Problem set: Band structure: graphene and carbon nanotubes

7.1. Electronic structure of graphene

A graphene sheet is a honeycomb lattice of carbon atoms (see figure). Let the distance between carbon atoms be $a$. A good model for graphene is to consider a single plane in which there is one valence electron per carbon atom. We will use the tight-binding approximation, in which this electron can occupy a single $p_z$ orbital at each carbon site. Let $\mathbf{R}$ denote the centers of the hexagons in the honeycomb: these form the underlying hexagonal Bravais lattice. Please notice that the latter is indeed a Bravais lattice differently from the graphene honeycomb lattice. The unit cell spanned by $a_1$ and $a_2$ contains two carbon atoms conventionally labelled as A and B atom, located at $\mathbf{R} + \mathbf{v}_A$, $\mathbf{R} + \mathbf{v}_B$, as shown in the figure. Denote the tight-binding hopping amplitude connecting these sites by $t$. Choose the zero of energy so that the energy of an isolated atomic orbital is zero. The entire Hamiltonian consists of the nearest-neighbor hopping.

(a) Find the reciprocal lattice, and construct the first Brillouin zone.

(b) Write down the tight-binding equations governing the system. How many bands do you find? What are the energy-wavevector relations?

\textbf{Hint:} You will need to solve a two-by-two matrix eigenvalue problem. This exercise was first attacked by Wallace in 1947.\footnote{You might want to read the original paper “P. R. Wallace, Phys. Rev. 71, 622 (1947)”. It is available online (when logged in the uni-r.de domain) under http://link.aps.org/abstract/PR/v71/p622 . Alternatively you can refer to some more recent formulation as, e.g., in Section 2.4 “Band structure of graphene” of Dr. Hauptmann’s PhD thesis (http://www.nbi.dk/~nygard/JonasSpeciale2003.pdf).}
(c) Show that the Fermi energy is equal to zero, by verifying that this gives the correct electron density. Find the set of $k$ points for which $\varepsilon(k) = 0$. Show that these correspond to the corners of the first Brillouin zone.

(d) Show that, near to a (first) Brillouin zone corner with wavevector $K$ (note that $K$ is the location of a BZ corner, not a reciprocal lattice vector), the spectrum is approximately

$$\varepsilon(k) \approx \pm v \sqrt{(k_x - K_x)^2 + (k_y - K_y)^2}.$$  

Determine the velocity $v$ in terms of $t$ and $a$. This behavior is intermediate between a metal (with a Fermi surface instead of points $K$) and an insulator (with a band gap). Indeed, graphite behaves as a semi-metal, with poor conductivity significantly higher than in an insulator.

(e) [Kür] Graphite is composed of a stack of graphene layers identically atop one another in the $z$ direction (a distance $d$ apart), and there is some small residual hopping $t_\perp$ between orbitals in neighboring layers at the same $(x, y)$ position. Sketch the Fermi surface, assuming $t_\perp \ll t$.

### 7.2. Electronic structure of single wall carbon nanotubes

Carbon nanotubes are made up of a section of the graphene lattice that has been wrapped up into a cylinder. You can specify the way the lattice is wound up by identifying the winding vector $\mathbf{W}$. The winding vector must be a Bravais lattice vector, and so can be specified by two integers:

$$\mathbf{W} = n \mathbf{a}_1 + m \mathbf{a}_2,$$

where $n$ and $m$ are integers. To construct a nanotube, take a graphene lattice and mark one atom (either A type or B type) as the origin. Shift the origin of the vector $\mathbf{W}$ on the chosen atom. The new vector $\tilde{\mathbf{W}}$ will point to another atom of the same type. Roll up the sheet perpendicular to $\tilde{\mathbf{W}}$ so that the second atom sits exactly on top of the first. You have constructed a $(n, m)$ nanotube!

A bit of nomenclature. We can specify some special tubes said achiral: they are $(n, n)$ tubes which are called armchair tubes, and $(n, 0)$ zig-zag tubes (Bruckmanldl would be probably more appropriate, but there is no mention of this in the literature yet...). All other tubes are said chiral.

(a) Build a $(5, 5)$ armchair tube (*i.e.* with scissors and adhesive tape!) by making use of the provided transparencies.$^2$

(b) Construct a $(8, 0)$ zig-zag tube.

