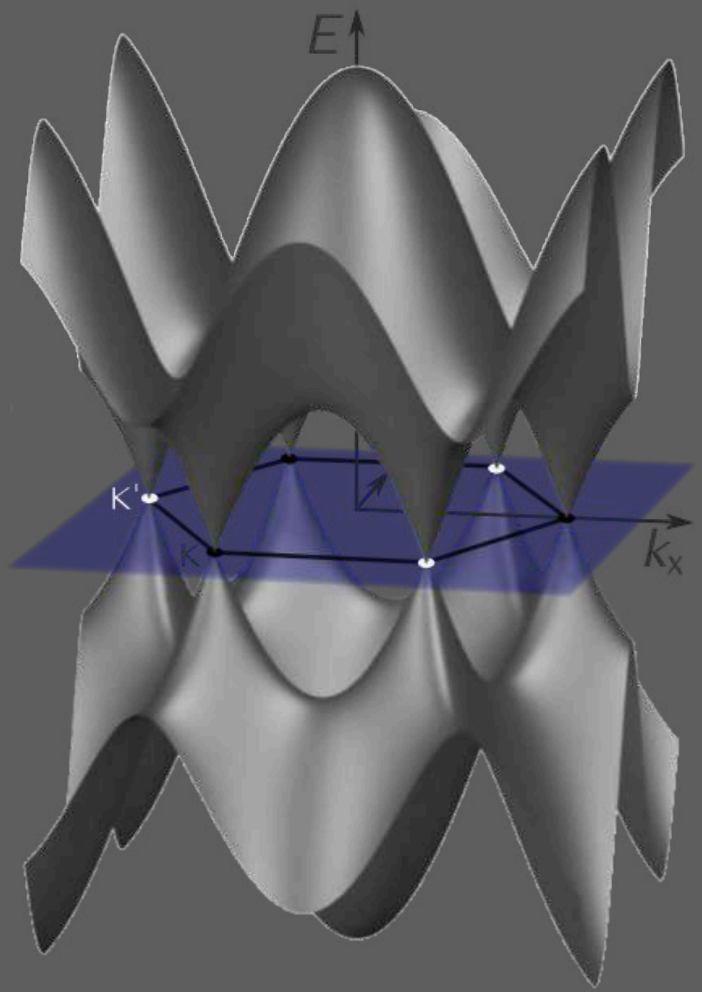
Semiclassical theory of Scanning Gate Microscopy for massless Dirac fermions

Presented by Pierre Guichard and Florian Maurer



Tutored by :
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— *Dietmar Weinmann*

IPCMS
Université de Strasbourg

Image source : Wikipedia, by Ponor

Objectives

- Theoretical understanding of experimental results using a semi-classical theory.

- Study and understand electronic transport in graphene.

- Compare electronic transport in graphene and in semiconductor heterostructure by studying the transmission.

Outline

I. Experimental motivations

II. Electronic transport in graphene

III. Classical method

IV. Results

V. Conclusion and outlook

I. Experimental motivations

II. Electronic transport in graphene

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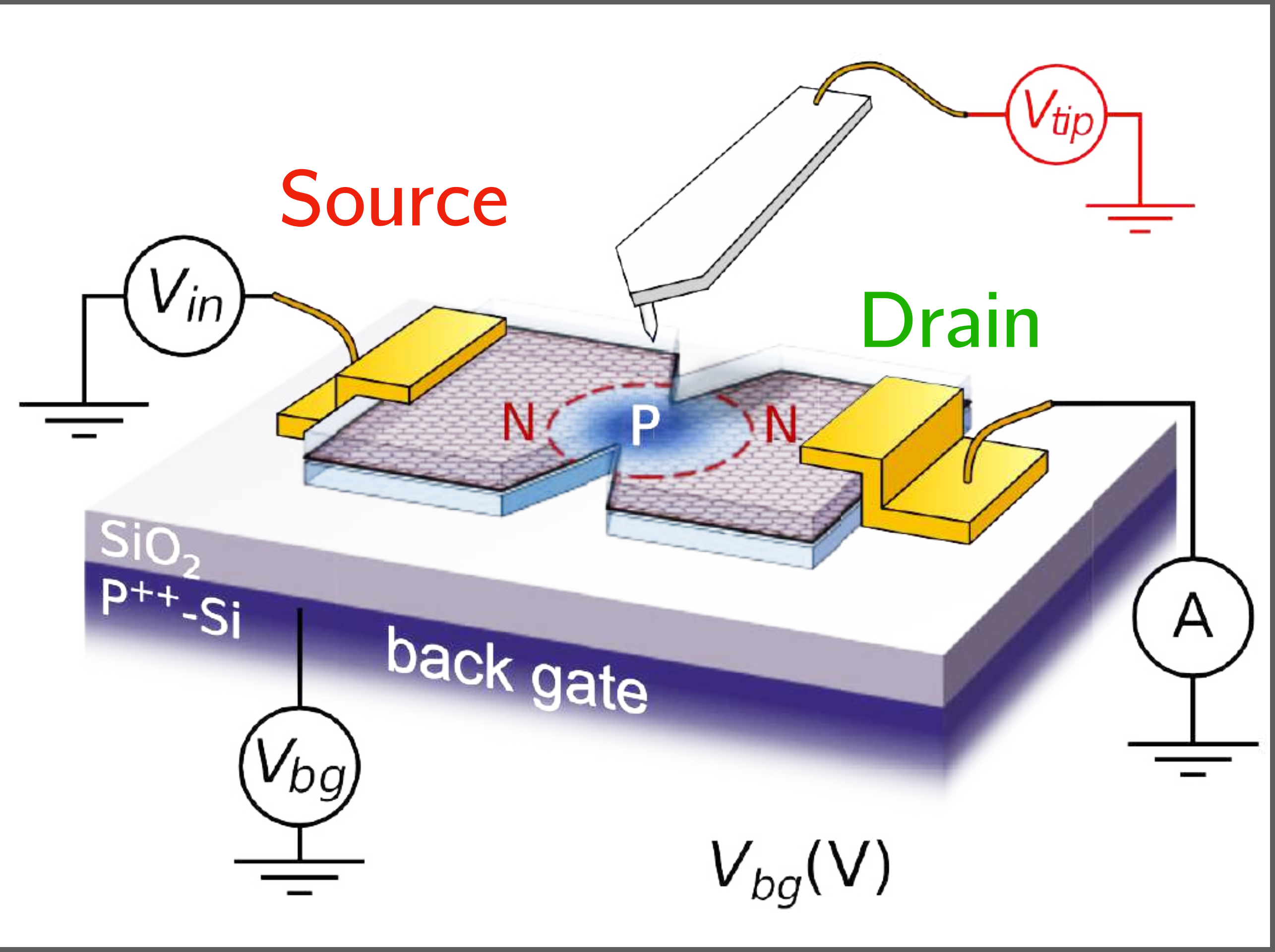
I — Experimental motivations

