

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

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# Tight Binding model

Hamiltonian in tight binding approximations can be written as:

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

where  $t$  is energy of hopping between nearest neighbours ( $\approx 2.8$  eV), and  $t'$  is energy of hopping between second nearest 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 creations (annihilation) operators on sublattice  $A$  ( $\hat{b}$  for sublattice  $B$ ).

# Tight Binding model

Hamiltonian for only neareset neighbours can be written as

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

$$\sum_{\langle i,j \rangle} \left( \hat{a}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{a}_i \right) = \sum_{i \in A} \sum_{\delta} \left( \hat{a}_i^\dagger \hat{b}_{i+\delta} + \hat{b}_{i+\delta}^\dagger \hat{a}_i \right), \quad (3)$$

where  $\delta$  means sum over nearest neighbours.

Next step involves switching operators to reciprocal space using Fourier transform

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

Hamiltonian after transformations can be written as

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

we can simplify this by introducing property:

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

Simplify hamiltonian takes form

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

which in simpler form is

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

where

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

and

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

Term

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

is nothing else than matrix representation of hamiltonian with elements

$$\Delta_{\mathbf{k}} = \sum_{\delta} e^{i\mathbf{k} \cdot \delta}. \quad (12)$$

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

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

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

$$= \dots = e^{-ik_x a} \left[ 1 + 2e^{i3k_x \frac{a}{2}} \cos\left(\frac{\sqrt{3}}{2} k_y a\right) \right]. \quad (15)$$

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  $V_{TG}$  and  $V_{BG}$  voltages. In calculations those voltages are applied by

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



Results should be similar to one from instruction:

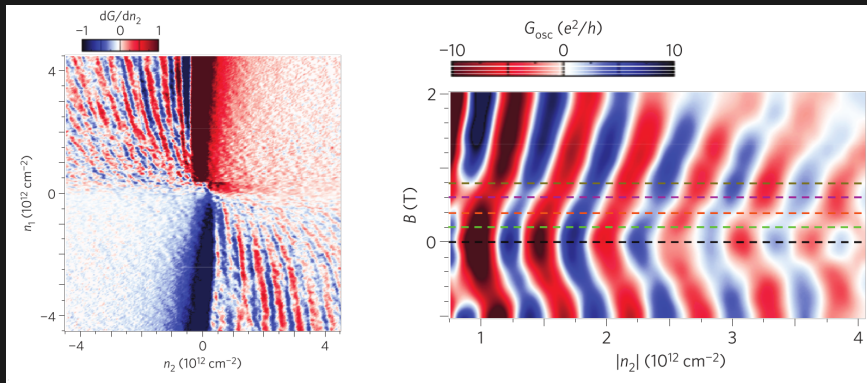


Figure: Measured values of conductance in graphene heterojunction.

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

    def __init__(self,
                  a_nm=0.25, # graphene primitive vector
                  sf=8.,     # scaling factor
                  t_eV=-3.0, # hopping potential
                  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  
    pereir = -self.B * (y1 + y2) * (x2 - x1) / 2  
  
    return self.t0 * np.exp(1j * pereir)
```

# make\_system() for graphene

---

```
sys = kwant.Builder()

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

sym1 = kwant.TranslationalSymmetry([-np.sqrt(3) * self.a0, 0])

