

Introduction to Graphene-Based Nanomaterials (additional material)

**From Electronic Structure to Quantum
Transport**

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Table of Instructions

Here we give some complementary information to the *Guide to the Book* presented at the end of Chapter 1 of Introduction to Graphene-Based Nanomaterials. We start with the pre-requisites and then follow with a few suggested paths through the book.

1.1 Pre-requisites

Throughout the book it is assumed that you have a general knowledge on Condensed Matter Physics at the level of an introductory course. If you need to refresh some concepts (lattices, Bloch's theorem, etc.) a few suggested textbooks are:

- *Solid State Physics* by Neil Ashcroft and N. David Mermin (Cengage Learning, 1976) is a classic textbook.
- *Solid-State Physics: An Introduction to Principles of Materials Science* by Harald Ibach and Hans Lüth (4th edition, Springer, 2009) is a popular textbook with a comprehensive overview of theoretical and experimental concepts.

A basic knowledge of quantum mechanics as required in a course on Condensed Matter Physics is also a pre-requisite. From our own teaching experience we noticed that sometimes students coming from disciplines other than Physics may need to refresh a few topics including Dirac bra-ket notation and Fermi Golden Rule. Dirac notation is a very convenient means to the formalism that should be in your toolbox, if you are not acquainted with it we suggest for you to follow the text book *Quantum Mechanics Vol. I* by C. Cohen-Tannoudji, B. Diu, and F. Lalöe (Wiley, New York, 1992). *Molecular Quantum Mechanics* by Atkins and Friedman (Oxford University Press, 2005) also contains a short introduction. Regarding Fermi Golden Rule you may want to follow any of the textbooks mentioned before.

1.2 Table of Instructions

Introduction to Graphene-Based Nanomaterials can be read in many ways and you are encouraged to make your own path through the book. Here we would like to suggest a few ways of doing it.

Path 1. The first one is to do it linearly from the first chapter to the end. This way the contents drive you from electronic structure to quantum transport in ballistic and disordered graphene-based nanomaterials. An overview on the applications is given in Chapter 8. The appendixes complement some of the topics in Chapters 2 and 3 and may be visited as needed.

Path 2. An alternative path is to frontload the overview of general concepts on quantum transport and then come to the specifics of graphene-based materials. Your path would then follow the order: Chapter 1, Chapter 3, Appendixes C-D, Chapter 2, Chapters 4-8.

Path 3. A third alternative is to hop through the entire set of material (comprising about 70 sections) according to a personalized **Table of Instructions**. To get yours we invite you answer a short questionnaire at:

www.introductiontographene.org

Please do not forget to check for the additional material in our website, we strongly encourage you to engage as early as possible in solving the exercises and problems. Learning by doing is by far the most effective and you can combine problem solving with reading of the necessary sections. In the following pages we include a selection of additional exercises and problems.

We hope that you find this book to be a useful companion for starting in this field and perhaps even for your day-to-day research.

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2⁺ Electronic properties of carbon-based nanostructures (Additional material)

Additional problems

2.13 Chirality revisited.

In this exercise we come back to [Section 2.2.2](#) of Introduction to Graphene-Based Nanomaterials which focuses on a low energy approximation for the electronic structure of graphene.

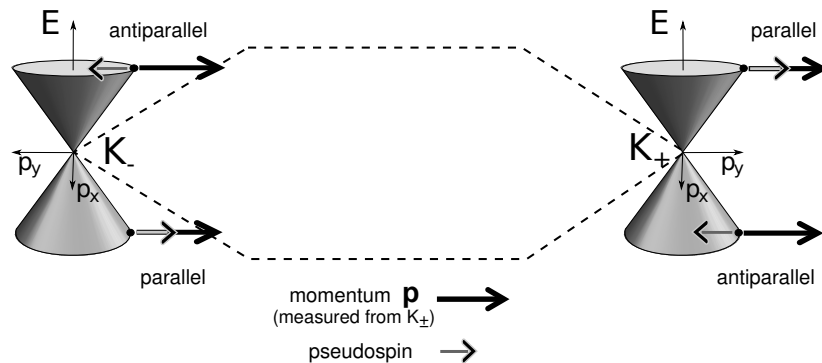


Figure 2.1 Sketch of the two inequivalent Dirac cones at K_+ and K_- points of the first Brillouin zone, together with direction of the pseudospin parallel or antiparallel to the momentum $\mathbf{p}$ of selected energies in conduction and valence bands. Reproduced from Introduction to Graphene-Based Nanomaterials [1].

First, let us recall that the eigenstates of the low-energy Hamiltonian have a fixed projection of the pseudospin (simply because the Hamiltonian itself is proportional to this projection!). The Hamiltonian in the vicinity of each inequivalent K point is proportional to $\hat{\sigma} \cdot \mathbf{p}$ (close to the K_+ point) and $\hat{\sigma}^t \cdot \mathbf{p}$ (close to the K_- point). This is, the low-energy Hamiltonians around each K point are identical except that in the first case one has the pseudospin operator which is given by the *right-handed* Pauli matrices, while in the last case one has the *left-handed* Pauli matrices ($\hat{\sigma}^t$). We note that in the previous reasoning the full eigenfunctions are described by 4-component spinors arranged in the form:

$$(|\Psi_{K_+,A}\rangle, |\Psi_{K_+,B}\rangle, |\Psi_{K_-,A}\rangle, |\Psi_{K_-,B}\rangle)^t.$$

Therefore, chirality is said to be reversed when passing from K_+ to K_- (see Fig. 2.1). The subtle point here is that helicity operator needs to be changed from right to left handed, *i.e.* it is not the same in both valleys (the Hamiltonian at K_- does not commute with $\hat{h}$ defined in Eq. (2.23)).