- What is Scanning Gate Microscopy ?
  - Imaging electron flow



Change of conductance with tip position

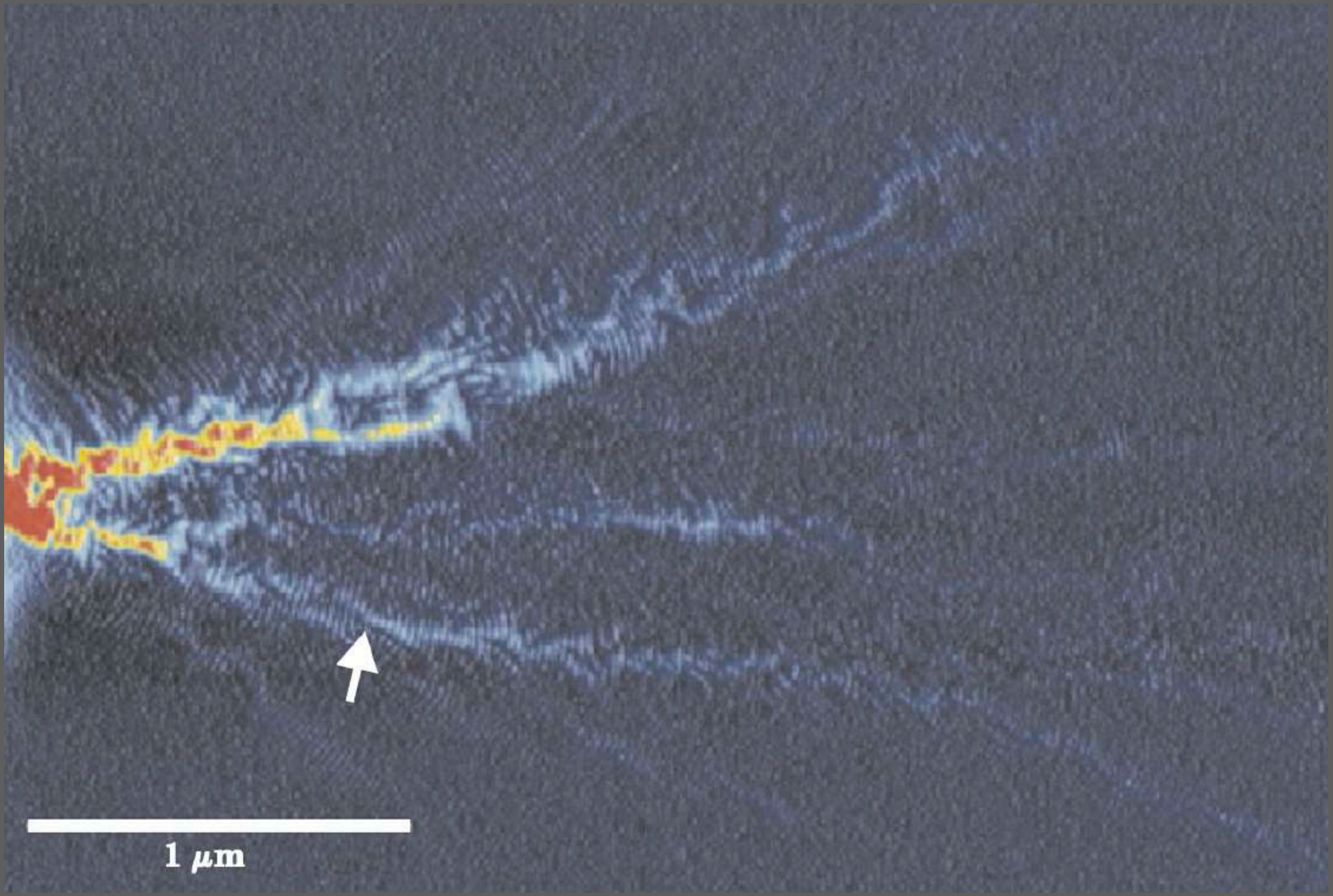
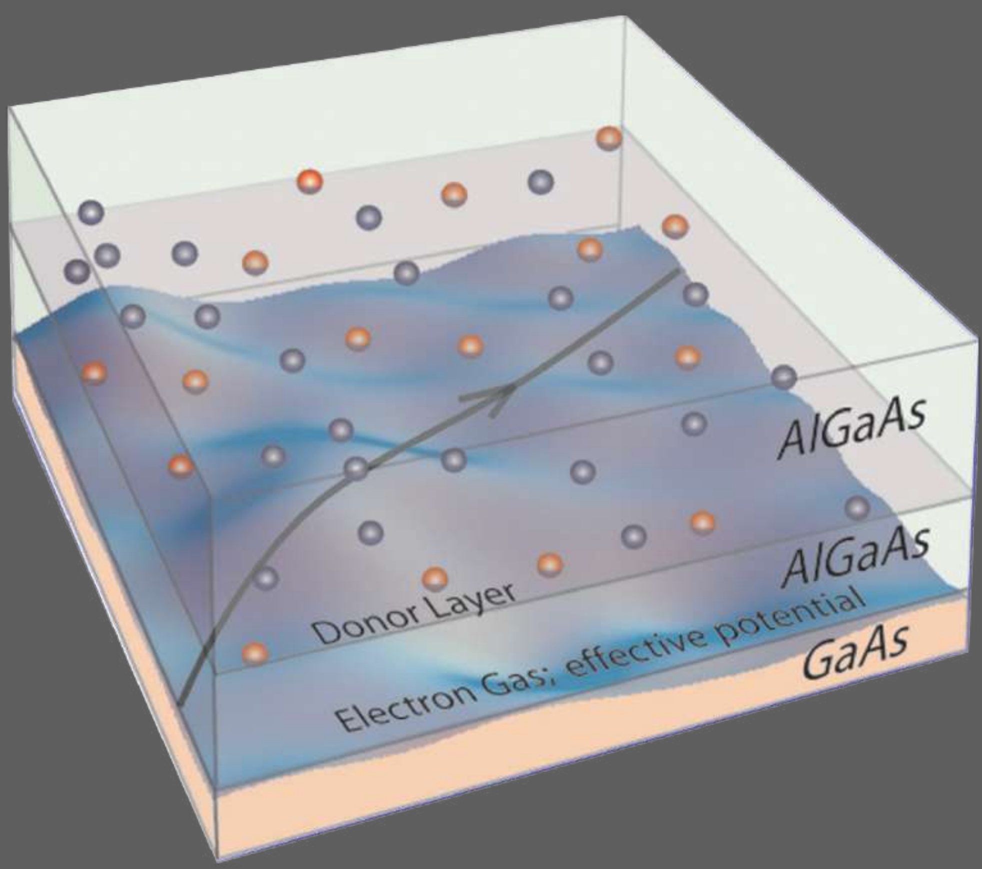


Image source : Left : B. Brun, Phys. Rev. B 100 (2019). Right : M. Topinka, Physics Today 56 (2003).

