# Fabry-Pérot oscillations in *npn* junctions in graphene

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# Tight Binding model

Hamiltonian in tight binding approximations can be written as:

$$\hat{H} = -t \sum_{<i,j>,\sigma} \left( \hat{a}^{\dagger}_{\sigma,i} \hat{b}_{\sigma,j} + \text{H.c.} \right) - t' \sum_{<<i,j>>,\sigma} \left( \hat{a}^{\dagger}_{\sigma,i} \hat{a}_{\sigma,j} + \hat{b}^{\dagger}_{\sigma,i} \hat{b}_{\sigma,j} + \text{H.c} \right), \tag{1}$$

where $t$ is the energy of hopping between nearest neighbours ($\approx 2.8$ eV), and $t'$ is the energy of hopping between second neighbours. Indexes $i$ and $j$ indicates locations in two sublattices - $A$ and $B$. Spin of particle is represented by $\sigma$. $\hat{a}^{\dagger}(\hat{a})$ are creation (anihilation) operators on sublattice $A$ ($\hat{b}$ for sublattice $B$).

# Tight Binding model

Hamiltonian for only nearest neighbours can be written as

$$\hat{H} = -t \sum_{<i,j>} \left( \hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right), \tag{2}$$

$$\sum_{<i,j>} \left( \hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right) = \sum_{i \in A} \sum_{\boldsymbol{\delta}} \left( \hat{a}_i^\dagger \hat{b}_{i+\boldsymbol{\delta}} + \hat{b}_{i+\boldsymbol{\delta}}^\dagger \hat{a}_i \right), \tag{3}$$

where $\delta$ means sum over nearest neighbours.

Next step involves switching operators to reciprocal space using Fourier transform

$$\hat{a}_i^\dagger = \frac{1}{\sqrt{N/2}} \sum_{\mathbf{k}} e^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}_i} \hat{a}_{\mathbf{k}}^\dagger. \tag{4}$$

Hamiltonian after transformations can be written as

$$\hat{H} = \frac{-t}{N/2} \sum_{i\in A} \sum_{\boldsymbol{\delta}\,\mathbf{k}\,\mathbf{k}'} \left[ e^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} e^{-\mathrm{i}\mathbf{k}'\cdot\boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^\dagger \hat{b}_{\mathbf{k}'} + \text{H.c.} \right], \tag{5}$$

we can simplify this by introducing property:

$$\sum_{i\in A} e^{\mathrm{i}(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}_i} = \frac{N}{2} \delta_{\mathbf{k}\mathbf{k}'}. \tag{6}$$

Simplified hamiltonian takes a form

$$\hat{H} = -t \sum_{\boldsymbol{\delta},\mathbf{k}} \left( e^{-\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}} \hat{a}_{\mathbf{k}}^{\dagger} \hat{b}_{\mathbf{k}} + e^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}} \hat{b}_{\mathbf{k}}^{\dagger} \hat{a}_{\mathbf{k}} \right), \tag{7}$$

which in a simpler form is written as

$$\hat{H} = \sum_{\mathbf{k}} \Psi^{\dagger} \hat{h}(\mathbf{k}) \Psi, \tag{8}$$

where

$$\boldsymbol{\Psi}^{\dagger} \equiv \begin{pmatrix} \hat{a}_{\mathbf{k}}^{\dagger} & \hat{b}_{\mathbf{k}}^{\dagger} \end{pmatrix} \quad \boldsymbol{\Psi} \equiv \begin{pmatrix} \hat{a}_{\mathbf{k}} \\ \hat{b}_{\mathbf{k}} \end{pmatrix} \tag{9}$$

and

$$\hat{h}(\mathbf{k}) \equiv -t \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^{*} & 0 \end{pmatrix}. \tag{10}$$

Term

$$\hat{h}(\mathbf{k}) \equiv -t \begin{pmatrix} 0 & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}}^* & 0 \end{pmatrix} \tag{11}$$

is nothing else than a matrix representation of hamiltonian with elements

$$\Delta_{\mathbf{k}} = \sum_{\boldsymbol{\delta}} e^{\mathrm{i}\mathbf{k}\cdot\boldsymbol{\delta}}. \tag{12}$$

