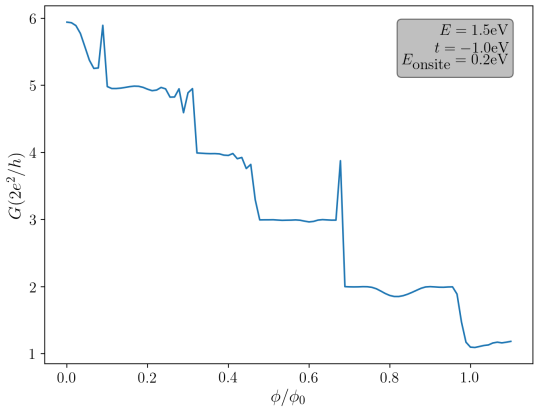

Figure 5: Transmission coefficient of a quantum point contact as a function of the external magnetic flux.

Graphene minimal conductivity

I studied an ideal strip of graphene of width W, and length L, with no impurities, or defects. To do this, I defined a bipartite graphene structure as shown in figure 6, then attached leads to it.

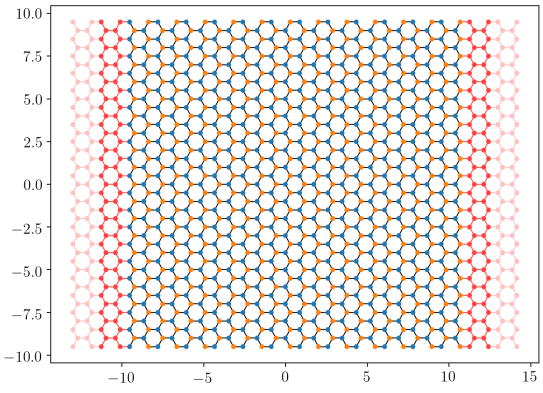

Figure 6: A bipartite graphene strip, defined in kwant, with leads attached to it.

With the help of kwant, I calculated the transmission probability of massless Dirac fermions through the strip in function of the gate voltage, V_{gate}.

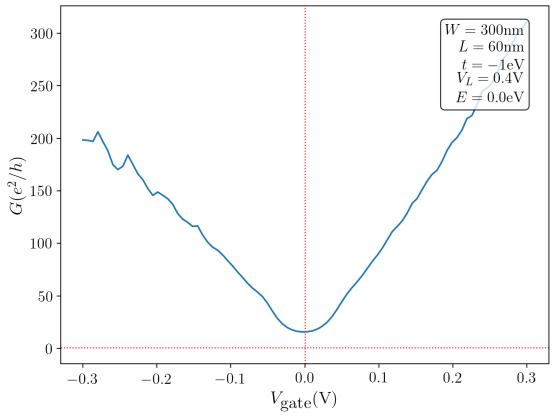

Figure 7: The transmission coefficient of a graphene strip in function of V_{gate} at a fixed $W/L = 5$ aspect ratio.

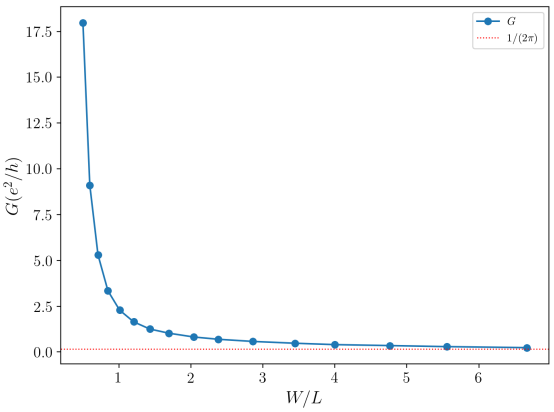

Figure 8: The transmission coefficient of a graphene strip in function of W/L ratio. The results are obtained using kwant.

Topological Anderson Insulators

My last was to test, and try to reproduce the results of the article [6] abot Topological Anderson Insulators. The article [6] defines the continuous Hamiltonian for a HgTe/CdTe heterostructure, as follows:

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^\dagger(-\mathbf{k}) \end{pmatrix},$$

where $h(\mathbf{k}) = \epsilon(k) + \mathbf{d}(\mathbf{k}) \cdot \sigma$, $\mathbf{k} = (k_x, k_y)$ and $\mathbf{d}(\mathbf{k}) = (Ak_x, Ak_y, M - Bk^2)$; $\epsilon(k) = C - Dk^2$.

The parameters used by my calculations are (following the article): $A = 364.5$meVnm, $B = -686$meVnm^2, $C = 0$, $D = -512$meVnm^2; $M = 12$meV for the "inverted" quantum well, and $M = -1$meV for the normal quantum well. The disorder was taken into consideration via a disorder Hamiltonian:

$$\mathcal{H}_{\text{disorder}} = \sum_i W_i \left|i\right\rangle \left\langle i\right|,$$

where W_i are random parameters uniformly distributed in the range $[-W/2, W/2]$.

Topological Anderson Insulators are materials, which are normally metallic. However, it can be shown experimentally, that disorder can create a topological insulator for parameters, where the system was metallic in absence of disorder. This phase is called Topological Anderson Insulator (TAI).