I — Experimental motivations

- SGM in semiconductor heterostructures

  - 2D motion of electrons
  - Current density



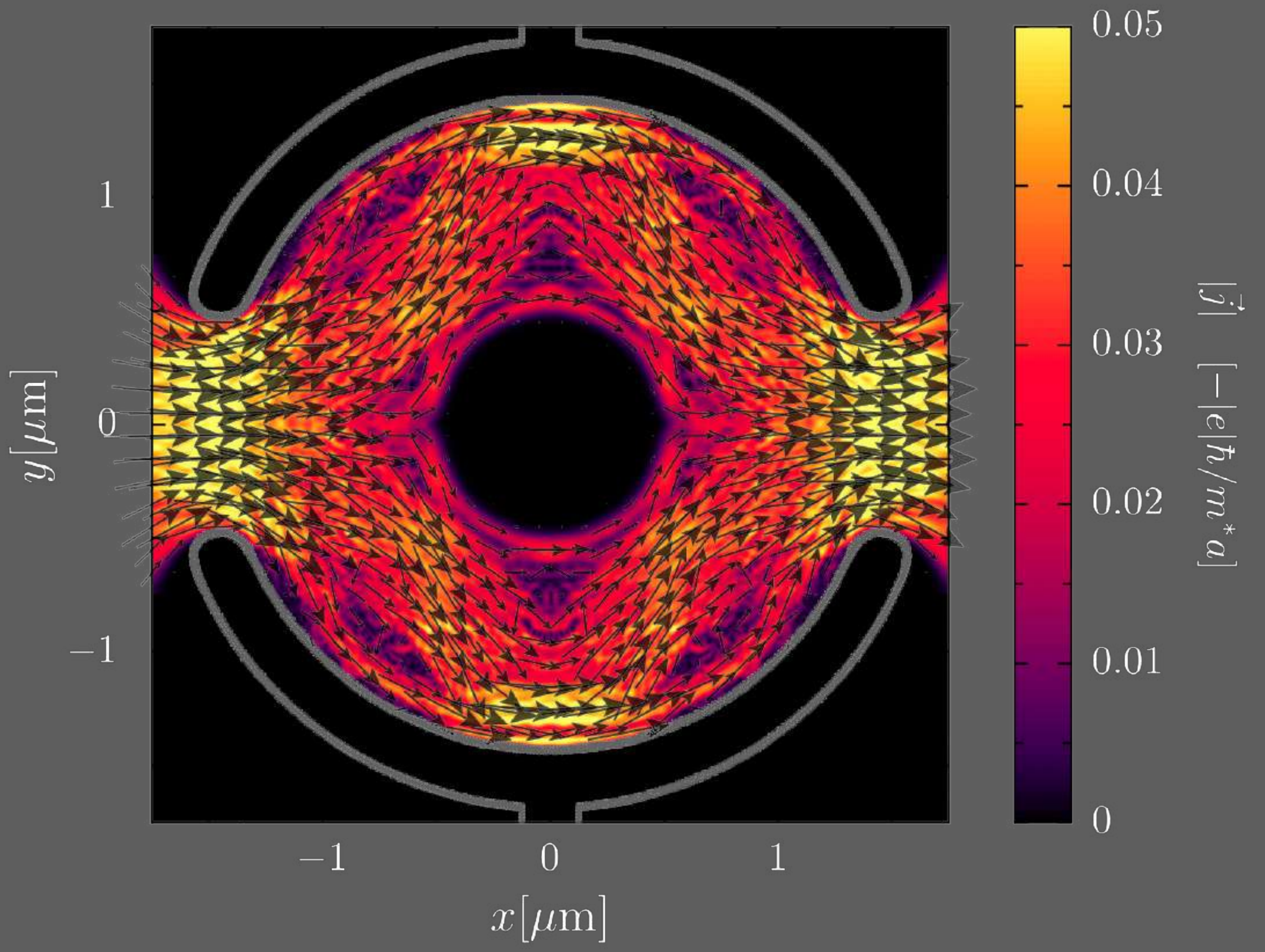


Image source : Left : M. Topinka, Physics Today 56 (2003). Right : C. Pöltl, Phys. Rev. B 94 (2016).