Show that a way of having the helicity operator defined in the same way in both valleys is to use the following ordering for the 4-component spinor:

$$(|\Psi_{K_+,A}\rangle, |\Psi_{K_+,B}\rangle, |\Psi_{K_-,B}\rangle, |\Psi_{K_-,A}\rangle)^t.$$

2.14 Berry's Phase.

Let us consider a system with a Hamiltonian $\mathcal{H}$ which varies in time through a set of parameters $\mathbf{X}(t) = (X_1(t), X_2(t), \dots)$, *i.e.* $\mathcal{H} = \mathcal{H}(\mathbf{X}(t))$. Let us assume that the time-variation is very slow as compared to all the other energy scales (adiabatic evolution).

In this approximation, it is useful to define, at each instant of time an orthonormal basis which follows the slow time evolution of the Hamiltonian, the basis of eigenstates of the instantaneous Hamiltonian:

$$\mathcal{H}(\mathbf{X}) |\phi_n(X)\rangle = \varepsilon_n(X) |\phi_n(X)\rangle$$

Even more, if the system is originally in an eigenstate of the Hamiltonian, it will remain in an eigenstate of $\mathcal{H}(t)$ as long as the time-variation is slow enough (this is the so-called adiabatic theorem). The state in such case will have the form

$$|\psi(t)\rangle = \exp(-i\alpha(t)) |\phi_n(t)\rangle,$$

where the phase $\alpha(t)$ is the only remaining degree of freedom. For a time-independent Hamiltonian this phase is just the *dynamical phase* given by the time-evolution and is fixed by the energy ε_n . One could naively expect that the same will happen in presence of a time-dependent variation. Strikingly, this is not the case and, as we will see in this exercise, the phase also contains an additional *geometrical phase* [2].

- (a) Consider the time-dependent Schrödinger equation for a system in the conditions described before:

$$\mathcal{H}(t)|\psi(t)\rangle = i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle.$$

Show that $|\psi(t)\rangle$ can be written in the form:

$$|\psi(t)\rangle = \exp\left(-\frac{i}{\hbar} \int_0^t \varepsilon_n(\mathbf{X}(t')) dt'\right) \exp(i\gamma_n(t)) |\phi_n(t)\rangle.$$

The phase $\gamma_n(t)$ is the so-called geometrical phase.

- (b) Obtain an expression for $\gamma_n(t)$. Show that the geometrical phase acquired over a closed path $\mathcal{C}$, the Berry phase, is given by:

$$\gamma_n = i \int_{\mathcal{C}} \langle \phi_n(\mathbf{X}) | \nabla_{\mathbf{X}} | \phi_n(\mathbf{X}) \rangle \cdot d\mathbf{X}.$$

Note that based on the previous equation one can define the analog of a vector potential:

$$\mathbf{A}_n = i\langle\phi_n(\mathbf{X})|\nabla_{\mathbf{X}}|\phi_n(\mathbf{X})\rangle,$$

such that

$$\gamma_n = \int_C \mathbf{A}_n \cdot d\mathbf{X}.$$

$\mathbf{A}_n$ is the so-called Berry vector potential or Berry connection.

- (c) Consider the case of graphene. Compute the Berry phase associated to a closed loop around a K point. Plot the Berry curvature for graphene near a K point. You may use the PythTB package (Python) from the group of David Vanderbilt at Rutgers University (<http://www.physics.rutgers.edu/pythtb/>) or any other software of your choice to compute this in a straightforward way.
- (d) Repeat the previous point for bilayer graphene.

Further reading: For a resource letter see [3]. In the context of graphene you may enjoy references [4, 5].

2.15 Landau levels in graphene.

Consider the low-energy approximation for electrons in graphene. Consider a magnetic field perpendicular to the graphene plane.

- (a) By using the Peierls substitution $\hat{\mathbf{p}} \rightarrow \hat{\mathbf{p}} + e\mathbf{A}$ (where $\mathbf{A}$ is the vector potential determining the magnetic field $\mathbf{B}$, $\mathbf{B} = \nabla \times \mathbf{A}$) solve for the spectra and obtain the Landau levels. What is the degeneracy of each Landau level?
- (b) Compare your response to (a) with that for the case of a normal metal.
- (c) The Landau level with $n = 0$ is a special one. Comment on this Landau level and the character of the corresponding wavefunction.

Hint: For a solution see Section 2.7.5 of Introduction to Graphene-Based Nanomaterials [1].

2.16 Stretching graphene.

Let us imagine that we stretch graphene. The effect of stretching on the electronic structure can be modeled as a change in the nearest neighbors hopping matrix elements. Therefore, instead of having a uniform value, say γ_0 , we would have in general γ_a , γ_b , and γ_c as shown in the scheme in Fig. 2.2.