(c) Build a chiral $(7, 3)$ tube.

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$^2$A pdf is also available under the following (clickable) link http://www-MCG.uni-R.de/downloads/graphene.pdf.
(d) Let’s determine the band structure of a nanotube. To do so, impose periodic boundary conditions on the wavefunction in the direction around the cylinder. Show that this means that $k \cdot W = 2\pi \ell$, where $\ell$ is an integer.

(e) Draw the graphene first Brillouin zone from the previous problem, indicating (a) the points $K$ (where the energy of the graphene layer is zero, $E = E_F$) and (b) the lines given by the quantization conditions –introduced in the previous point– for $(n, m) = (3, 3)$ and $(n, m) = (2, 0)$.

(f) Plot the energy versus $k_x$ for the allowed values of $k_y$ in the $(3,3)$ tube above. Then plot the energy versus versus $k_y$ for the allowed values of $k_x$ in the $(2,0)$ tube.

For each case, is the nanotube metallic or insulating according to band theory?

(g) For which $n$ and $m$ are the Brillouin zone corners allowed wavevectors for a nanotube? Show that the tubes satisfying this condition are metallic!

(h) In reality, one expects that the curvature of the nanotube cylinder affects the tight-binding matrix elements slightly. Consider this effect for the special cases of armchair, and zig-zag tubes. In these cases, the curvature effect can be modeled by making the hopping matrix element slightly different (= $t'$) on transversal bonds (parallel to the winding vector in the case of the armchair tubes) than the other ones (= $t$). How does this affect the metallicity of the armchair and zig-zag tubes?
From geometrical considerations it is not difficult to identify the vectors that define the Bravais lattice with:

\[
\vec{a}_1 = \begin{pmatrix} \frac{-\sqrt{3}}{2} a \\ \frac{3}{2} a \end{pmatrix}, \quad \vec{a}_2 = \begin{pmatrix} \frac{\sqrt{3}}{2} a \\ \frac{3}{2} a \end{pmatrix}
\]

The vectors that define the reciprocal lattice are defined by the relation:

\[
\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}
\]

Thus if we indicate at first \(b_4 = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}\)

\[
b_4 \cdot a_2 = 0 = \frac{\sqrt{3}}{2} \alpha a + \frac{3}{2} \alpha b_x
\]

\[
b_4 \cdot a_4 = 2\pi = -\frac{\sqrt{3}}{2} \alpha a + \frac{3}{2} \beta b_x
\]

In matrix notation:

\[
\alpha \begin{pmatrix} \sqrt{3} & 3/2 \\ -\sqrt{3} & 3/2 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 2\pi \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \frac{2\pi}{a} \frac{2}{3\sqrt{3}} \begin{pmatrix} 3/2 & -3/2 \\ \sqrt{3} & \sqrt{3} \end{pmatrix} \begin{pmatrix} 0 \\ 2\pi \end{pmatrix} = \frac{2\pi}{a} \begin{pmatrix} -\sqrt{3} b_x \\ \sqrt{3} b_x \end{pmatrix}
\]

\[
b_3 = \frac{2\pi}{a} \begin{pmatrix} -\sqrt{3} b_x \\ \sqrt{3} b_x \end{pmatrix}
\]
In the same way: $b_2 = \begin{bmatrix} a \\ b \end{bmatrix}$

\[ b_2 \cdot a_4 = 0 = -\frac{\sqrt{2}}{2} \alpha x + \frac{\sqrt{2}}{2} q_b \]

\[ b_2 \cdot b_2 = 2R = \frac{\sqrt{2}}{2} \alpha x + \frac{\sqrt{2}}{2} q_b \]

In matrix notation:

\[ a \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \end{bmatrix} \begin{bmatrix} x \\ q_b \end{bmatrix} = 2\pi \begin{bmatrix} 0 \\ 1 \end{bmatrix} \Rightarrow \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \frac{\sqrt{2} \pi}{\alpha} \begin{bmatrix} \sqrt{2} - \frac{q_b}{\sqrt{2}} \\ -\frac{\sqrt{2}}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{2\pi}{\alpha} \begin{bmatrix} \sqrt{2} \\ -\frac{q_b}{\sqrt{2}} \end{bmatrix} \]

\[ b_2 = \frac{2\pi}{\alpha} \begin{bmatrix} \sqrt{2} \\ -\frac{q_b}{\sqrt{2}} \end{bmatrix} \]