This approach leads to finding a dispersion relation in graphene by finding eigenenergies of a simplified hamiltonian.

$$\Delta_{\mathbf{k}} = e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_1})} + e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_2})} + e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_3})} \tag{13}$$

$$= e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_3})} \left[1 + e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_1}-\boldsymbol{\delta_3})} + e^{\mathrm{i}(\mathbf{k}\cdot\boldsymbol{\delta_2}-\boldsymbol{\delta_3})}\right] \tag{14}$$

$$= \cdots = e^{-\mathrm{i}k_x a} \left[1 + 2e^{\mathrm{i}3k_x\frac{a}{2}} \cos\left(\frac{\sqrt{3}}{2}k_y a\right)\right]. \tag{15}$$

Final dispersion relation can be written as:

$$E_{\pm}(\mathbf{k}) = \pm t\sqrt{1 + 4\cos\left(\frac{3}{2}k_x a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right) + 4\cos^2\left(\frac{\sqrt{3}}{2}k_y a\right)}. \quad (16)$$

Main goal of project is to analyse Klein Tunelling across $n-p-n$ $(p-n-p)$ junctions in graphene. Because of zero energy gap in graphene $n/p$ interfaces act as semi-transparent mirrors. Thus charge carriers propagating across a bipolar junction can perform multiple reflections - as in Fabry-Perot interferometer.
Density of carriers is usually changed by applying $V_{\mathrm{TG}}$ and $V_{\mathrm{BG}}$ voltages. In calculations those voltages considered by

- applying and changing amplitude of potential barrier ($V_{\mathrm{TG}}$),
- changing energy of an incident electron ($V_{\mathrm{BG}}$).

Results should be similar to the one from the instruction:

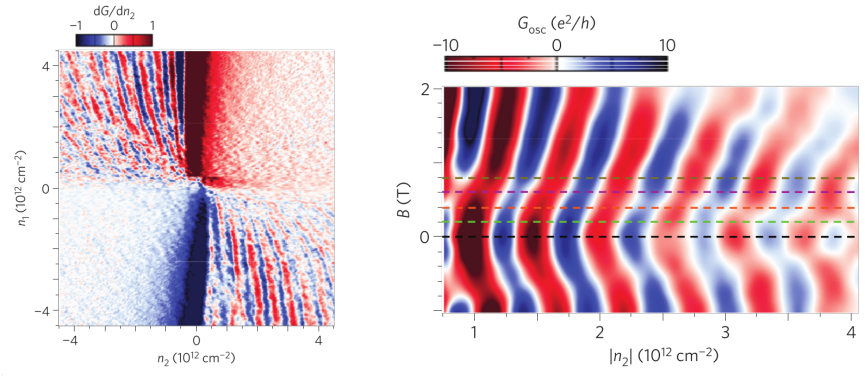



Figure: Measured values of conductance in graphene heterojunction.

```
class Graphene:
u = utl.Utils()

def __init__(self,
             a_nm=0.25, # graphene primitive vector
             sf=8.,     # scaling factor
             t_eV=-3.0, # hopping pottential
             W = 100,   # width of cell  (y dim)
             L = 200,   # length of cell (x dim)
             B = 0.,    # magnetic field
             V_np = 1., # potential amplitude
             d = 10.    # smothness of potential
             ):
...
```

# Graphene lattice

```
self.graphene = kwant.lattice.general(
    [(0, self.a0), (cos_30 * self.a0, sin_30 * self.a0)],
    [(0, 0), (self.a0 / np.sqrt(3), 0)],
    norbs=1,
)
self.a_sub, self.b_sub = self.graphene.sublattices
```

# make_system() for graphene

```
def pote_x(x):
    lt_term = np.tanh((x + self.L/8)/self.d)
    rt_term = np.tanh((x - self.L/8)/self.d)

    return self.V_np * ( lt_term - rt_term ) / 2

def nn_hopping(site1, site2):
    x1, y1 = site1.pos
    x2, y2 = site2.pos
    phase = -self.B * (y1 + y2) * (x2 - x1) / 2

    return self.t0 * np.exp(1j * phase)
```