I — Experimental motivations

- SGM in graphene

  - Quantum simulations yet no semi-classical model for the motion

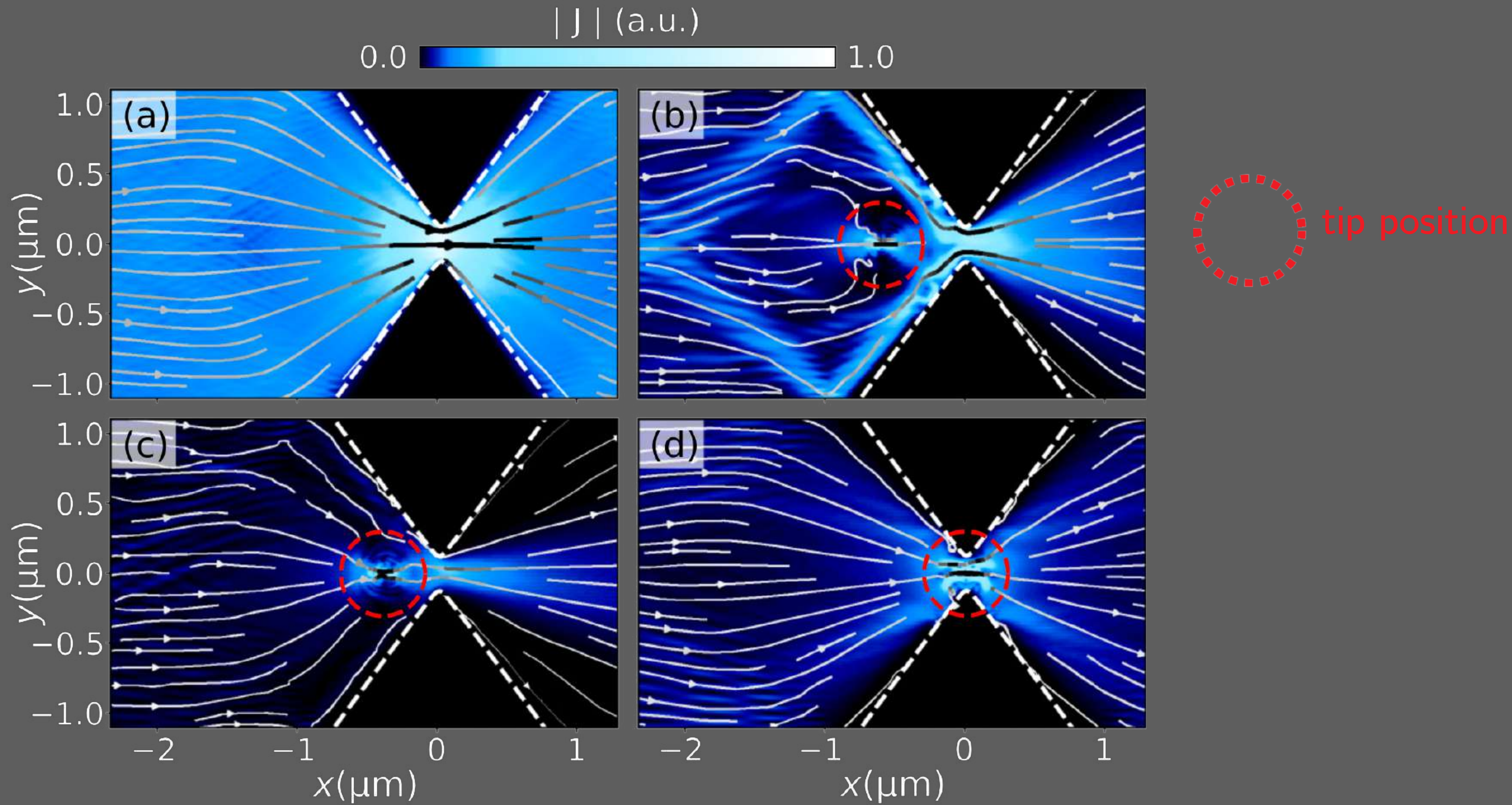


Image source : B. Brun, Phys. Rev. B 100 (2019).

I. Experimental motivations

II. Electronic transport in graphene

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II — Electronic transport in graphene

- What is graphene ?
  - Unveiled in 2004 for the first time 
  - 2D material : monolayer of Carbon atoms

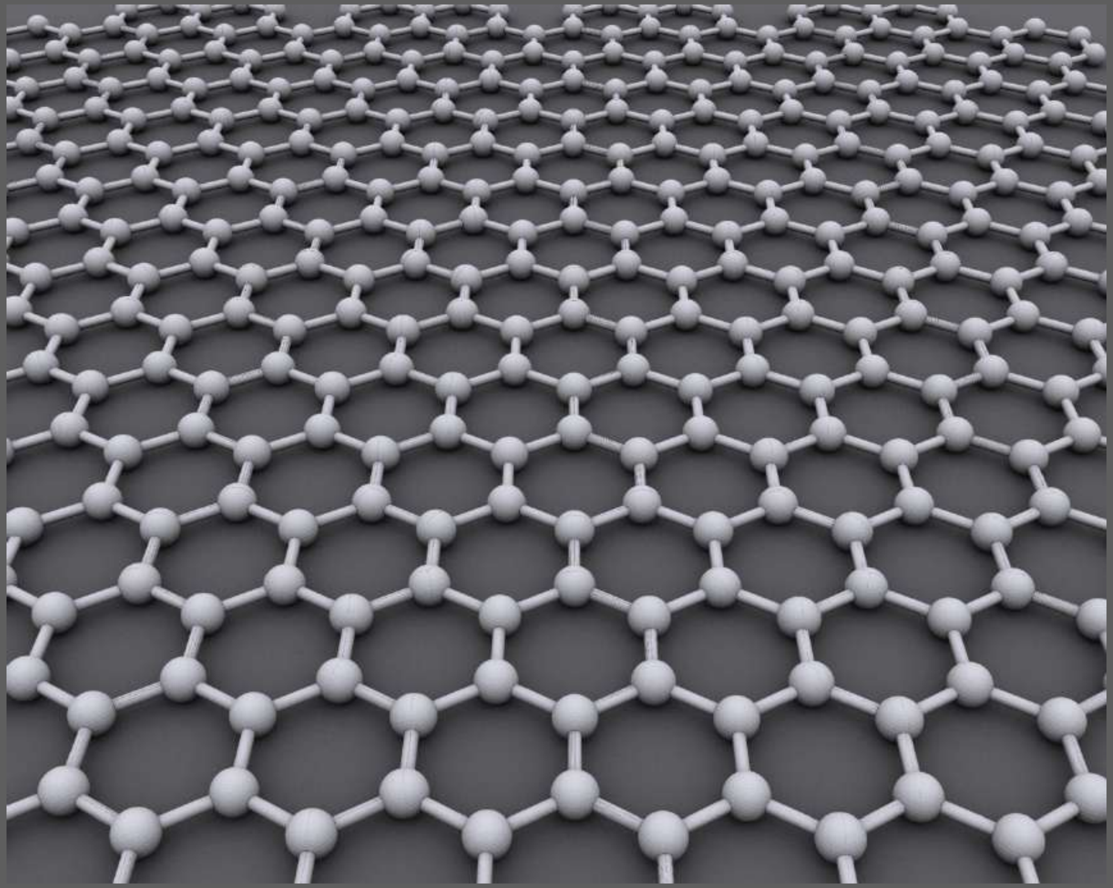


Image source : Wikipedia, by Alexander AIUS

II — Electronic transport in graphene

- What is graphene ?
  - Honeycomb lattice : not a Bravais lattice
  - Two atoms per cell