Now the construction of the first Brillouin zone:

\[ \| b_1 \| = \sqrt{2\pi} \left( \frac{1}{3} + \frac{1}{\sqrt{2}} \right) = \frac{2\pi}{3\alpha} = \| b_2 \|. \]

In polar coordinates:

\[ b_2 = (\rho_2, \Theta_2) \]

\[ \Theta_2 = \frac{b_{2x}}{\rho_2} = \frac{3\alpha}{\sqrt{2}} \cdot \frac{\pi}{2} \begin{bmatrix} -1 \\ \sqrt{2} \end{bmatrix} = -\frac{\sqrt{2}}{2} \]

\[ 2\| \Theta_2 \| = b_{2y} = \frac{3\alpha}{4\pi} \cdot \frac{\pi}{\alpha} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{2} \]

\[ \Theta_2 = \frac{\pi}{\alpha} \]

\[ \rho_2 = \| b_2 \| \]

The easiest way of constructing a Brillouin zone is to consider all the $\vec{w} = \alpha b_2 + \beta b_2$ with $\alpha \in [0, 1)$ and $\beta \in [0, 1)$.
But this is not the only Brillouin zone that one can construct. It turns out to be more useful to define a new one symmetrically:

\[ A' = A - \vec{b}_1 - \vec{b}_2 \]

in the sense that each point in \( A' \) can be reached from 1 and only 1 point in \( A \) via \( -\vec{b}_1 \) and \( -\vec{b}_2 \).

\[ B' = B - \vec{b}_4 \]

\[ C' = C - \vec{b}_2 \]

This ensures that the red area is closer to the surface.

1b) If \( H \) is the Hamiltonian for the electronic system and we take \( \alpha \) basis to describe the system the orbitals \( \phi_\alpha (r - R - N \alpha) \) with \( \alpha = A, B, A \), \( R \in k \vec{a}_1 + m \vec{b}_2 \) with \( n, m \in \mathbb{Z} \)

we assume in tight binding that only matrix elements between wavefunctions centered on the same site or in nearest neighbors.

\[ \phi_{\alpha}(r) = \text{the orbital } \phi_\alpha \text{ of the hydrogen atom} \]
Instead of using the basis we just introduced, it is useful to consider the Bloch basis:

$$\Phi_{\alpha k} (r) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \Phi_{\alpha} (r - \mathbf{R}) e^{-ik \cdot \mathbf{R}}$$

$$\Phi_{\beta k'} (r) = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \Phi_{\beta} (r - \mathbf{R}) e^{-ik' \cdot \mathbf{R}}$$

where $k \in \mathbb{R}^2$ (first Brillouin zone) and $\mathbf{R}$ run over all the $N$ Bravais lattice sites. The localized basis set and the Bloch basis are connected by a unitary transformation (the discrete Fourier transform) and are thus equivalent. We now construct all the matrix elements of the Hamiltonian in terms of the Bloch basis: (in the limit $N \to \infty$)

$$\langle \Phi_{\alpha k} | H | \Phi_{\beta k'} \rangle$$

$\alpha, \beta = A, B$ and $k, k' \in \mathbb{R}^2$

**AA**

$$H_{AA} (k, k') = \int \, \frac{1}{N} \sum_{\mathbf{R}, \mathbf{R}'} \Phi^*_{\alpha} (r - \mathbf{R}) H \Phi_{\beta} (r - \mathbf{R}' - \mathbf{R}) e^{-ik R + i k' R'}$$

for $R \neq R'$, $-R - N_A$ and $-R' - N_A$ cannot be nearest neighbors

$$= \varepsilon \frac{1}{N} \sum_{\mathbf{R}} e^{-i(k - k') \cdot R} = \varepsilon \delta_{kk'}$$

**BB**

$$H_{BB} (k, k') = H_{AA} (k, k') = \varepsilon \delta_{kk'} \quad \text{no difference, for symmetry}$$

