

Chapter 2

Tight-Binding Description of Graphene Nanostructures

In graphene, the four electrons in the outer shell of carbon atoms are arranged in a planar hybridization sp_2 , with three orbitals oriented towards the vertices of a regular triangle. Three electrons form covalent bonds with the neighbouring atoms, thus building a hexagonal lattice. The remaining electron, corresponding to the non-hybridized p orbital perpendicular to the structure, is responsible for the conductivity of the system. This is due to the non-negligible overlap between the orbitals of neighbouring atoms, which allows the electron to form extended states spanning over multiple sites.

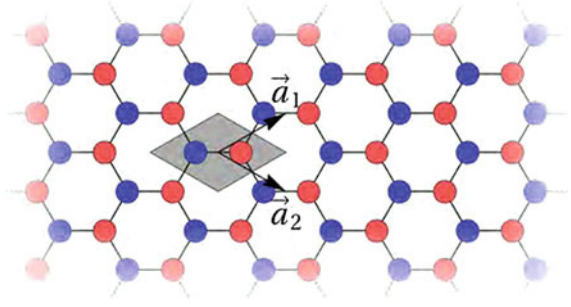
2.1 Dispersion Relation of Graphene

The electronic properties of graphene can be described using a simple TB model [1]. The electrons in the covalent bonds form deep fully filled valence bands, and thus their effects on the conductivity can be safely disregarded. The unhybridized p orbital is only slightly perturbed by the neighbouring atoms. Therefore, the wave function of an electron in the system can be written as a Linear Combination of Atomic Orbitals (LCAO). Using these orbitals as the basis set to represent the wave function, the Hamiltonian that governs the dynamics of the electron is given by:

$$\mathcal{H} = \sum_i \epsilon_i |\phi_i\rangle \langle \phi_i| - \sum_l \sum_{\{(i,j)\}_l} t_l (|\phi_i\rangle \langle \phi_j| + |\phi_j\rangle \langle \phi_i|), \quad (2.1)$$

where ϵ_i represents the onsite energy at the i th atom, $|\phi_i\rangle$ the atomic orbital in the same site, $\{(i, j)\}_l$ the set of couples of l th-nearest neighbours, and t_l the hopping parameter between them that represents the overlap between orbitals. The number of neighbours included in the calculation depends on the required accuracy, and usually ranges from 1 to 3. For brevity, t_1 is redefined as t .

Fig. 2.1 Characteristic hexagonal lattice of graphene. Different colours are used for atoms belonging to different sublattices. A primitive cell is shown in grey along with the lattice vectors a_1 and a_2



If the system is assumed to be infinite, and all the onsite energies are equal (system without disorder), then the Bloch theorem can be applied. As a consequence, extended states with a well-defined $\mathbf{k}$ vector can be defined, with a wave function given by the following *ansatz*:

$$|\psi_B(\mathbf{k})\rangle = \sum_{m,n} \left[|\phi_{m,n}^a\rangle + c |\phi_{m,n}^b\rangle \right] e^{i\mathbf{k}\cdot\mathbf{R}_{m,n}} \quad (2.2)$$

where c is a complex variable, $\mathbf{R}_{m,n} = m\mathbf{a}_1 + n\mathbf{a}_2$ is the position of the centre of the $\{m, n\}$ -cell and $|\phi_{m,n}^{a(b)}\rangle$ represents the atomic orbital on the first (second) atom of that cell (see Fig. 2.1). Both the arbitrary global phase of the wave function and its normalization have been used to remove the coefficient associated to $|\phi_{m,n}^a\rangle$. Plugging this wave function in the usual eigenvalue equation $\mathcal{H}|\psi_B\rangle = E|\psi_B\rangle$ and projecting it over $\langle\phi_{0,0}^a|, \langle\phi_{0,0}^b|$, leads to a system of two equations and two unknowns, E and c . This allows for the writing of the dispersion relation $E(k_x, k_y)$. The analytic expressions derived can be written in a compact way for $l = 1, 2$ [2]. In the case $l = 1$,

$$E(\mathbf{k}) = \pm t \sqrt{3 + 2 \cos(\sqrt{3}k_y a_0) + 4 \cos\left(\frac{\sqrt{3}}{2}k_y a_0\right) \cos\left(\frac{3}{2}k_x a_0\right)} \quad (2.3)$$

$$c(\mathbf{k}) = E(\mathbf{k}) \left[e^{ik_x a_0} + 2e^{-ik_x a_0/2} \cos\left(\sqrt{3}k_y a_0/2\right) \right]^{-1}, \quad (2.4)$$

$a_0 \simeq 0.142$ nm being the distance between neighbouring carbon atoms in graphene.