- (a) Explore how the electronic structure changes when the hoppings are altered due to the stretching. Use a simple tight-binding model and assume $\gamma_a = \gamma_b$.
- (b) Consider the situation when γ_c is larger/smaller than $\gamma_a = \gamma_b$. Is it possible to introduce a gap at the Dirac point? Plot the energy dispersions for a few typical cases and comment on your results.

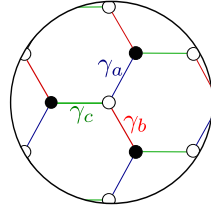


Figure 2.2 Scheme of a honeycomb lattice with non-uniform hopping matrix elements.

2.17 Charge density in graphene.

- Compute the charge density in graphene for Fermi energies $E_F = 10meV$ and $E_F = 100meV$ at zero temperature.
- Plot the charge density as a function of temperature.
- Derive the dependence of the charge density on temperature at the charge neutrality point.
- Search the literature to get the typically reachable values of E_F , n .

2.18 Hands-on the electronic structure of graphene nanoribbons and carbon nanotubes.

In this exercise you will get some hands-on experience on the electronic structure of graphene ribbons and carbon nanotubes.

- Consider the simplest tight-binding model where only nearest neighbors interactions are included. You are asked to consider armchair and zigzag nanoribbons/nanotubes and compute the dispersion relations for a few cases of your choice.

Hint: You could use the PythTB package (Python) from the group of David Vanderbilt at Rutgers University (<http://www.physics.rutgers.edu/pythtb/>). If you have further questions please post them in our website and we will try to help you or expand on this.

- Interpret the results obtained for carbon nanotubes in terms of the zone folding approximation. Convince yourself that in this case the different bands can be obtained just by cutting the 2D graphene dispersion relation along a given path in the $k_x - k_y$ plane.
- Note the appearance of flatbands close to the charge neutrality point for the case of zigzag nanoribbons. Can you obtain these bands by slicing the dispersion relation of 2D graphene as noted in (b) for nanotubes? Comment on this.

Hint: You may want to read again the introduction to Section 2.4 of Introduction to Graphene-Based Nanomaterials [1].

- As a follow up of (c) (or as an additional hint in case you may need one to answer (c)) you may want to plot the probability density associated to the states in the flatband of a zigzag nanoribbon. (PythTB also allows you to do this in a simple way.)
- Numerically **explore** other possible terminations for the graphene nanoribbons. Suggested reading: [6, 7].

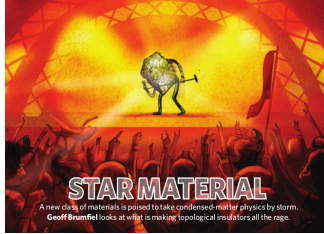


Figure 2.3 Topological insulators, a new class of star materials, share many peculiarities with graphene. Some of their striking properties can be understood from simple models on hexagonal lattices. Reprinted by permission from Macmillan Publishers Ltd: Nature (G. Brumfiel, Nature **466**, 310-311 (2010)), copyright (2010).

2.19 Low energy model for graphene nanoribbons.

Consider a low-energy approximation for the electronic structure of graphene as considered in [Section 2.2.2](#) of Introduction to Graphene-Based Nanomaterials [1]. Determine the solutions for zigzag and armchair graphene ribbons by imposing appropriate boundary conditions at the sample edges. Compare your results for the spectra with those obtained by using a tight-binding model. Comment on the advantages/limitations of this approach.

2.20 Eigenmodes of infinite carbon nanotubes and graphene ribbons.

Consider the tight-binding Hamiltonian for armchair graphene nanoribbons and zigzag nanotubes.

- Find a suitable decomposition of the Hamiltonian in the nearest neighbors approximation such that the problem is casted as several one-dimensional problems in parallel.
Hint: For a solution we refer to [Section 4.2.2](#) of Introduction to Graphene-Based Nanomaterials [1].
- Use the results obtained in (a) to derive the condition for metallicity of the corresponding nanotubes/nanoribbons. Compare your results with those presented in Chapter 2.
- Plot the density of states and the dispersion relations.

2.21 Haldane's model (Topological Insulators)

In 1988 Haldane [8] introduced a simple model on a graphene lattice which exhibited striking properties. This model precluded the birth of what is known today as Topological Insulators [9] (Fig. 2.3). In this exercise we will explore some of its properties.

Haldane's model is sketched in Fig. 2.4. Two terms are added in addition to the usual ones in the simple tight-binding model for graphene: (i) *Complex second nearest neighbors hoppings breaking time-reversal symmetry*. The second nearest neighbors hoppings are given by $\gamma_2 \exp(-i\epsilon_{ij}\phi)$, $\epsilon_{ij} = \text{sign}(\mathbf{d}_1 \times \mathbf{d}_2)_z$, $\mathbf{d}_1$ and $\mathbf{d}_2$ are unit vectors along the direction of the two bonds connecting the next nearest neighbors sites and ϕ is a chosen flux (like in the Peierls substitution introduced in [Section 2.7](#) of Introduction to Graphene-Based Nanomaterials [1]). The sign of such phases is indicated in the figure. (ii) *A mass term which breaks inversion symmetry*. This

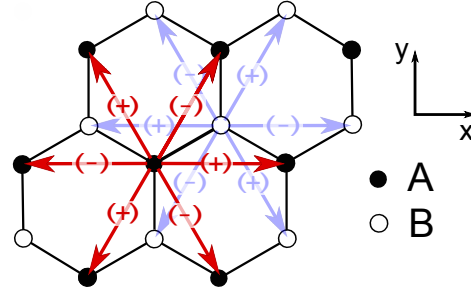


Figure 2.4 Scheme showing the connectivity between the lattice sites in the Haldane model. Complex second nearest neighbors hoppings are added to graphene's lattice, the sign of the corresponding phases is indicated in the figure. Furthermore, lattice sites A and B have onsite energies $+\Delta$ and $-\Delta$ respectively.

term is simply a staggered on-site energy, which is taken to be equal to $+\Delta$ for the A-sites and $-\Delta$ for the B-sites.