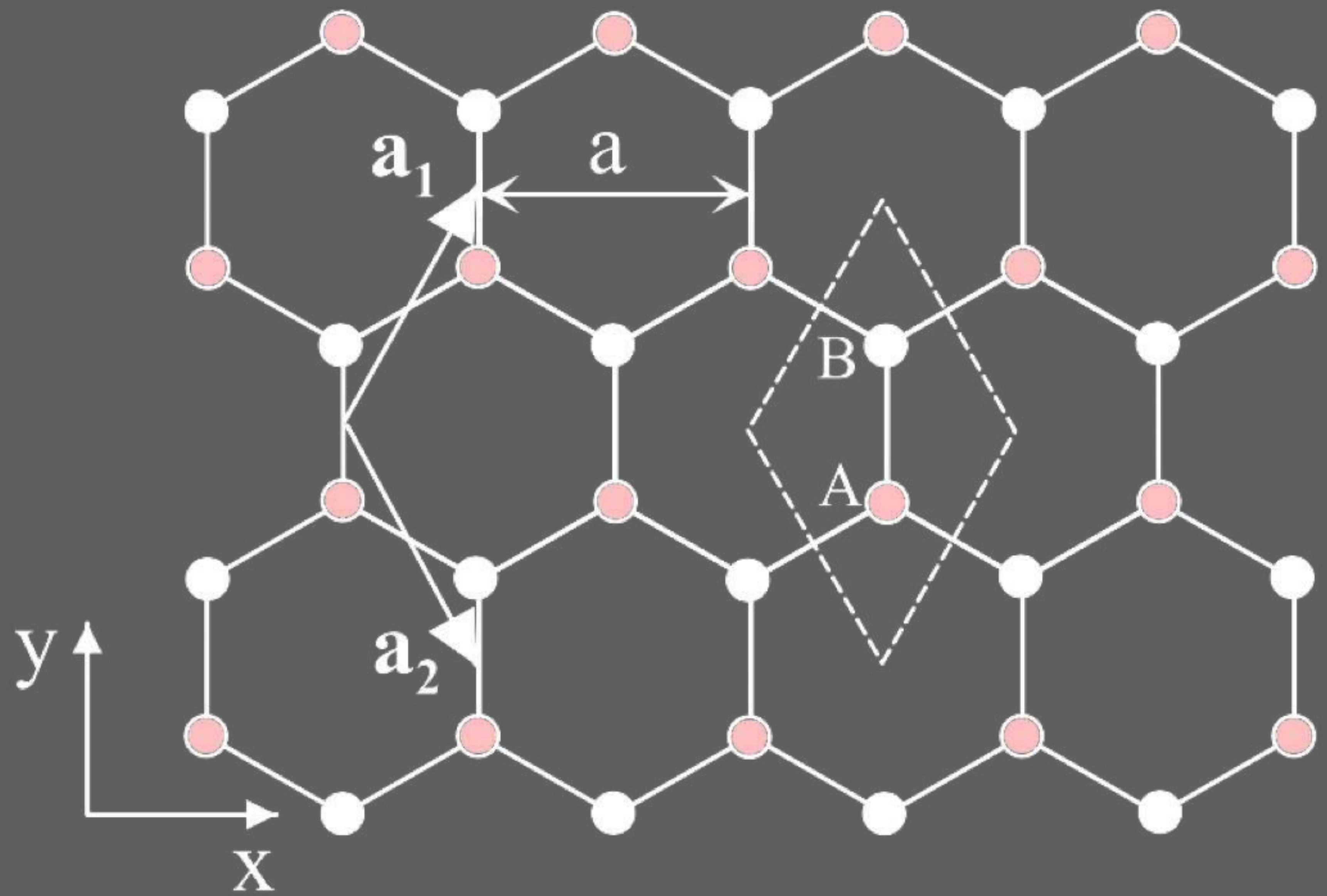
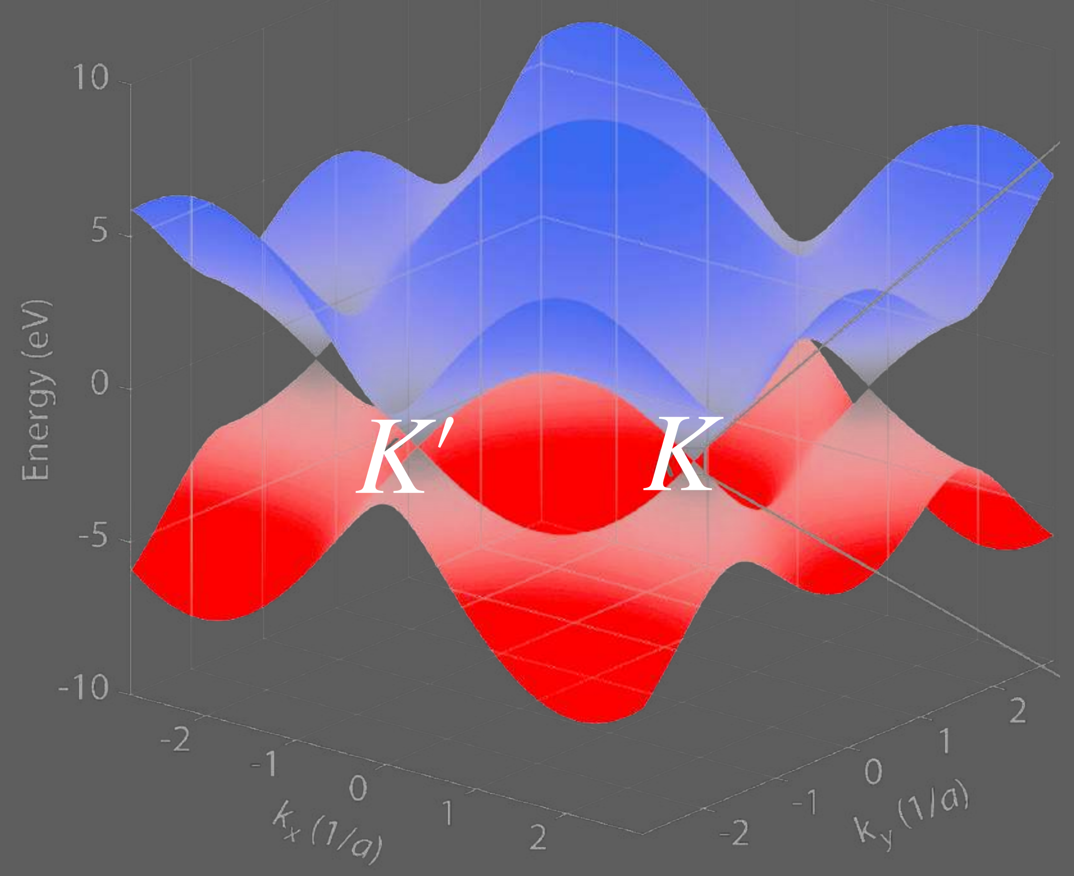
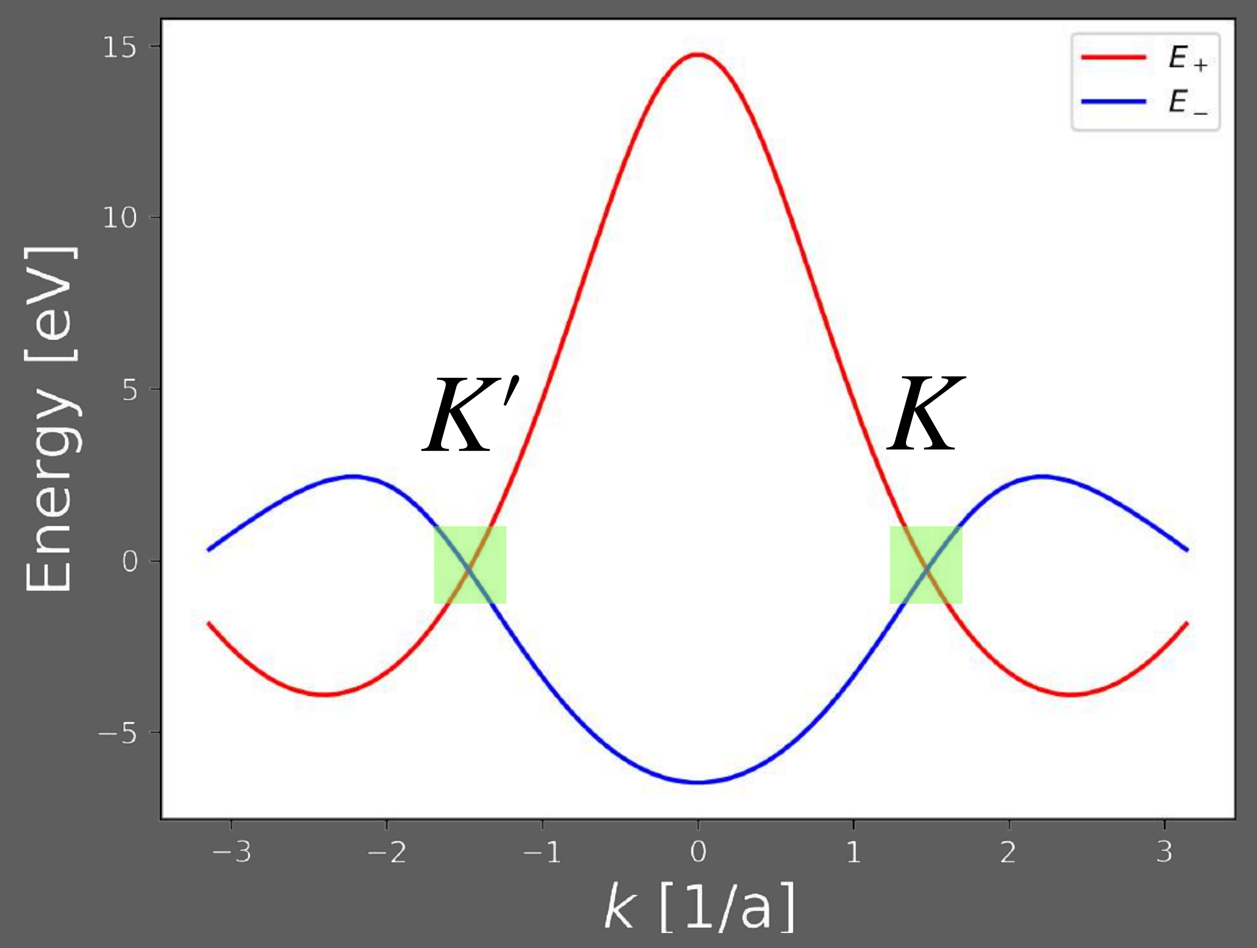