**AB**

$$H_{AB} (k, k') = \int \, \frac{1}{N} \sum_{\mathbf{R}} \Phi^*_{\alpha} (r - \mathbf{R} - N_A) H \Phi_{\beta} (r - \mathbf{R}' - N_B) e^{-ik R + i k' R'}$$

$-N_A + R$ is nearest neighbor of $-N_B + R'$ for $R = R'$

$$\int \, \Phi^*_{\alpha} (r - \mathbf{R} - N_A) H \Phi_{\beta} (r - \mathbf{R}' - N_B) = \Gamma$$
\[ H_{AB}(k,k') = \frac{1}{N} \sum \frac{1}{R} e^{-i(k-k')R} + \frac{1}{N} \sum \frac{1}{R} e^{-i(k-k')R + ik'q_2} \]
\[ = \frac{1}{N} \sum \frac{1}{R} e^{-i(k-k')R + ik'q_2} \]
\[ = \frac{1}{N} \sum \frac{1}{R} e^{-i(k-k')R} (1 + e^{ik_1} + e^{ik_2}) = \frac{1}{N} \sum f(k) \]

The general state \( \psi \) can be written as
\[ \psi(r) = \sum_{\mathbf{k}} c_{\mathbf{k}} \Phi_{\mathbf{k}}(r) \]

The Schrödinger equation then takes the form (time independent)
\[
\begin{pmatrix}
\epsilon & \frac{1}{N} f(k) \\
\frac{1}{N} f^*(k) & -1
\end{pmatrix}
\begin{pmatrix}
c_{\mathbf{k}}^i \\
c_{\mathbf{k}}^i
\end{pmatrix}
= E_i(k)
\begin{pmatrix}
c_{\mathbf{k}}^i \\
c_{\mathbf{k}}^i
\end{pmatrix}
\]

written \( \forall \mathbf{k} \in \mathbb{R}^2 \). It is thus a natural consequence to have a branch since we obtain in general 2 eigenvalues \( \forall \mathbf{k} \):
\[
E_1(k) = \epsilon + \sqrt{\frac{1}{N} \left| f(k) \right|^2}
\]
\[
E_2(k) = \epsilon - \sqrt{\frac{1}{N} \left| f(k) \right|^2}
\]
10. The Fermi energy, at least at zero temperature, is defined as the energy of the highest occupied energy state. In practice, we have 2 electrons per unit cell and 2 (2-fold spin degenerate) bands. Since the number of states in the momentum space is equal to the number of states in real space, half of the states (the lower half) is always occupied.

\[ \varepsilon + \sqrt{1} f(k)^2 \leq \varepsilon + \sqrt{1} f(k)^2 \quad (\tau < 0) \Rightarrow \text{the Fermi energy is defined as } \max_{k \in \text{FBZ}} \varepsilon + \sqrt{1} f(k)^2. \]

Since \( \tau < 0 \) and \( |f(k)|^2 \) vanish in the FBZ, \( \varepsilon_F \rightarrow \varepsilon \) (or, measuring the energy from the onsite energy \( \varepsilon_{F=0} \))

\[ f(k) = 0 : \quad k = \alpha b_1 + \beta b_2 \]

\[ \Rightarrow \quad a + e^{i\alpha \text{Re} \tau} + e^{i\beta \text{Im} \tau} = 0 \]

There is a non-trivial solution of the equation above.

\[ a \neq 0 \]

Solution 1 \( \alpha = \frac{\tau}{3}, \beta = \frac{\beta}{3} \)

Solution 2 \( \alpha = \frac{\tau}{3}, \beta = \frac{\beta}{3} \)

if \( \alpha, \beta \in [0, 1] \)

In the "diamond-like" FBZ, the Fermi surface is thus represented by 2 points.
Which are these two points?

The thick curve is by constructing the vector \(\frac{2}{3}b_1 + \frac{1}{3}b_2\).

Point \(E\) is by symmetry corresponding to \(\frac{1}{3}b_1 + \frac{2}{3}b_2\).