The full tight-binding Hamiltonian reads:

$$\mathcal{H} = \Delta \sum_j \xi_j c_j^\dagger c_j + \gamma_0 \sum_{\langle i,j \rangle} c_i^\dagger c_j + \gamma_2 \sum_{\langle\langle i,j \rangle\rangle} e^{-i\epsilon_{ij}\phi} c_i^\dagger c_j,$$

where the double brackets in the last summation indicate sum over second-nearest neighbors and $\xi_j = +1$ when $j \in A$, $\xi_j = -1$ when $j \in B$.

- Compute the electronic structure for an infinite sheet for different values of ϕ and Δ and compare with those for graphene and graphene with a mass term (Δ terms in the above Hamiltonian).
- Repeat point (a) for the case of a ribbon. Show that graphene with a mass term differs from Haldane's model *at the edges*.
- Plot the probability associated to the wave-functions in (b) at different energies. Discuss your results. Argue why the Haldane model does not give an ordinary band insulator.

Hints and solutions to selected problems

2.2 Electronic structure of Graphene and Boron-Nitride: The $\pi - \pi^*$ model.

Hint

Figure 2.5 shows typical results obtained with a simple tight-binding model.

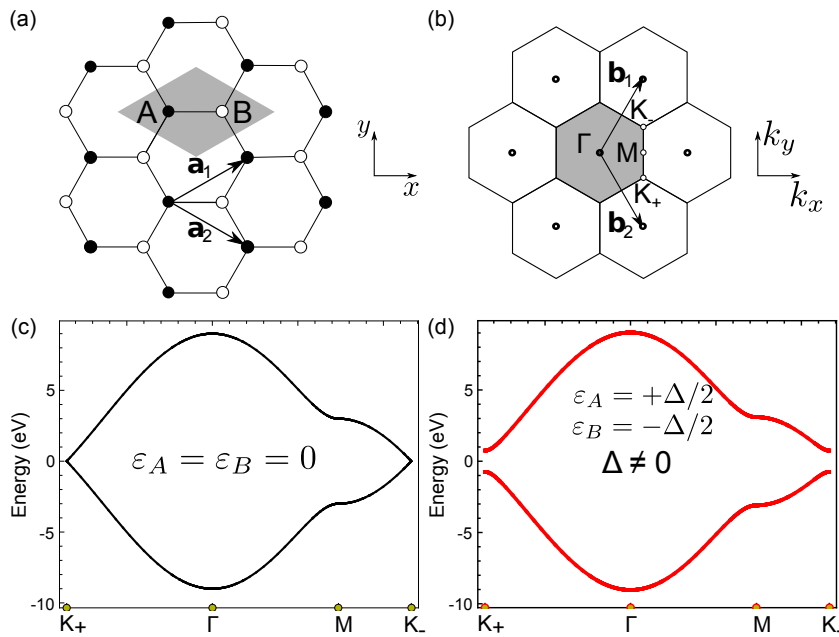


Figure 2.5 (a) Graphene lattice featuring the basis vectors, the corresponding reciprocal lattice is shown in (b). (a) and (b) are reproduced from Introduction to Graphene-Based Nanomaterials [1]. (c-d) Electronic band structures of a simple model of graphene when $\epsilon_A - \epsilon_B = \Delta = 0$ (c) and when the two atoms from the two different sublattices are different (when $\epsilon_A - \epsilon_B = \Delta \neq 0$ (d)). When $\Delta \neq 0$, the symmetry between the two sub-lattices is broken, inducing the appearance of a band gap equal to Δ . This symmetry breaking also imposes the loss of the intrinsic linear dispersion at the K -point of the irreducible Brillouin zone. In these panels, only nearest neighbors coupling was considered and the corresponding matrix element was taken equal to 3 eV. The overlap between neighboring orbitals was neglected. This is the simplest model for the electronic structure of graphene. In Figs. 2.6 and 2.7 you can see how the electronic structure changes when more accurate models are used.

2.3 Electronic structure of Graphene: A tight-binding study.

Solution

As a result of this exercise you should obtain a figure like Fig. 2.6 (which is also reproduced in Fig. 2.6 of Introduction to Graphene-Based Nanomaterials) [1].