Image source : Fig. 8.1, Graphene Nanoelectronics, E. McCann

II — Electronic transport in graphene





- Linear dispersion relation near K and K'

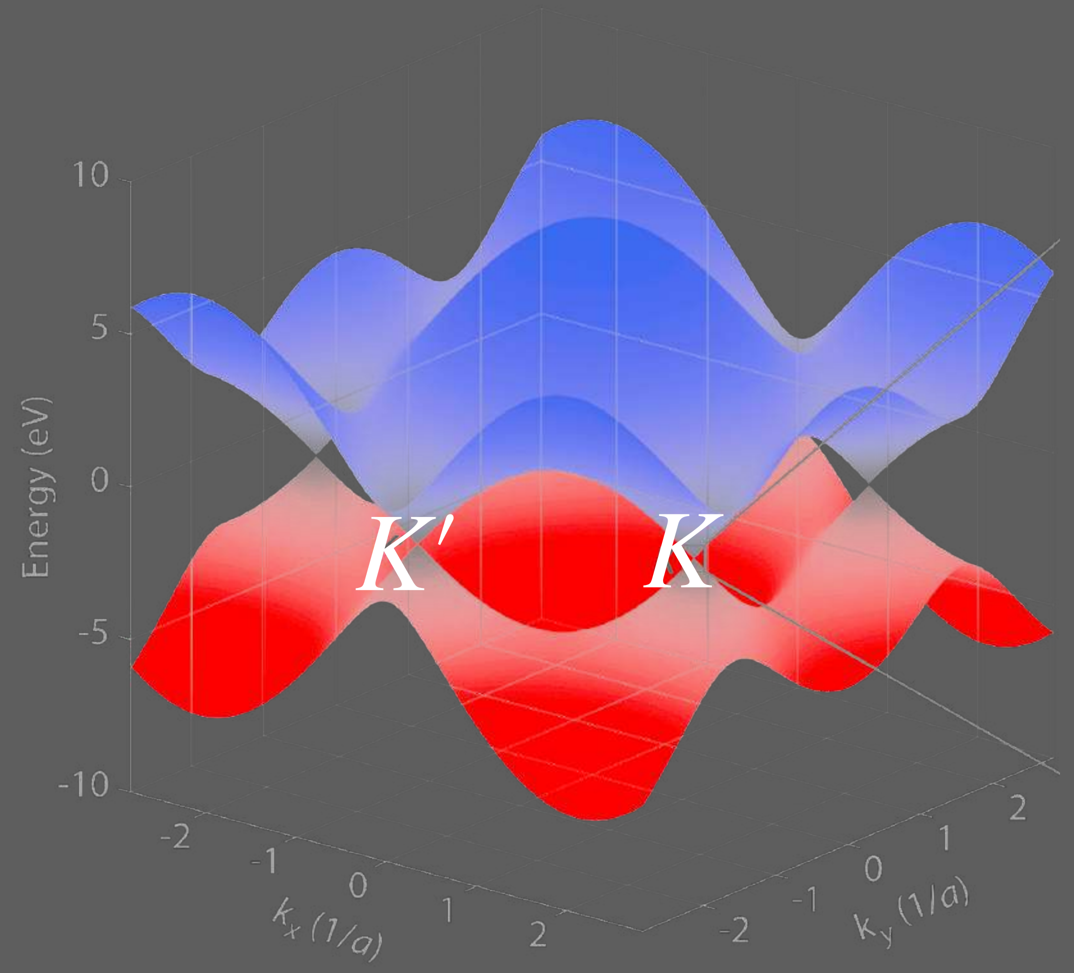
$$E_\pm = \pm v_\mathrm{F} |\overrightarrow{p}|$$