lead1 = kwant.Builder(sym1)
lead1[graphene.shape(lead_shape, (0, 0))] = pote_x(self.x_min)
lead1[graphene.neighbors()] = nn_hopping
```

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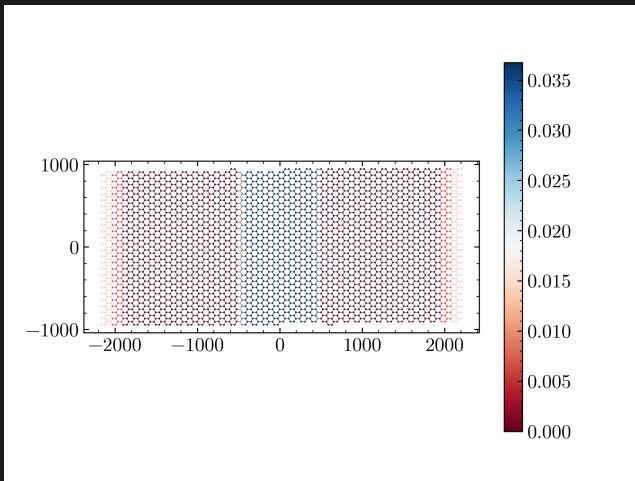


Figure: Graphene lattice for  $sf = 16$ . This scaling factor was too large.

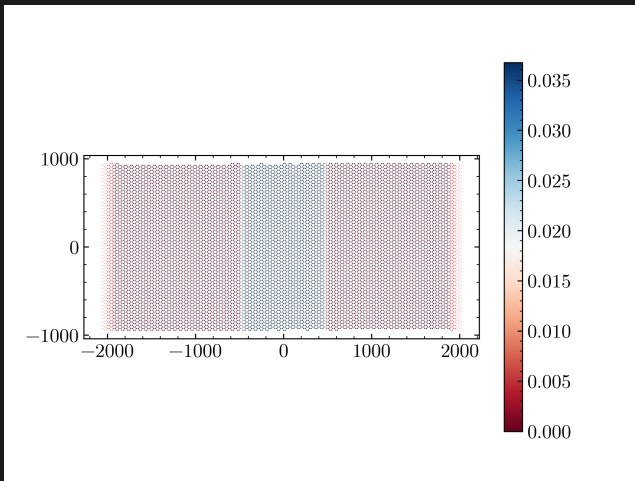
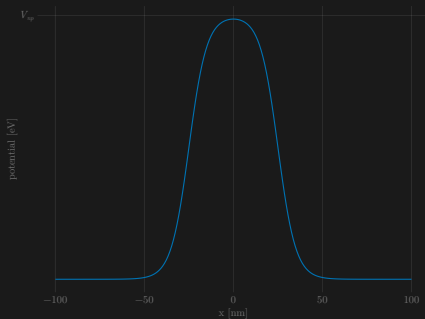
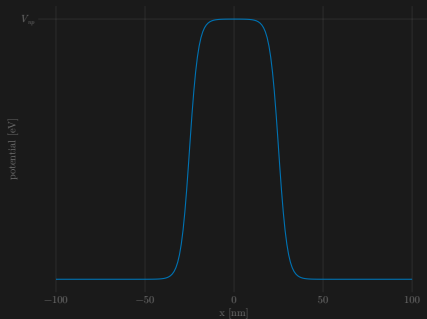


Figure: Graphene lattice used in simulation. Color indicates potential value.

# Smoothness parameter



(a)

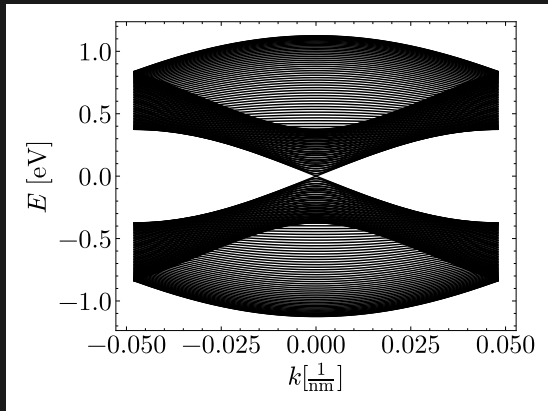


(b)

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



As a first check dispersion relation has been calculated.



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

Figure: Dispersion relation in graphene layer.

In order to check a range of calculations simple currents has been calculated.

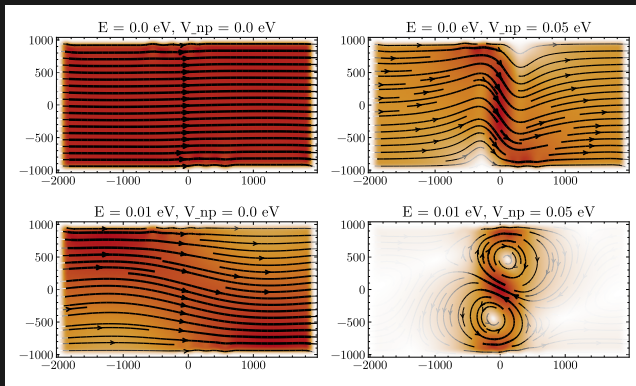


Figure: Currents in system with changing incident electron energy and potential barrier height.

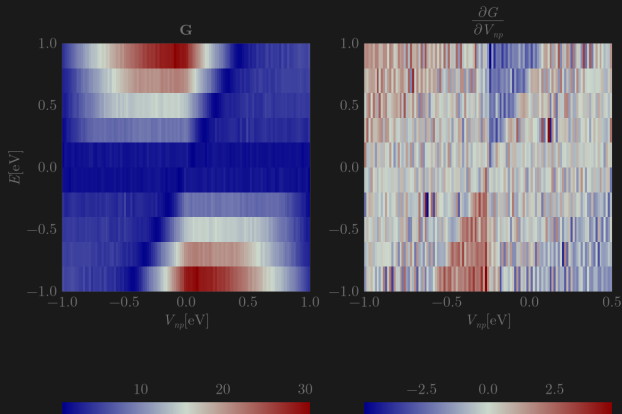


Figure: Conductance scan over incident electron energy  $E$  and amplitude of potential barrier  $V_{np}$ .

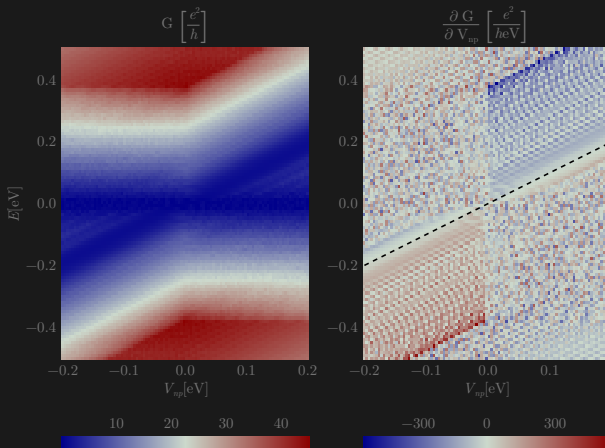