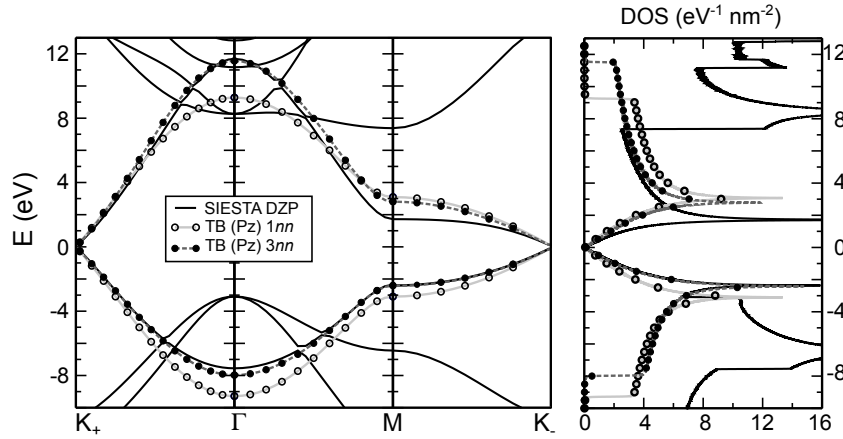


Figure 2.6 Electronic band structures and density of states computed using a first nearest-neighbors model (1 nn, blue lines with open square symbols), a third nearest-neighbors model (3 nn, black lines with filled circle symbols), and an *ab initio* code (red lines) along the $K - \Gamma - M - K$ path of the irreducible Brillouin zone. The Fermi energy is set to zero. Adapted with permission from [10]. Copyright (2012) by the American Physical Society. By courtesy of A. Lherbier

2.4 Electron-hole symmetry in bipartite lattices.

Solution

A *bipartite* lattice can be divided in two interpenetrating sublattices. An example is the honeycomb lattice, where we have two atom types (A and B) as shown in Fig. 2.2 of Introduction to Graphene-Based Nanomaterials [1], but here we will keep the problem general and not assume any particular lattice as long as it is bipartite.

Assuming that one sublattice (say A) couples only to the other sublattice (say B) we can write the associated Hamiltonian in the generic block-form:

$$\mathcal{H} = \begin{pmatrix} \mathcal{H}_{AA} & \mathcal{H}_{AB} \\ \mathcal{H}_{BA} & \mathcal{H}_{BB} \end{pmatrix},$$

where the blocks $\mathcal{H}_{AA}$ and $\mathcal{H}_{BB}$ are proportional to the identity matrix. For simplicity we assume that the on-site energies of both sublattices are equal and set that value as the energy reference (*i.e.* $\mathcal{H}_{AA} = \mathcal{H}_{BB} = 0$)¹. Then, if $(\phi_A, \phi_B)^T$ is the eigenfunction corresponding to the eigen-energy E ,

¹ After following the solution presented here, you are challenged to consider what happens if we lift the assumption that the on-site energies of both sublattices are equal.

$$\begin{pmatrix} 0 & \mathcal{H}_{AB} \\ \mathcal{H}_{BA} & 0 \end{pmatrix} \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix} = E \begin{pmatrix} \phi_A \\ \phi_B \end{pmatrix},$$

then one can verify that

$$E^2 \phi_A = \mathcal{H}_{AB} \mathcal{H}_{BA} \phi_A.$$

Therefore if $(\phi_A, \phi_B)^T$ is an eigenfunction with energy E then $(\phi_A, -\phi_B)^T$ is also an eigenfunction with an energy which is the opposite, $-E$, i.e. there is particle-hole symmetry.

2.11 Electronic structure of Graphene: An ab initio study

Solution

After following steps a-c as explained in the text of Problem 2.11, you should obtain the result shown in Fig. 2.7

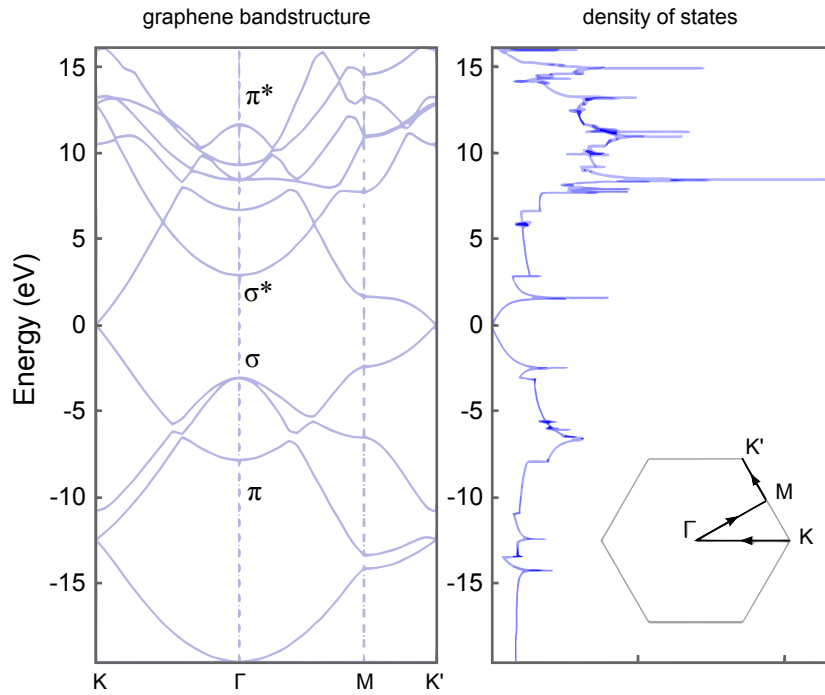


Figure 2.7 *Ab initio* electronic band structures and density of states of graphene computed using the ABINIT code. The band structure is calculated along high-symmetry lines ($K - \Gamma - M - K'$ path) of the irreducible Brillouin zone. The Fermi energy is set to zero.