Using $t_2 = -0.2t$, $t_3 = 0.025t$, as obtained in [3] using *ab-initio* calculations, the dispersion relation was calculated, and plotted in Fig. 2.2. As the system is modelled using two orbitals per unit cell, two energy bands show up in the dispersion relation. Contrary to the expression derived in Eq. (2.3), in this case there is strong asymmetry between the bands due to the non-nearest neighbour interactions.

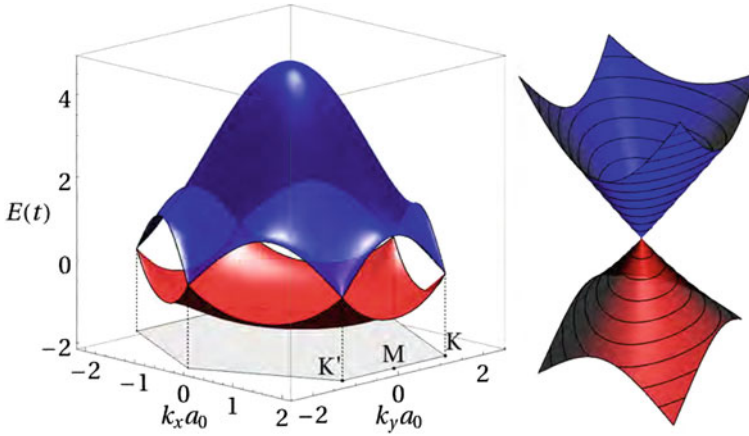


Fig. 2.2 Dispersion relation of graphene in the first Brillouin zone, calculated using a TB model considering up to third-nearest neighbours interaction and hopping parameters t , $t_2 = -0.2t$, $t_3 = 0.025t$. Six Dirac points are observed, with only two of them— K , K' —being inequivalent. A zoom in one of the Dirac points is shown in the *right plot*, where the linear dispersion relation can be observed

2.1.1 Dirac Points and Dirac Cones

The calculated bands touch each other at six points, located in the vertices of the hexagon corresponding to the first Brillouin zone. Due to the boundary conditions in the reciprocal space, only two of them are non-equivalent. They are denoted as K , K' . Contrary to the usual parabolic shape, the dispersion relation near the band edges is linear, as seen in the zoom around K , in the right part of the same figure.

These points are called Dirac points, and the neighbouring regions, Dirac cones. This nomenclature has its roots in the field of theoretical physics, where linear dispersion relations arose as solutions of the Dirac equation for massless fermions. In fact, for each cone a massless Dirac Hamiltonian can be derived as an effective Hamiltonian for states close to the Dirac point [4]. This effective description is used in Chap. 5. Interestingly, due to the presence of two atoms per unit cell, a new variable appears which is analogous to the spin of a fermion, thus being called pseudospin. Some unusual effects can be explained by means of this effective description, such as the Klein tunnelling [5], i.e., the perfect transmission of a particle through electrostatic barriers of arbitrary height and width, for normal incidence. The anomalous integer quantum Hall effect, i.e., the shift by $1/2$ in the position of the Hall plateaus with respect to the usual sequence, due to the presence of a Landau level at $E = 0$, can also be explained using the Dirac equation.

The physical nature of the pseudospin comes from Eq. (2.4), which is a bivalued function with constant absolute value $|c(\mathbf{k})| = 1$. This function has branch points in the edges of the Brillouin zones, and therefore a closed loop around one of these

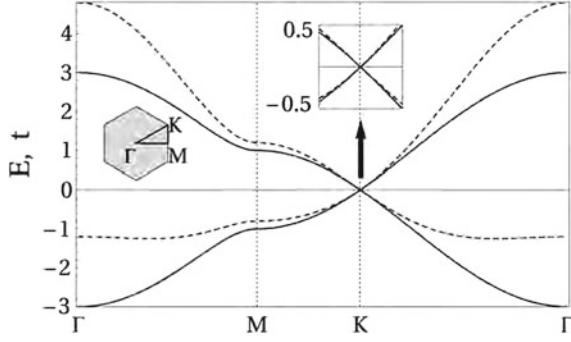


Fig. 2.3 Comparison of the dispersion relation of graphene along the path Γ – M – K – Γ using two different sets of TB model parameters: a simple nearest-neighbour with hopping parameter t —*solid line*, and another with interaction up to third-nearest neighbours and parameters $t, t_2 = -0.2t, t_3 = 0.025t$ —*dashed line*. In spite of the strong shifts of the bands, the simplest model captures to a very high accuracy the behaviour close to the neutrality point, with both models showing the Dirac point and the linear dispersion relation

points introduces a change of sign in $c(\mathbf{k})$, which is analogous to the behaviour of the spin in fermions under 2π spatial rotations.