It is interesting to note that \(\mathbf{a}\) and \(\mathbf{e}\) are a "broken" print of the expected Brillouin zone. The other 4 points can be easily traced to be of \(\mathbf{a}\) or \(\mathbf{e}\) type since they are connected to \(\mathbf{a}\) or \(\mathbf{e}\) by the vectors \(b_1\) and/or \(b_2\). Explicitly:

\[
\begin{align*}
\mathbf{C} &= \mathbf{A} - b_2 \\
\mathbf{F} &= \mathbf{B} - b_1 \\
\mathbf{E} &= \mathbf{A} - b_2 - b_1 \\
\mathbf{D} &= \mathbf{B} - b_1 - b_2
\end{align*}
\]

1d) The dispersion relation is:

\[
\varepsilon(k) = \pm \gamma \sqrt{1 + f(k)^2} = \pm \gamma \left| 1 + e^{i k a_1} + e^{i k a_2} \right|
\]

If \(k = k + \Delta k\) where (for example) \(k = \frac{1}{3} b_1 + \frac{2}{3} b_2\)

and \(\Delta k = \alpha b_1 + \beta b_2\) with \(\alpha, \beta < 1\)

\[
\varepsilon(k') = \pm \gamma \left( 1 + e^{-\frac{2\pi i}{3}} - 2 \pi i b_1 e^{\frac{2\pi i}{3}} + e^{-\frac{2\pi i}{3}} - 2 \pi i b_2 e^{-\frac{2\pi i}{3}} \right)^{1/2}
\]

\[
= \pm \gamma \left( 1 + e^{\frac{2\pi i}{3}} - 2 \pi i b_1 e^{-\frac{2\pi i}{3}} + e^{\frac{2\pi i}{3}} - 2 \pi i b_2 e^{\frac{2\pi i}{3}} \right)^{1/2}
\]

\[
= \frac{1}{4 \pi} \left( 1 + b_1 \cdot b_2 \right)^{1/2} = \frac{\gamma v}{2} \Delta k
\]

\[
\gamma = \frac{3 \times 10^5}{2 \times 10^4}
\]
The solution to this problem comes from the identification of the unit cell for the system.

ABB\'s are the 4 atoms belonging to the unit cell. The problem is not really 2D since we have only 2 layers of graphene.

The tight binding hamiltonian in terms of the 4 Bloch functions corresponding to the 4 atoms of the unit cell reads:

\[ H(k) = \begin{bmatrix}
    E f(k) & t_1 & 0 & 0 \\
    t_1^* & E & 0 & 0 \\
    0 & 0 & E f(k) & t_1^* \\
    0 & 0 & t_1 & E f(k)
\end{bmatrix} \]

\[ \text{det}(H(k) - \epsilon \mathbf{1}) = 0 \]

\[ 0 = \epsilon - \lambda \cdot \text{det} \begin{bmatrix}
    \epsilon - \lambda & t_1 \\
    t_1^* & \epsilon - \lambda
\end{bmatrix} - \text{bf}(k) \text{det} \begin{bmatrix}
    \text{bf}(k) & t_1 \\
    t_1^* & \epsilon - \lambda
\end{bmatrix} + \text{bf}(k) \text{det} \begin{bmatrix}
    \epsilon - \lambda & t_1 \\
    t_1^* & \epsilon - \lambda
\end{bmatrix} \]

\[ = (\epsilon - \lambda)^2 - 2t_1^* (\epsilon - \lambda)^2 - 2 \text{bf}(k)^2 (\epsilon - \lambda)^2 - 2t_1^2 \epsilon f(k)^2 + t_1^4 \epsilon f(k)^4 + t_1^4 \]

\[ = (\epsilon - \lambda)^2 - t_1^2 \text{bf}(k)^2 - t_1^2 - 2t_1^2 \epsilon f(k)^2 - (\epsilon - \lambda)^2 - 2t_1^2 \epsilon f(k)^2 + 2t_1^2 t_1 f(k)^2 \]

\[ = \left( (\epsilon - \lambda)^2 - (t_1 f(k) + t_1^2)^2 \right) \left( (\epsilon - \lambda)^2 - (t_1 f(k) - t_1^2)^2 \right) \]

\[ = \left( \lambda - \epsilon - t_1 f(k) - t_1 \right) \left( \lambda - \epsilon - t_1 f(k) + t_1 \right) \left( \lambda - \epsilon - t_1 f(k) + t_1 \right) \left( \lambda - \epsilon + t_1 f(k) - t_1 \right) \]
The 4 eigenvalues thus read:

\[ \lambda_1 = \epsilon + t_1 f' (t) + t_2 \quad \text{since} \quad t_2 < t \quad \lambda_2 < \lambda_3 < \lambda_4 \]

\[ \lambda_2 = \epsilon + t_1 f' (t) - t_2 \]

Since \( \nu \) the 4 eigenvalues are evenly distributed around \( \epsilon \) and the system is at half filling we obtain \( \epsilon_s = \epsilon \).