3⁺ Quantum transport, general concepts (Additional material)

"Two seemingly incompatible conceptions can each represent an aspect of the truth ... They may serve in turn to represent the facts without ever entering into direct conflict."

Louis de Broglie.

Additional problems

3.4 Scattering through a resonant state.

Let us consider a simple one-dimensional tight-binding Hamiltonian where a state with energy E_0 is coupled to two ordered semi-infinite chains (see scheme in Fig. 3.1):

$$\mathcal{H} = \begin{pmatrix} \ddots & \gamma & 0 & 0 & 0 \\ \gamma & 0 & \gamma_L & 0 & 0 \\ 0 & \gamma_L & E_0 & \gamma_R & 0 \\ 0 & 0 & \gamma_R & 0 & \gamma \\ 0 & 0 & 0 & \gamma & \ddots \end{pmatrix}$$

- (a) Compute the transmission and reflection probabilities ($T(\varepsilon)$ and $R(\varepsilon)$) as a function of the incident's electronic kinetic energy ε .

*Hint: This can be done by using different methods. One instructive way is to propose *plane-waves* on each side of the scatterer and solve for the corresponding transmission and reflection amplitudes. In this case, assume electrons incoming from the left and consider also the reflected and transmitted plane waves (the probability amplitude at the scatterer is also unknown) and then*

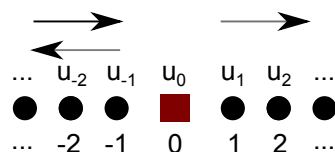


Figure 3.1 Scheme of the one-dimensional scatterer considered in the text.

replace the proposed solution in the Schrödinger equation. This alternative follows the steps in [11] (Sec. 13-6).

Another way is to use Green's functions (see Appendix C).

- (b) Plot $T(\varepsilon)$ for different values of the parameters γ_L, γ_R . Show that for suitable parameters there is a resonance close to E_0 and show that the line shape is a Lorentzian in the appropriate limit. Interpret the finite width of the resonance.
- (c) **Optimal transmittance and symmetry of the contacts.** From the result obtained previously obtain an expression for the maximum of T in terms of γ_L and γ_R . What is the condition to achieve the maximum possible value ($T(E_{res}) = 1$)? Note that this imposes a condition on the symmetry of the contacts (see for example [12]).
- (d) *Current at finite bias voltage.* Compute the current as a function of the bias voltage (you may want to approximate your results in the limit where the resonance width is much smaller than all the other energy scales). Analyze the large bias voltage limit.
- (e) *Current in the low bias limit.* Compute also the conductance in the low-bias limit (linear response). What is the effect of temperature on your results? Give an expression for the linear-response conductance at finite temperature. How large is the thermal smearing of the conductance?
- (f) **Transmission Phase.** Up to now nothing was said about the phase of the transmitted electrons. The transmission phase is related to quantities such as the density of states and also gives dynamical information [13]. You are asked to compute the phase shift or transmission phase for the simple model as a function of ε . What do you expect for a one-dimensional system with many resonant states?
- (g) **Wigner Time Delay.** The energy derivative of the phase shift δ gives a time-scale:

$$\tau_W = \hbar \frac{d\delta}{d\varepsilon},$$

the so called (Wigner time-delay) which can be regarded as a measure of the time-delay due to tunneling (see for example [14]). Compute the Wigner time-delay and comment on your results.

3.5 Symmetries of the S-matrix and phase rigidity.

The scattering matrix (or S-matrix) is a useful concept in scattering theory. Let us assume a situation where we have leads with a single mode each. The matrix element $S_{m,n}$ of the scattering matrix S gives the probability amplitude associated with the transmission from lead n to lead m (generalization to a situation where there are many modes on each lead is straightforward), *i. e.* $T_{m,n} = T_{m \leftarrow n} = |S_{m,n}|^2$.

- (a) **Unitarity.** Show that current conservation requires the unitarity of the S matrix: $\sum_m |S_{m,n}|^2 = 1$. Interpret the result.
- (b) **Reciprocity.** Show that in the presence of a magnetic field B , the scattering matrix satisfies: $S(B) = S^t(-B)$, where t denotes the transpose.

- (c) **Phase rigidity.** Consider a metallic ring connected to two leads (L and R) and threaded by a magnetic field. Expand the two-terminal conductance in Fourier series:

$$G(\phi) = G_{\text{avg}} + A \cos(2\pi\phi/\phi_0 + \delta) + \dots$$

where ϕ is the magnetic flux and ϕ_0 is the magnetic flux quantum. Show that because of symmetry reasons there are only cosine terms in the expansion and that in this two-terminal setup the phase shift δ in the Aharonov-Bohm oscillations can only be 0 or π (this is called *phase rigidity*). Argue how this result breaks down the argument that views the conductance of the Aharonov-Bohm ring as interference of partial waves traveling on each arm [15, 16].

Further reading:

- [Symmetry of electrical conduction \[17\]](#).
- See Chapter 3 of Datta's book [18].