This analogy with massless fermions is of practical importance if the linear dispersion is stable, in contrast to being just a mathematical consequence of an over-simplified model considering only nearest-neighbour interactions. Considering interaction up to third-nearest neighbours, the expansion of the dispersion relation around the Dirac point K can be made, using $\mathbf{k} = \mathbf{K} + k_\rho \mathbf{u}_\theta$:

$$E(k_\rho, \theta) = (3t_2 - \epsilon_0) \pm \frac{3}{2} (t_1 - 2t_3) k_\rho - \frac{18t_2 \pm 3 \sin(3\theta) (t_1 + 4t_3)}{8} k_\rho^2 + \mathcal{O}(k_\rho^3), \quad (2.5)$$

where the different signs stand for the two bands. The expansion around K' only changes the sign of θ . The linear term proves the stability of the Dirac cone centred in $\mathbf{K}$. It is also clear from Eq. (2.5) that t_2 shifts the energy spectrum and t_3 changes the slope of the dispersion relation, but no angular dependence of the spectrum is observed until terms of order k_ρ^2 . This effect is named trigonal warping and, as it is proportional to $t_1 \gg t_2, t_3$, is the main non-linear effect to be taken into account as the energies of interest move away from the Dirac point [6] (Fig. 2.3).

2.1.2 Opening Gaps in Graphene

Despite its impressive properties, graphene is not well suited for applications in digital electronics due to two closely related properties: the absence of a band gap and the difficulties to confine carriers using electrostatic potentials.

A number of methods have been proposed in the literature to circumvent these issues:

- Stacks of graphene layers [7–9]: placing graphene layers in stacks, with optional back gate voltages, can induce band gaps in the resulting system.
- Chemical doping: the adsorption of molecules by the p orbitals in a patterned way, e.g., by using Moiré patterns caused by the substrate [10–12], allows for the formation of heterostructures with band gaps.
- Strain induced band gaps [13, 14] and patterned defects [15].
- Band gaps induced by lateral confinement [16, 17]: graphene strips have a band gap due to the lateral confinement of the charge carriers, which increases as the system is narrowed down.

In Chaps. 3–5 the latter method is used to create devices with band gaps.

2.2 Electronic Properties of Graphene Nanoribbons

Due to the importance of opening a gap in graphene for many applications, a number of research groups are involved in the production of nanoribbons. There are currently a variety of techniques which allow for atomic precision in graphene growth, which range from the initial attempts using lithographic methods [17], to the bottom-up growth via cyclodehydrogenation after surface-assisted coupling of molecular precursors into linear polyphenylenes [18, 19] or the unzipping of carbon nanotubes [20, 21].

Despite the finite size of any sample, a useful method to understand its electronic properties is to consider one of the dimensions of the sample of infinite length, keeping the other finite. Then, the system becomes quasi one-dimensional, considering unit cells with length equal to the periodicity of the structure and same width as the structure. Then, the electronic transport can be studied using the dispersion relation $E(k)$, which can be obtained using a modified Transfer Matrix Method (TMM) [22]. Further details of this method are given in appendix A.

2.2.1 Relationship Between Dispersions of the 1-D and 2-D Systems

It is interesting to understand the results obtained for the nanoribbons in terms of the properties of bulk graphene. There is a fundamental rule connecting both systems, which states that the propagating eigenmodes of a one-dimensional system can be written as a linear combination of the eigenmodes of its two-dimensional counterpart, provided that complete primitive cells are used to construct the 1-D system. This is valid as long as no edge deformation is taken into account. Within the TB model, the boundary conditions of one cell with $n = 1, \dots, N$ rows of atoms are equivalent to