Figure: Finer conductance scan over incident electron energy  $E$  and amplitude of potential barrier  $V_{np}$ . Black dashed line has  $\frac{\pi}{4}$  slope and has been added as reference.

Calculations results can be compared to other theoretical calculations.

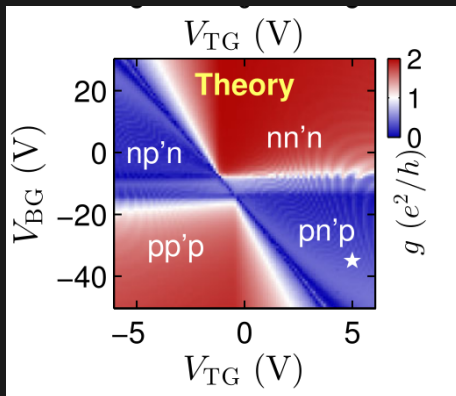


Figure: Figure 1e from [10.1103/PhysRevLett.113.116601](https://doi.org/10.1103/PhysRevLett.113.116601). Similarities between plot are clearly visible, however obtained in one project has much lower range

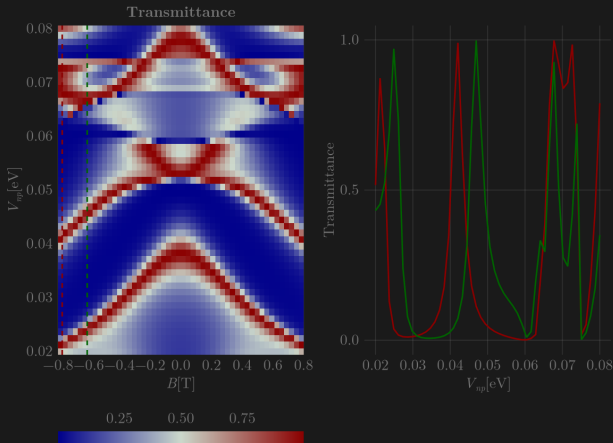


Figure: Transmittance scan over external magnetic field  $B$  and amplitude of potential barrier  $V_{np}$ . Incident electron energy has been set to 0.01 eV. For two values lines has been plotted for better visualisation of transmittance maxima.

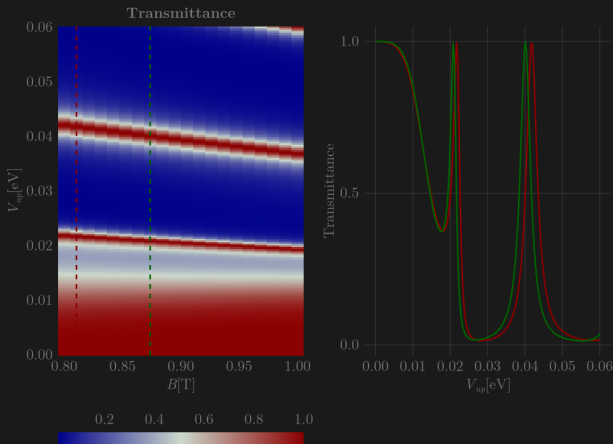


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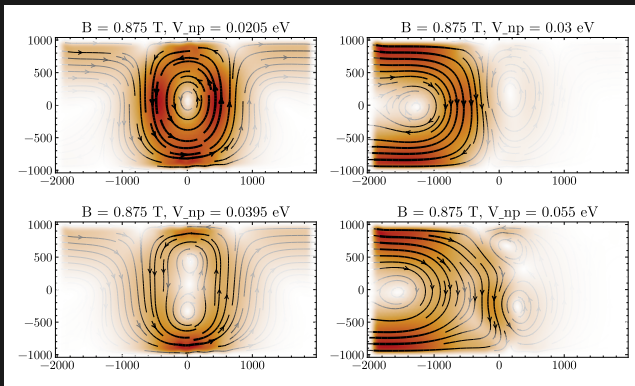


Figure: Currents in system with external magnetic field and changing potential barrier height. Incident electron energy is equal to  $0.01$  eV. Parameters have been chosen in order to obtain maxima and minima of transmittance.



Calculations proved that:

- conductance oscillations 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 oscillations,

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