# make_system() for graphene

```python
sys = kwant.Builder()

graphene = self.graphene
sys[graphene.shape(rect, (0, 0))] = potential
sys[graphene.neighbors()] = nn_hopping

syml = kwant.TranslationalSymmetry([-np.sqrt(3) * self.a0, 0])

leadl = kwant.Builder(syml)
leadl[graphene.shape(lead_shape, (0, 0))] = pote_x(self.x_min)
leadl[graphene.neighbors()] = nn_hopping
```

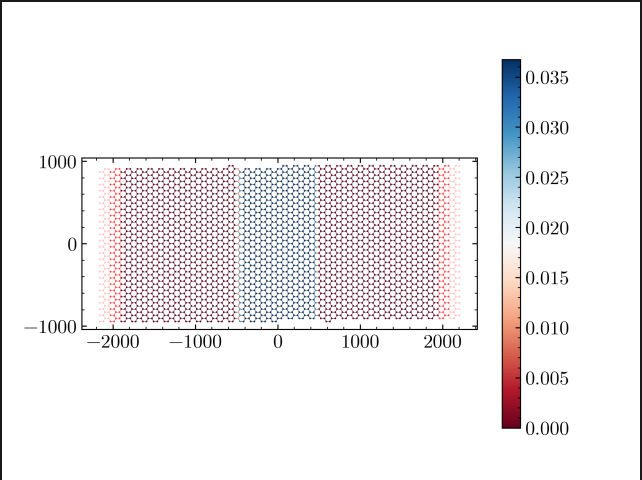



Figure: Graphene lattice for $sf = 16$. This scaling factor was to large.

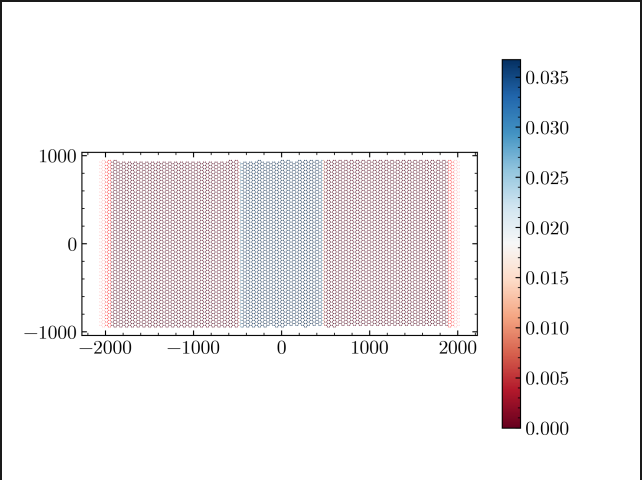
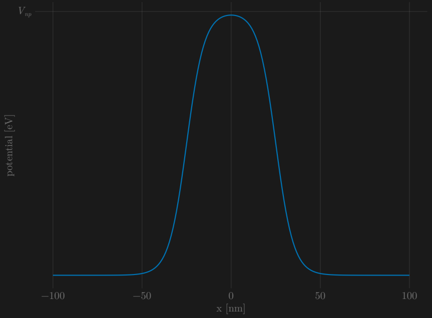
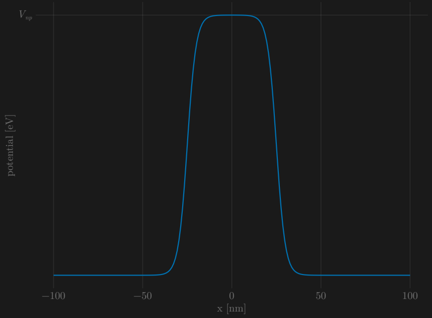



Figure: Graphene lattice used in simulation. Color indicates potential value.

# Smoothness parameter




(a)




(b)

Figure: Smooth potential barrier used in simulation $d =$ (a) 10 nm, (b) 5 nm.