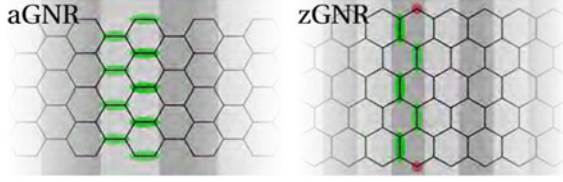


Fig. 2.4 *Left panel* shows the unit cell of an armchair graphene nanoribbon ($N = 4$ cells wide) and *right panel*, a zigzag graphene nanoribbon ($N = 3$ cells wide). The primitive cells of these structures are marked with alternate grey tones, the primitive cells of bulk graphene, in green, and the unpaired carbon atoms, in red

setting the wave function to be 0 at $n = 0, N + 1$. Then, a wave function in the 1-D system can be directly connected to a set of wave functions in the 2-D system.

The discussion above can be easily applied to the two types of graphene nanoribbons, with armchair edges—aGNRs, left plot of Fig. 2.4—and with zigzag edges—zGNRs, right plot in the same figure. The confinement in the vertical direction creates a new periodicity in both systems, $a = 3a_0$ for aGNRs and $a = \sqrt{3}a_0$ for zGNRs. The primitive cells of these systems are marked with alternate grey tones. For aGNRs, this cell is made up of primitive cells of the 2-D system, marked in green, while for zGNRs, two atoms—in red—are unpaired. Therefore, for aGNRs,

$$\mathbf{e}_n^{1D}(k_x, E) = \int dk_y c_n(k_x, k_y, E) \mathbf{e}^{2D}(k_x, k_y, E), \quad (2.6)$$

that is, the n th propagating eigenmode $\mathbf{e}_n^{1D}(k_x, E)$ can be written as a linear combination of the eigenmodes of the two-dimensional one, as they are a complete basis set for the aGNR. On the other hand, for zGNRs, the above equation does not hold.

These arguments are tested in Fig. 2.5, by projecting the dispersion relation of graphene in k_x —aGNRs, red—and k_y —zGNRs, blue. For ribbons with armchair edges, the comparison with the 1-D dispersion—black lines in the left panel—shows a perfect agreement, contrary to the case of zGNRs—right panel. In both cases, the width of the GNR was chosen to be $N = 23$ cells.

Some additional properties can be derived from this procedure. First, the projection always mixes states from Dirac cones. In aGNRs, these cones are inequivalent, i.e., not connected by reciprocal vectors, whereas for zGNRs, the mixed cones are equivalent. Furthermore, the eigenmodes for aGNRs can be directly connected to lines of the 2-D dispersion with constant k_y ; the reflections in the boundary of the Brillouin zone are due to the shrinking of the zone by a factor 2.

2.2.2 Dependence of the Dispersion Relation on the Model Used

Using the simplest TB model with nearest-neighbour interactions, very different dispersion relations can be obtained, depending on the geometry of the system [23]. If zGNRs are chosen (black lines in the right plot of Fig. 2.5), no band gap shows

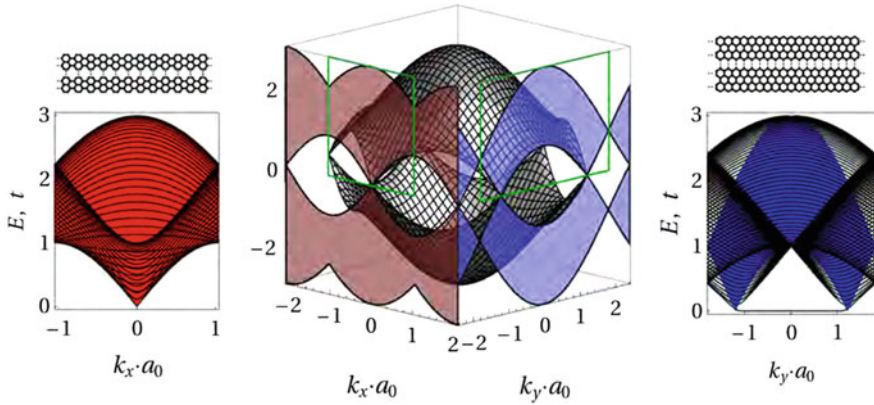


Fig. 2.5 Central panel in grey, dispersion relation of graphene in the first Brillouin zone, calculated using a TB model with nearest neighbours interaction. The projection of all the possible energy values for a constant k_x (k_y) are plotted in red (blue) on the same panel, including the contribution of the different Brillouin zones. Left panel projection of the dispersion relation of graphene—red region—and dispersion relation of an aGNR $N = 23$ cells wide—black lines. Right panel projection of the dispersion relation of graphene—blue region—and dispersion relation of a zGNR $N = 23$ cells wide—black lines

up, and the dispersion relation presents edge states (extended states fading away far from the edge) with energy $E = 0$.