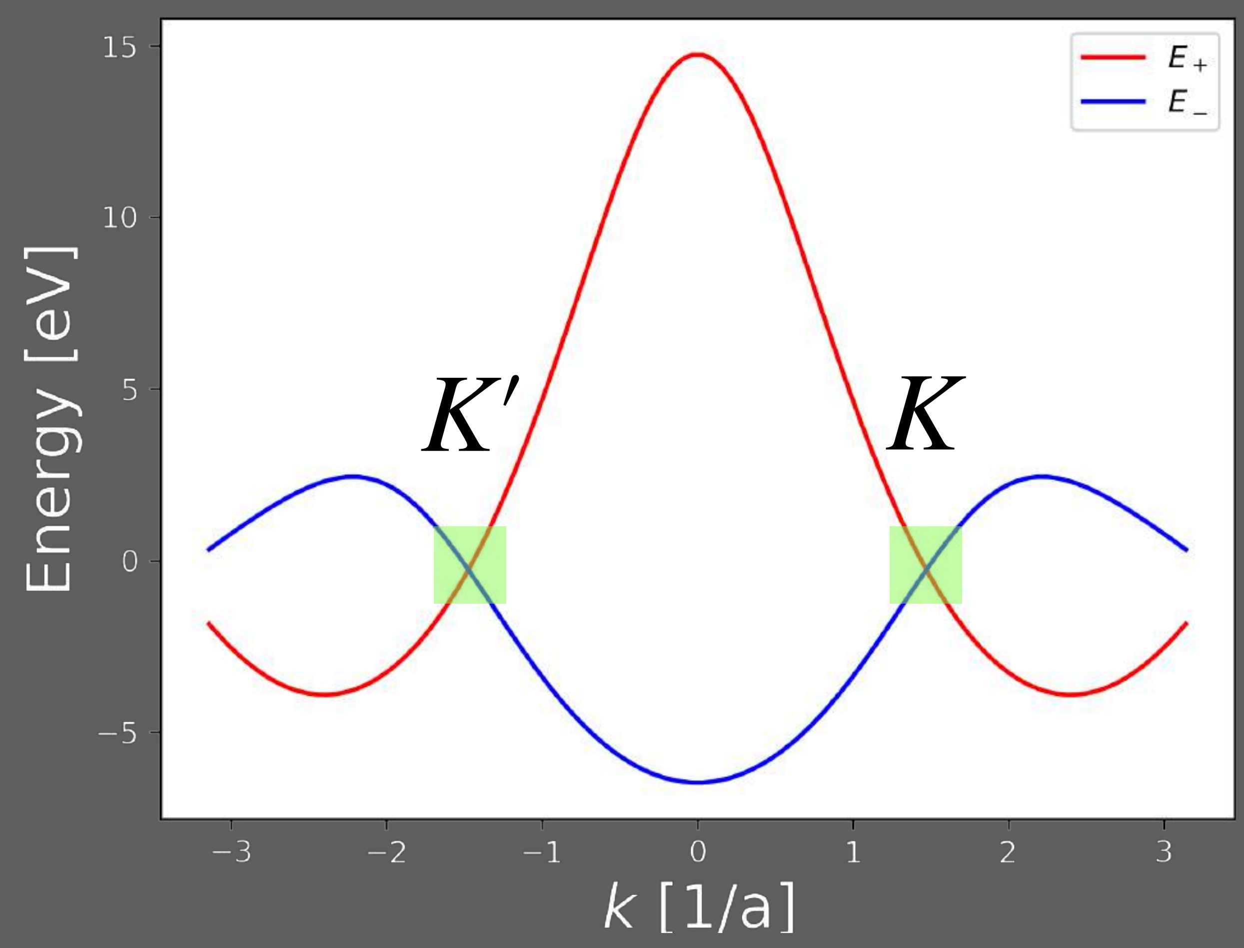
Massless Dirac fermions

$$v_\mathrm{F} \simeq \frac{c}{300}$$

Pseudo-relativistic

II — Electronic transport in graphene





- Linear dispersion relation near K and K'

$$E \neq \frac{|\overrightarrow{p}|^2}{2m}$$

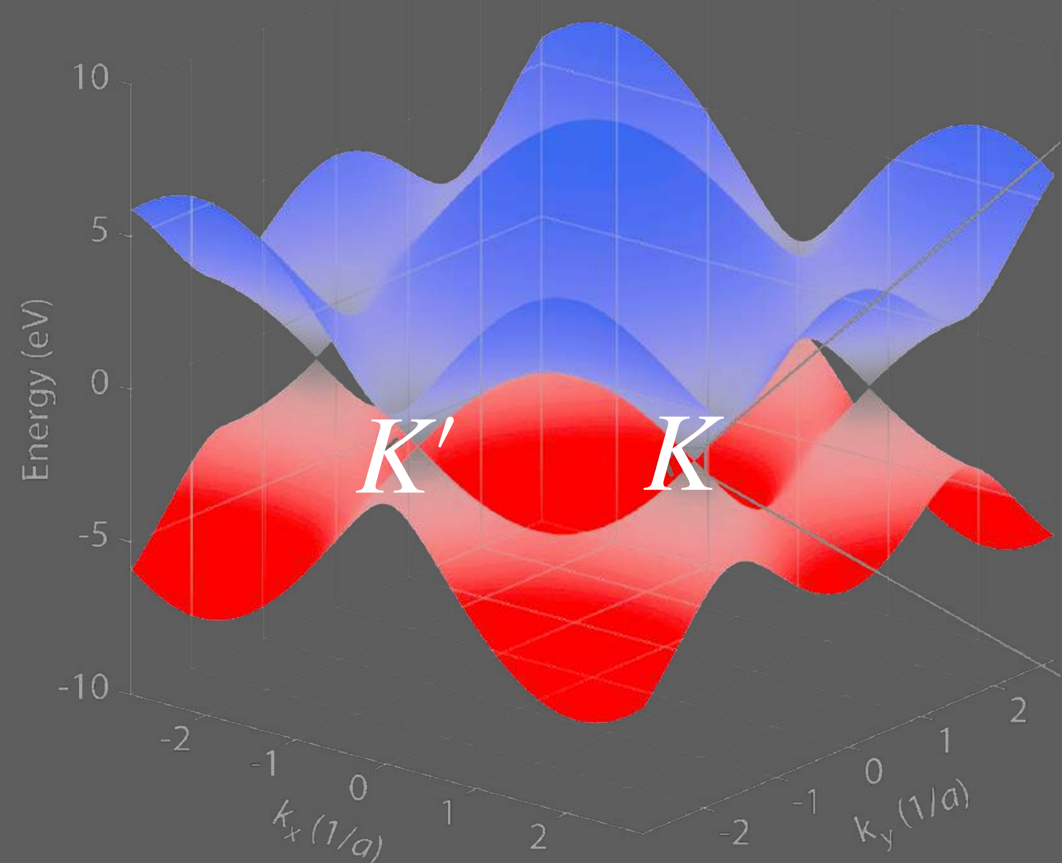
$$E_\pm = \pm v_\mathrm{F} |\overrightarrow{p}|$$