The Fermi surface is described now by the equation \( \epsilon_k = \epsilon \).

We write this equation for each of the eigenvalues and we obtain only a trivial equation:

\[ |f(t)| = \frac{t_1}{t} \quad (a) \]

Since \( t_1 < t \) we can use the information derived at point (c) to say that eq. (a) has small circles of radius \( r_k = \frac{\sqrt{2} t_1}{3a} \) around the Fermi points of the simple graphene sheet.

2a, b, c) They are intended just to visualize the definition of the chiral vector.

2d) The graphene wavefunction is:

\[ \Psi (\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{K}} \sum_{\frac{\pi}{a}} c_i \phi_{2g} (\vec{r} - \vec{N}_d - \vec{R}) e^{ik \cdot \vec{R}} \]

\[ \Psi (\vec{r} + \vec{W}) = \frac{1}{\sqrt{N}} \sum_{\vec{K}} \sum_{\frac{\pi}{a}} c_i \phi_{2g} (\vec{r} - \vec{N}_d - \vec{R} + \vec{W}) e^{ik \cdot \vec{R}} = R' = R - W \]

\[ = \frac{1}{\sqrt{N}} \sum_{\vec{K}} \sum_{\frac{\pi}{a}} c_i \phi_{2g} (\vec{r} - \vec{N}_d - \vec{R}') e^{ik \cdot (\vec{R}' + \vec{W})} = \Psi (\vec{r}') \leq \delta \quad e^{ik \cdot \vec{W}} = 1 \]
2f) According to band theory the (3,3) sublattice is metallic. The (2,0) sublattice, for metallicity at least, one of the bands must cross $E_F$. In that case there is no gap between occupied and unoccupied states. (See page 13 for plots)

2g) The Brillouin zone can be represented by the points:

$$k = \frac{2}{3} b_1 + \frac{1}{5} b_2$$

$$k = \frac{1}{3} b_1 + \frac{2}{3} b_2$$

$$W = n a_1 + m a_2$$

The periodic boundary condition for bands touching the Fermi surface yields:

$$\left(\frac{2}{3} + \frac{5}{3}n\right) m = \lambda$$

or

$$\left(\frac{1}{3} + \frac{2}{3}m\right) n = \lambda$$

where $n, m, \lambda \in \mathbb{Z}$. $2n + m$ can be obtained by $\lambda$
In order to fix the ideas let us consider first the armchair tube.

The chiral vector is \((n,n)\) and thus we can write the tight binding hamiltonian in the form:

\[
H_0(n) = \begin{pmatrix}
\varepsilon & f(n) \\
f^*(n) & \varepsilon
\end{pmatrix}
\]

where \(f(k) = t \left( \frac{t'}{t} + e^{i\kappa_1} + e^{i\kappa_2} \right)\).

The band structure is still of the form \(\varepsilon(n) = \varepsilon \pm |f(n)|\) and the Fermi points are defined by the equation

\[
\frac{t'}{t} + e^{i\kappa_1} + e^{i\kappa_2} = 0 \quad t' \leq t \Rightarrow \frac{t'}{t} \leq 1
\]

\[k = \alpha b_1 + \beta b_2 \rightarrow \text{we obtain } 2 \text{ solutions } \alpha = \frac{t}{3} + \delta \quad \beta = \frac{t}{3} - \delta \]

The metallicity condition is

\[n \left(\frac{t}{3} + t + \delta\right) + m \left(\frac{2}{3} + 2 - \delta\right) = \varepsilon \quad \text{which, for } n = m \]

\[n \left(\frac{t}{3} + \delta\right) + n = \varepsilon
\]

Analogously for the zig-zag tube, but in this case the metallicity relation is broken since the 5 terms do not cancel out.
Dispersion relation for graphene
The points are equivalent.