For aGNRs (left plot of Fig. 2.5), the dispersion relations are centred around $k_x = 0$, and their band edges are in general parabolic. An important exception occurs for widths $N = 3n - 1$, $n \in \mathbb{N}$, where a gapless mode with linear dispersion appears, whereas for $N \neq 3n - 1$, a gap opens, as in the case plotted in the figure.

Nevertheless, if more elaborated models are used, the properties of the dispersion relation are modified [3]. In the case of aGNRs, the three different families persist, defined by N modulo 3, but the gapless modes fade away, and the lower edge of the dispersion relation becomes parabolic. This is shown in Fig. 2.6, where the band gap is plotted as a function of the width for models with increasing complexity: only nearest neighbours—left, interactions up to third-nearest neighbours—centre, and after the addition of hydrogenic impurities that relaxate the edges—right.

In spite of the differences between families, the band gap of each of them approximately depends on the width as N^{-1} . This is a consequence of the confinement energy of a Dirac fermion in an infinite well being inversely proportional to the width of the well [24]. This dependence has been obtained using first—principles calculations [16] and experimentally verified [17]. Note that this behaviour is different from the usual N^{-2} observed in other lattices, which stems from the solution of the Schrödinger equation for a massive particle confined in a well.

Changes in the dispersion relation of zGNRs due to the different models are not addressed here. This is due to the controversy regarding fundamental aspects such as edge reconstruction [25], or the presence of a net magnetic moment, which would make the dispersion relation spin-dependent [26, 27].

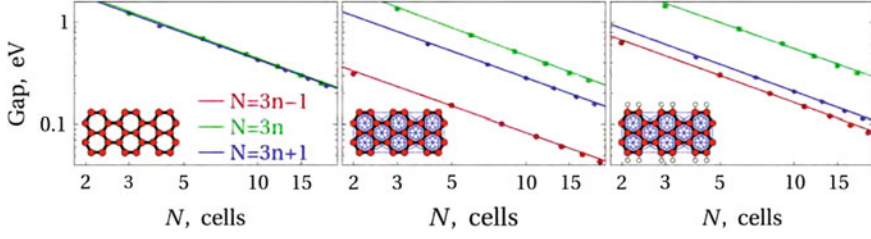


Fig. 2.6 Band gap as a function of the system width for aGNRs, calculated using three different models: nearest neighbour—*left*, third-nearest neighbours—*middle*, and third-nearest neighbours with hydrogenation in the edges—*right*

2.3 Electronic Transport Through Quantum 1-D Systems

The Landauer-Büttiker scattering formalism [28–30] has been used to calculate transport properties of the devices proposed in this work. Below, a brief summary of this formalism is given.

First, an infinite 1-D system with N propagating channels without scattering, that is, with perfect transmission, is considered, each channel having an associated dispersion relation, $E_n(k)$. The density of states of each mode n per unit of length and energy is given by

$$\rho_n(E) = \frac{2}{2\pi} \frac{1}{\partial E_n / \partial k} = \frac{1}{\pi \hbar} \frac{1}{v_{g,n}(E)}, \quad (2.7)$$

where $v_{g,n}(E)$ is the group velocity of the n th mode. The degeneracy due to the spin has already been included. Then, the current density per unit of energy associated to this mode can be expressed as:

$$j_{n,0} = e \rho_n(E) v_{g,n}(E) = \frac{e}{\pi \hbar} = \frac{2e}{h}, \quad (2.8)$$

which is independent of the dispersion relation. If the number of propagating channels at energy E is $N(E)$, the total current flowing from left to right in that perfect sample can be written as:

$$I_0 = \frac{2e}{h} \int N(E) [f_l(E, V_{SD}) - f_r(E, V_{SD})] dE, \quad (2.9)$$

where the Fermi functions of the left and right contacts are given by $f_l(E, V_{SD}) = [1 + \exp((E_F - E)/k_B T)]^{-1}$ and $f_r(E, V_{SD}) = [1 + \exp((E_F - eV_{SD} - E)/k_B T)]^{-1}$ respectively, V_{SD} is the source-drain voltage applied across the whole sample in the x direction.