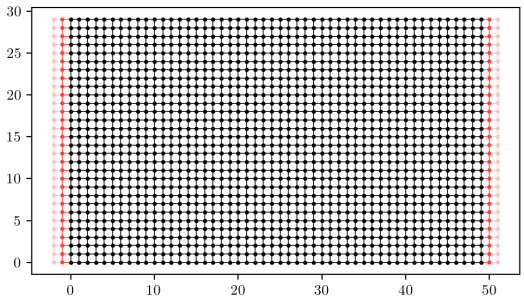

Figure 9: The HgTe scattering region is modeled with a sqare lattice with lattice constant $a = 5$. This is a small example, with $L_y = 30a$ and $L_x = 50a$, the original strip used for calculations was larger.

To test TAI numerically, I considered a strip of square lattice (figure 9). The parameters of the strip I used for calculations are $a = 5$, $L_y = 500a$, $L_x = 2500a$. The Hamiltonian for the system is defined above, and is discretized automatically by `kwant.continuum.discretize`.

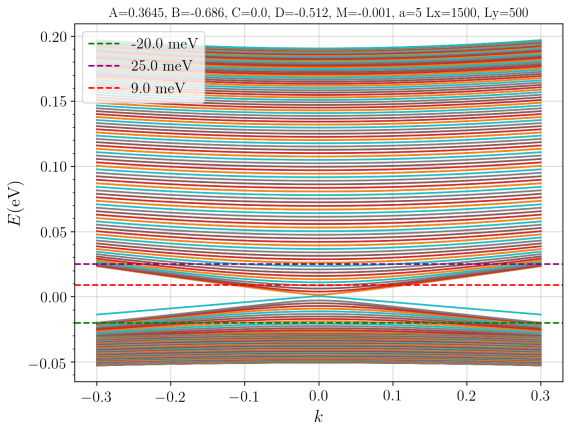

Figure 10: Band structure for the "inverted" quantum well, with $M = -1$meV

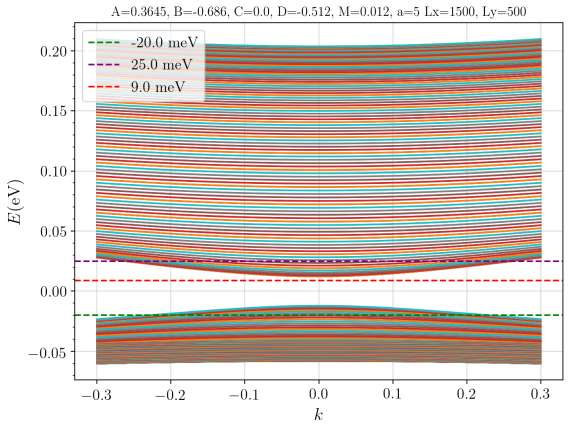

Figure 11: Band structure for the "normal" quantum well, with $M = 12$meV

The band structure for the normal configuration is shown on figure 10, while the "inverted" configuration is shown on figure 11.

The results should indicate that there is a plateau after $W = 100$meV in the case of $E_F = 25$meV, this is expected based on the article [6]. Figure 12. shows these results in the original paper.

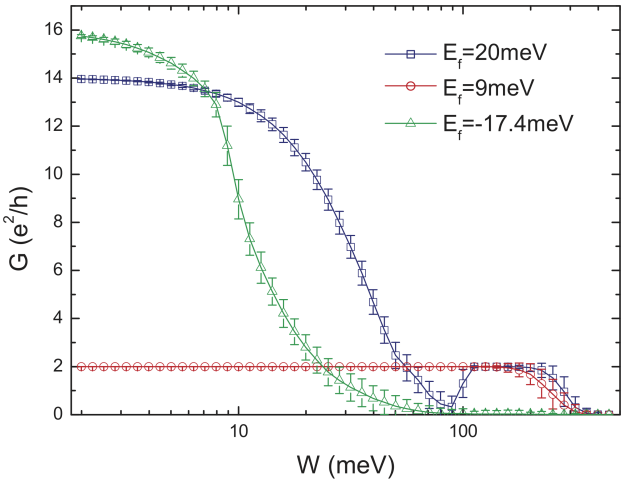

Figure 12: The results for conductance against disorder parameter presented in the original paper [6].

Figure 13. shows my results computed with kwant, on a system that corresponds to the "normal" phase ($M = 12$meV). This should have a plateau at around $W = 100$meV, but there is no plateau found. This may be due to some misconfiguration of the system, or the lack of statistics (more cycles of computation).

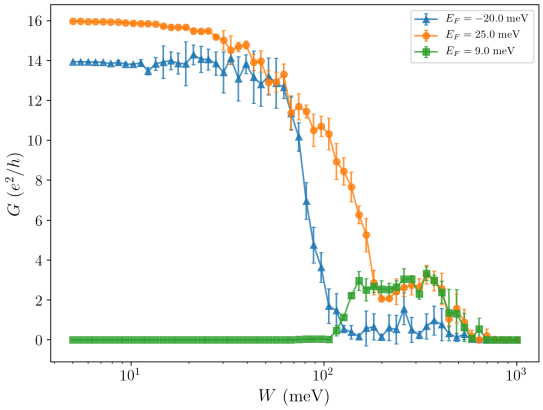

Figure 13:

Conclusion

In this semester, during my work, I learned about the kwant package. Furthermore, I learned some basic concepts of numerical materials science, computational physics and some basic concepts of mesoscopic transport phenomena. I was able to define tight-binding systems using kwant, do some basic calculations on them. I investigated quantum point contacts, the effect of magnetic field, the minimal conductivity

of a graphene strip. A slightly more advanced topic was the topological Anderson-insulator, and the effect of disorder in mesoscopic systems. My results are often a little different from the literature, but this is probably due to the lack of time and computational power.

References

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