As a first check dispersion relation has been calculated.

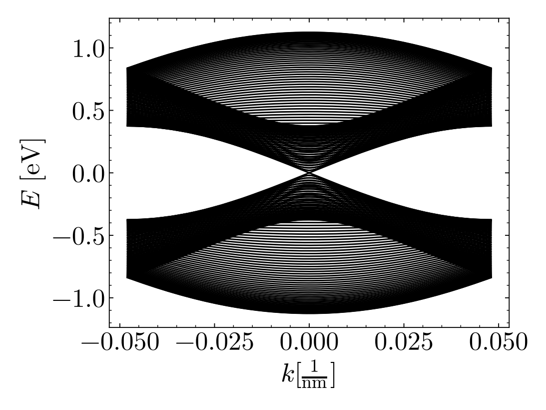



Figure: Dispersion relation in graphene layer.

Obtained linear dispersion relation near dirac cone is characteristic for graphene.

In order to check the range of calculations, simple currents have been calculated.

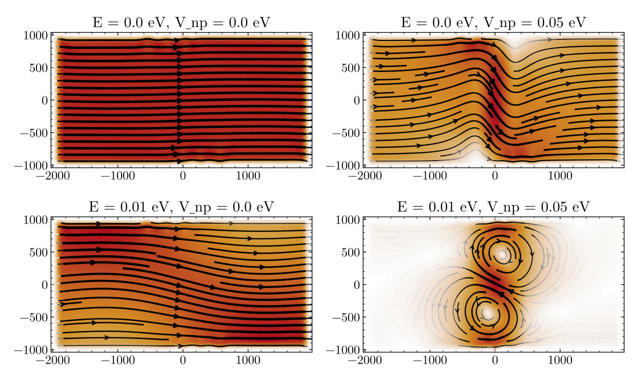



Figure: Currents in the system with changing incident electron energy and potential barier height.

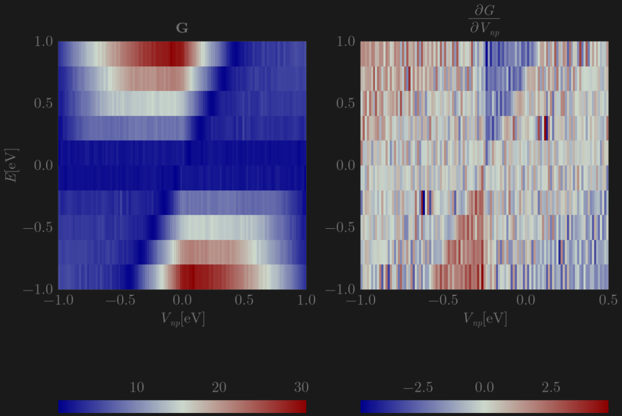



Figure: Conductance scan over an incident electron energy $E$ and an amplitude of potential barrier $V_{np}$.

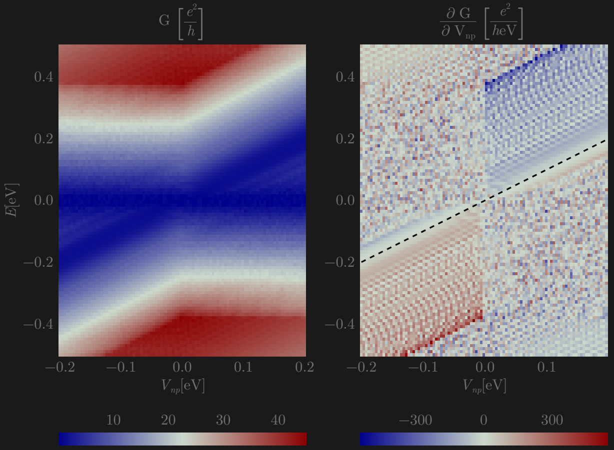



Figure: Finer conductance scan over an incident electron energy $E$ and an amplitude of potential barrier $V_{np}$. Black dashed line has $\frac{\pi}{4}$ slope and has been added as a reference.

Calculations results can be compared to other theoretical calculations.