3.6 Beyond two-terminals: Multiterminal conductance.

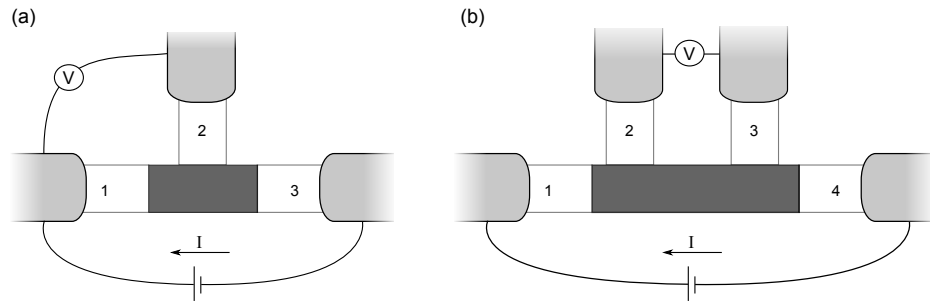


Figure 3.2 (a) Sketch of a three terminal device including the current and voltage measuring probes. (b) Sketch of a four-terminal device including the current and voltage measuring probes as considered in the text.

- (a) **Three-terminal conductance.**

Consider a mesoscopic/nanoscale device as the one shown in Fig. 3.2 where the central region is connected to three leads or terminals. In this case there are several ways to measure the current and voltage through the device, one of them is represented in Fig. 3.2. By using the Landauer-Büttiker equation (see chapter of Introduction to Graphene-Based Nanomaterials [1]) in the low-bias and zero temperature limit, determine the resistance measured in the configuration shown in Fig. 3.2. Assume that the transmission probabilities between the different leads is known.

- (b) **Four-terminal conductance.**

Let us consider a four-terminals device as the one represented in Fig. 3.2. As in the previous exercise, you are asked to use the Landauer-Büttiker equation in

the low-bias and zero temperature limit to derive an expression for the (four-terminal) resistance in this configuration. How does your response change if you invert the voltage and current measuring probes?

- (c) Discuss your results and compare with the two-terminals case. What is measured when you measure the resistance in a two-terminals and four-terminals configurations?

Hints and solutions to selected problems

3.1 Landauer conductance of pristine carbon-based materials.

Hint

Check our website for more on this exercise.

If you are on the process of debugging your code we would like to stress that debugging for the case of a pristine system should be one of the first steps of any transport calculation. Fortunately, when you have reflectionless contacts you could use the fact that the conductance is quantized in your favor. Indeed, any departure from this quantization beyond the numeric precision should be scrutinized: It may hint of possible mistakes or inefficient implementations (the Devil is in the details!).

3.2 Conductance through carbon-based materials using the Kubo formula.

Hint

The recursion methods covered in Appendix D of Introduction to Graphene-Based Nanomaterials [1] may serve as the basis for highly efficient computational implementations.

Before starting this exercise revise [Chapter 3](#) and [Appendix D](#). Then start by implementing it for the calculation of the DOS for a pristine system.

Check our website for more on this exercise, we will be adding a few suggestions and a sample code:

www.introductiontographene.org

4⁺ Klein tunneling and ballistic transport in graphene and related materials (Additional material)

“Es gibt keinen Gott und Dirac ist sein Prophet.”

Wolfgang Pauli.¹

Additional problems

4.8 Transport regimes in graphene and carbon nanotubes.

Ballistic transport, transport with negligible or low scattering, has been observed in a variety of graphene-based devices, including carbon nanotubes, graphene and graphene nanoribbons. This much sought-for property shows the exceptional control of the quality of the sample-metal contacts in these materials as well as their low-disorder. In Chapters 3 and 4 of Introduction to Graphene-Based Nanomaterials [1] we mentioned several experiments where different transport regimes are observed. In this exercise you are asked to explore the literature in the search of experimental evidence for different transport regimes in carbon nanotubes, graphene and graphene nanoribbons. Specifically: (i) Find a few experiments where seemingly ballistic transport can be explained in terms of Landauer's theory. (ii) Find results departing from ballistic transport and/or Landauer's theory. Argue on their possible origin. (iii) Look for experiments where the transition from coherent to sequential tunneling is observed in the same sample. Indicate the different regimes and a control variable tuning the transition between them.

¹ Remark attributed to Wolfgang Pauli during the Fifth Solvay International Conference (October 1927).

5⁺ Quantum transport in disordered graphene-based materials (Additional material)

Additional problems

5.6 Influence of disorder in the conductance of two-dimensional materials: The role of topology.

In this exercise we will explore topological protection of the edge states as found in problem 2.21.

- (a) Following exercise 3.1, consider a graphene nanoribbon where disorder is added to a central region of length L as in Fig. 5.1. Numerically compute the two-terminal conductance for different disorder strengths.
- (b) Repeat (a) for the case of Haldane's model introduced problem 2 (additional exercises of Chapter 2). Compare your answers and rationalize the observed behavior.

Hint: Consider a simple tight-binding Hamiltonian and start by placing vacancies at random in the central region (this can be done just by increasing the onsite energies to a very high value). Then compute the two-terminal conductance by using Landauer's theory as a function of the Fermi energy.

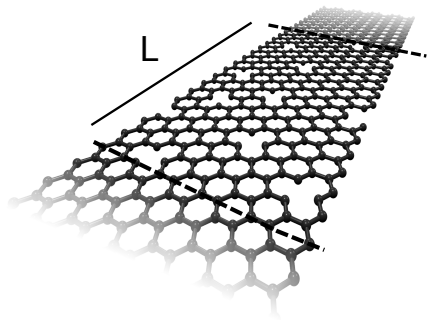


Figure 5.1 Scheme of the situation considered in the text: Transport through an infinite graphene ribbon containing a disordered region of length L .