Now, instead of the infinite homogeneous system, a sample between two semi-infinite homogeneous leads is considered. Scattering within the sample makes the current density per mode j_n drop, due to the back-scattered waves. Therefore, by defining the transmission coefficient as

$$T(E) = \sum_n \frac{j_n}{j_{n,0}} \equiv \sum_n T_n(E) \leq N(E), \quad (2.10)$$

and plugging this definition in Eq. (2.9), the following total current is obtained:

$$I = \frac{2e}{h} \int T(E) [f_l(E, V_{SD}) - f_r(E, V_{SD})] dE. \quad (2.11)$$

2.3.1 Spin-Dependent Transport in 1-D Systems

For systems with spin-dependent response, it is useful to define new parameters beyond the transmission and current. Assuming that no spin flip occurs within the considered system, the spin-dependent transmissions $T_{\pm}$ are defined as the transmission through the system of a charge carrier with spins up and down, respectively, and the transmission polarization,

$$P_T = \frac{T_+ - T_-}{T_+ + T_-}. \quad (2.12)$$

The current defined in Eq. (2.11) can be straightforwardly extended to a spin-dependent intensity,

$$I_{\pm} = \frac{e}{h} \int T_{\pm}(E, U_G) [f(E, \mu_S) - f(E, \mu_D)] dE. \quad (2.13)$$

Then, the total current through the device is calculated as

$$I = I_+ + I_-, \quad (2.14)$$

and its polarization, as

$$P = \frac{I_+ - I_-}{I_+ + I_-}. \quad (2.15)$$

2.3.2 Current Density of a Mode Within the Tight Binding Model

In a TB calculation, the usual output is the wave function ψ itself. Therefore, it is necessary to calculate the transmission, i.e., the current density associated to ψ . In a quasi-one-dimensional system this can be easily done by using the continuity

equation, which relates the time evolution of the probability density $\rho(x, t) = |\psi(x, t)|^2$ with the divergence of the probability current [31]:

$$\frac{\partial}{\partial t} \rho(x, t) = -\frac{\partial}{\partial x} j(x, t), \quad (2.16)$$

which for a discrete system with period a can be expressed as

$$j(n, t) - j(n + 1, t) = a \frac{\partial}{\partial t} \rho(n, t). \quad (2.17)$$

The system needs to be divided in slices in such a way that atoms in the n th slice can only be connected to the atoms in the neighbouring slices $n - 1, n + 1$, that is, the blocks of the Hamiltonian $\mathcal{H}$ fulfil $\mathcal{H}_{m,n} \neq 0 \Leftrightarrow |m - n| \leq 1$. The wave function at n is defined as $|\psi_n\rangle = \sum_i c_{n,i} |\phi_{n,i}\rangle$. Then,

$$\begin{aligned} \frac{\partial}{\partial t} \langle \psi_n | \psi_n \rangle &= \left(\frac{\partial}{\partial t} \langle \psi_n | \right) |\psi_n\rangle + \langle \psi_n | \left(\frac{\partial}{\partial t} |\psi_n\rangle \right) \\ &= \frac{i}{\hbar} \sum_m (\langle \psi_m | \mathcal{H}_{m,n} | \psi_n \rangle - \langle \psi_n | \mathcal{H}_{n,m} | \psi_m \rangle) \\ &= -\frac{2}{\hbar} \text{Im} (\mathbf{c}_{n-1}^* \mathcal{H}_{n-1,n} \mathbf{c}_n) + \text{Im} (\mathbf{c}_{n+1}^* \mathcal{H}_{n+1,n} \mathbf{c}_n), \end{aligned} \quad (2.18)$$

with $\mathbf{c}_n \equiv (c_{n,1}, \dots, c_{n,i}, \dots)$. In the last step the hermiticity of the Hamiltonian, $\mathcal{H}_{m,n}^* = \mathcal{H}_{n,m}$, has been used. By simple comparison of Eqs. (2.17) and (2.18), the following expression is obtained:

$$j(n) = \frac{2a}{\hbar} \text{Im} (\mathbf{c}_{n-1}^* \mathcal{H}_{n-1,n} \mathbf{c}_n). \quad (2.19)$$

For stationary solutions, the current density is constant along the sample, $j(n) = j$.

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Modelling of Plasmonic and Graphene Nanodevices

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