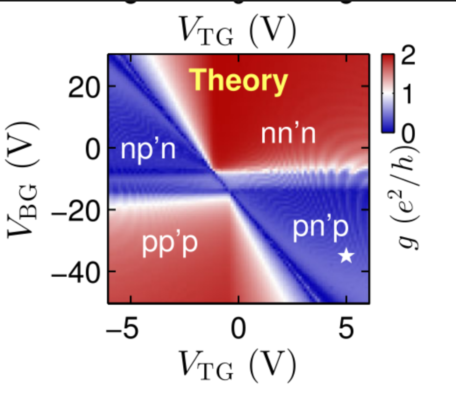



Figure: Figure 1e from 10.1103/PhysRevLett.113.116601. Similarities between plot are clearly visible, however obtained in this project has much lower range.

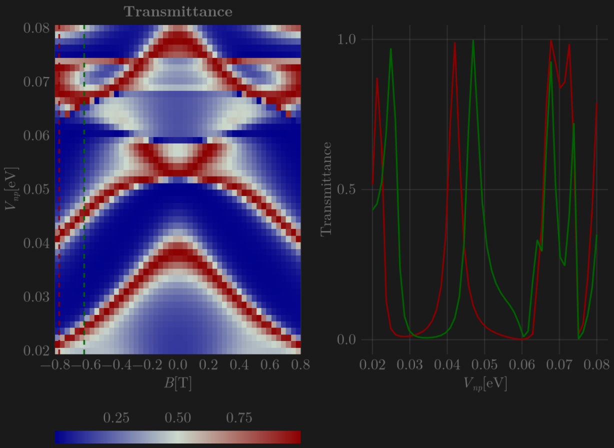
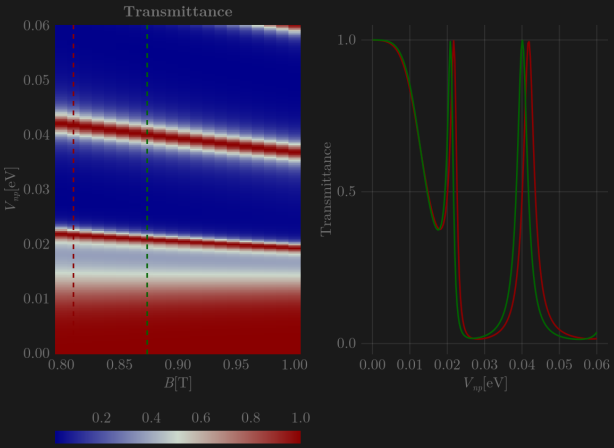



Figure: Transmittance scan over external magnetic field $B$ and amplitude of potential barrier $V_{np}$. Incident electron energy has been set to 0.01 eV. For two values lines have been plotted for better visualisation of transmittance maxima.

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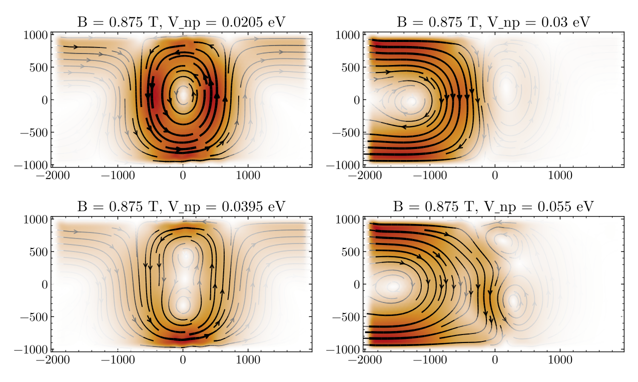


Figure: Currents in the system with external magnetic field and changing potential barier height. Incident electron energy is equal to 0.01 eV. Parameters have been chosen in order to obtain maxima and minima of transmittance.

Calculations proved that:

- conductance oscilations are theoretically observable in graphene heterojunctions,
- introducing smooth potential barrier for electrons may act as material with different refractive index for photons (optics analogy),
- external magnetic field acts on electrons and shifts oscilations,

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