5.7 Mean free path.

Imagine a cubic lattice of a given metal with interatomic distance a .

- (a) We start with the three-dimensional case. Assuming there is 1% of substituted impurities, give an estimate of the mean free path.
- (b) Does the mean free path display some energy-dependence which could be revealed by some external means (gate voltage for instance)?
- (c) Same questions as (a) and (b) for a two-dimensional square lattice.
- (d) Same questions as (a) and (b) for a one-dimensional lattice.
- (e) Give an estimate of the localization length for the 1D lattice case.
- (f) Select the Gaussian impurity disorder model (see [Section 5.2.5](#)), for which you can tune the impurity density but also several parameters of the scattering potential. Assume a situation with strong intervalley scattering and choose potential parameters accordingly.
- (g) Using the recursion method (see Appendix D and [Section 3.4](#)), elaborate the corresponding 1D, 2D and 3D Hamiltonians and compute numerically the energy-dependence of the mean free path. Check your qualitative estimates.
- (h) Compute numerically the elastic mean free path in graphene for the Gaussian impurity model. Use the tight-binding simplified model.

5.8 [Project] Quantum Hall effect in graphene: Landau levels, edge states and multiterminal conductance.

Forenote: Beware that this exercise may take more effort than others presented in the book. This could be used as a project for a course at a Master's level.

Let us consider an *all-graphene* device where a central region is connected to leads in a Hall bridge configuration as shown in Fig. 5.2. Your task will be to compute the Hall response and test its robustness against disorder. Specifically, you are asked to compute R_{xx} (resistance between terminals 2 and 3) and G_{xy} (conductance between terminals 4 and 2 for example) for both pristine and disordered systems, and interpret your results.

This is a numerical counterpart of the experiment carried out in [19] (Yes, you will have the chance of comparing your results with the experiments!).

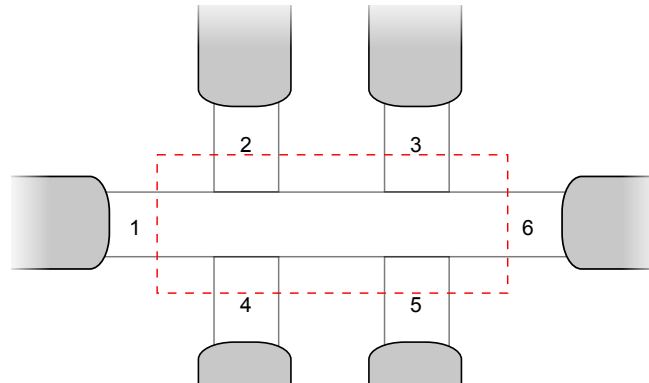


Figure 5.2 Scheme showing a Hall bridge configuration for measuring the Hall response. Six terminals are connected to the central region where a perpendicular magnetic field is applied to the region delimited by the red dashed rectangle. Your task will be to compute the Hall response of such a device (which we assume to be *all-graphene*).

On the way to completing this project you will get practical experience on modeling magnetic fields through the Peierls substitution (Section 2.7 of Introduction to Graphene-Based Nanomaterials [1]), the Landauer-Büttiker formalism and multiterminal conductance (see Chapter 3 of [1] and additional exercises) and modeling of disorder.

Check www.introductiontographene.org for updates or to ask questions regarding this project.

6⁺ Quantum transport beyond dc (Additional material)

*"Now, here, you see, it takes all the running you can do, to keep in the same place.
If you want to get somewhere else, you must run at least twice as fast as that!"*

Lewis Carroll, Through the Looking Glass.

Additional problems

6.4 Time reversal symmetry.

Consider a system in the presence of a time-dependent term proportional to $\sin(\Omega t)$. Show that it preserves time-reversal symmetry. Show that combining it with another out-of phase term ($\propto \sin(\Omega t + \phi)$, $\phi \neq 0$) time-reversal symmetry is broken.

6.5 Time-evolution operator over one driving period.

Consider a time-periodic Hamiltonian as in Section 6.3 of Introduction to Graphene-Based Nanomaterials [1].

- (a) Prove Eq. (6.18), this is, that the time-evolution operator over one period of the potential, $\hat{U}(T, 0)$, is related to the Floquet Hamiltonian through:

$$\hat{U}(T, 0) = \exp\left(-\frac{i}{\hbar} \hat{\mathcal{H}}_F T\right).$$

Therefore, a Floquet state with quasienergy ε_α acquires a phase $\exp(-i\varepsilon_\alpha T/\hbar)$ after one period T .

- (b) Argue on how the result in (a) allows to compute the stroboscopic evolution of a system under such a time-periodic Hamiltonian. Compare with the situation in which the Hamiltonian has a general time-dependence.

Hints and solutions to selected problems

6.3 Laser-illuminated graphene.

Check our website for more on this exercise, suggestions and a sample code:

www.introductiontogroupene.org

Further reading:

- For more details on the electronic properties of illuminated graphene see [20, 21].
- A recent realization of laser-induced bandgap at the surface of a topological insulator was reported in Science [22].
- A recent paper on Floquet chiral edge states (a laser-induced counterpart of the topological states you saw earlier for the Haldane model) see [23].

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