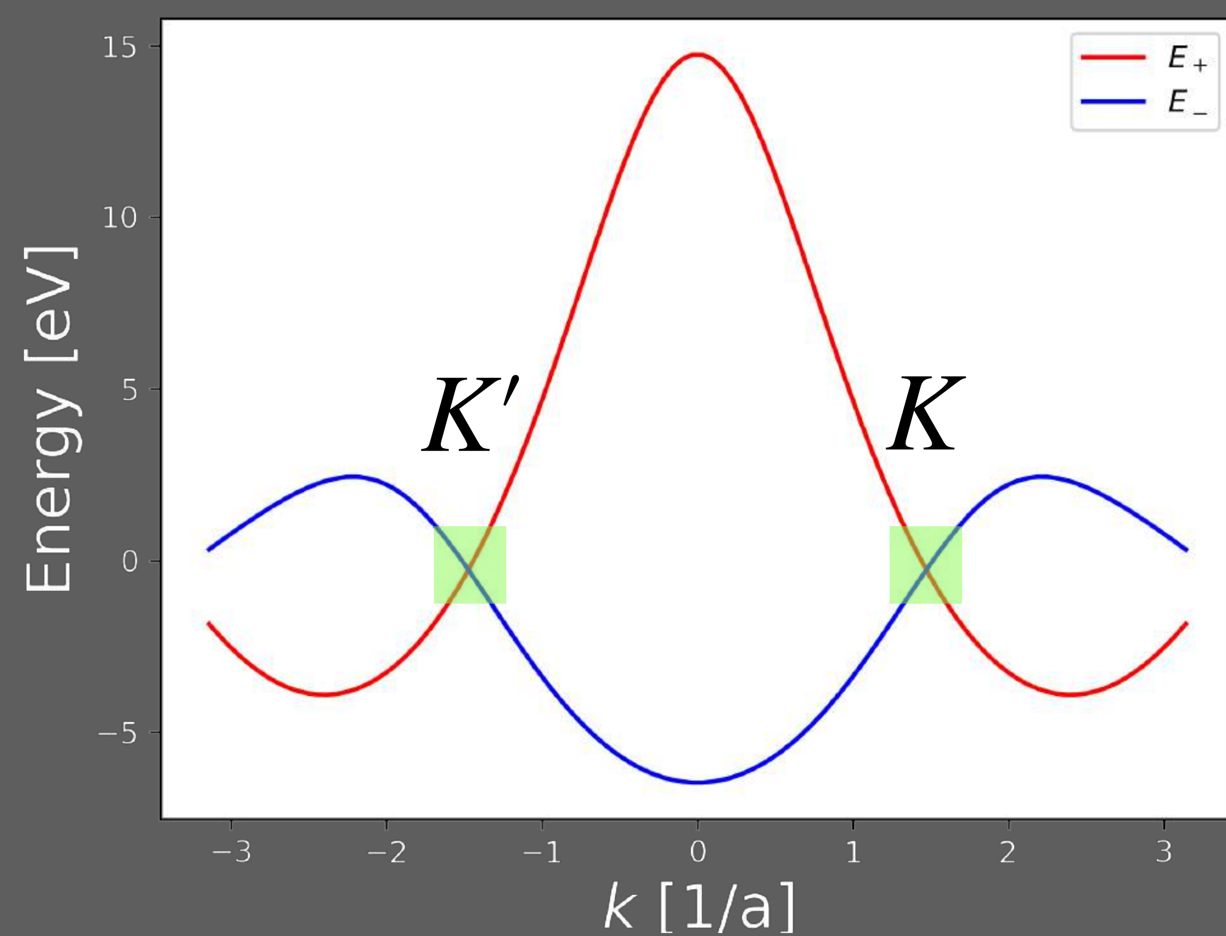
Massless Dirac fermions

$$v_\mathrm{F} \simeq \frac{c}{300}$$

Pseudo-relativistic

II — Electronic transport in graphene





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$$E \neq \frac{|\overrightarrow{p}|^2}{2m}$$

$$E_\pm = \pm v_\mathrm{F} |\overrightarrow{p}|$$

$$v_\mathrm{F} \simeq \frac{c}{300}$$

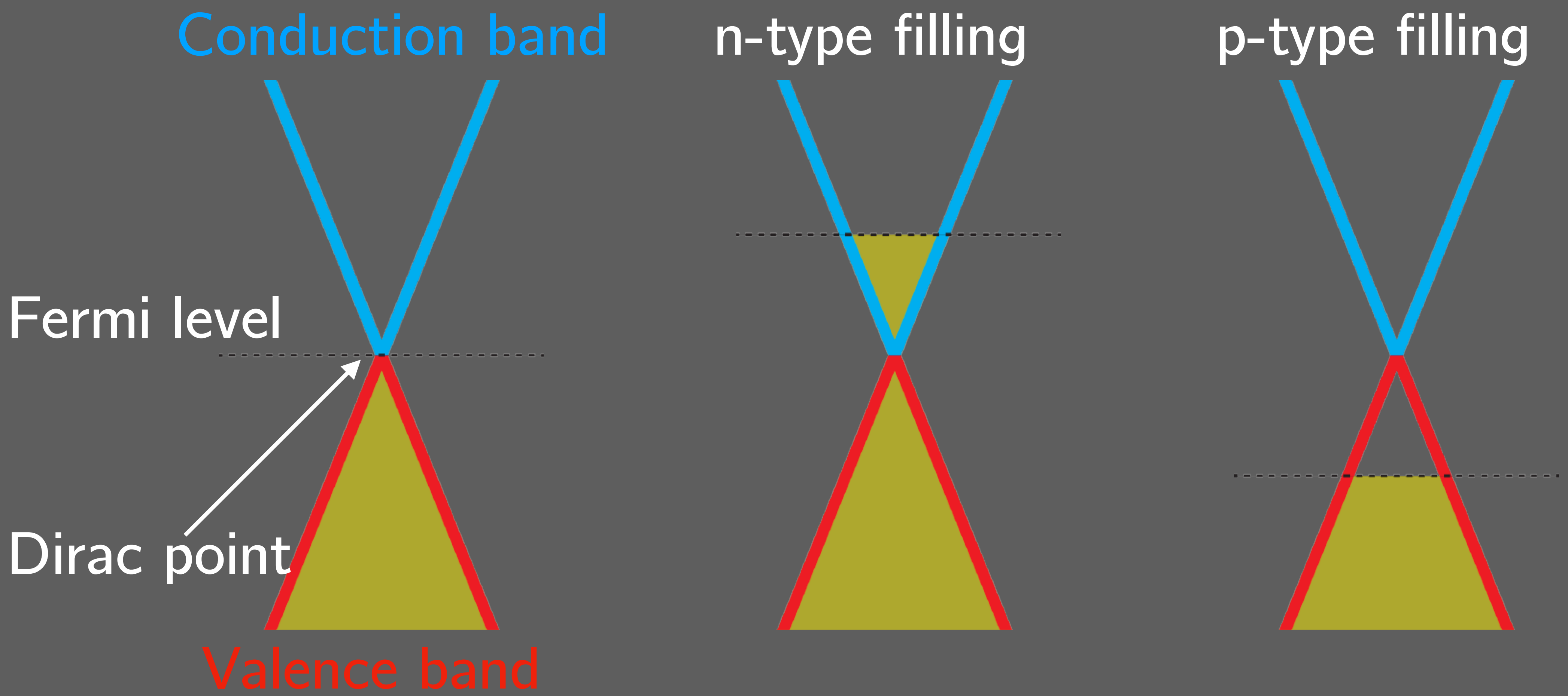
Massless Dirac fermions

Pseudo-relativistic

$$E_\pm = \pm\sqrt{c^2|\overrightarrow{p}|^2 + m^2c^4}$$

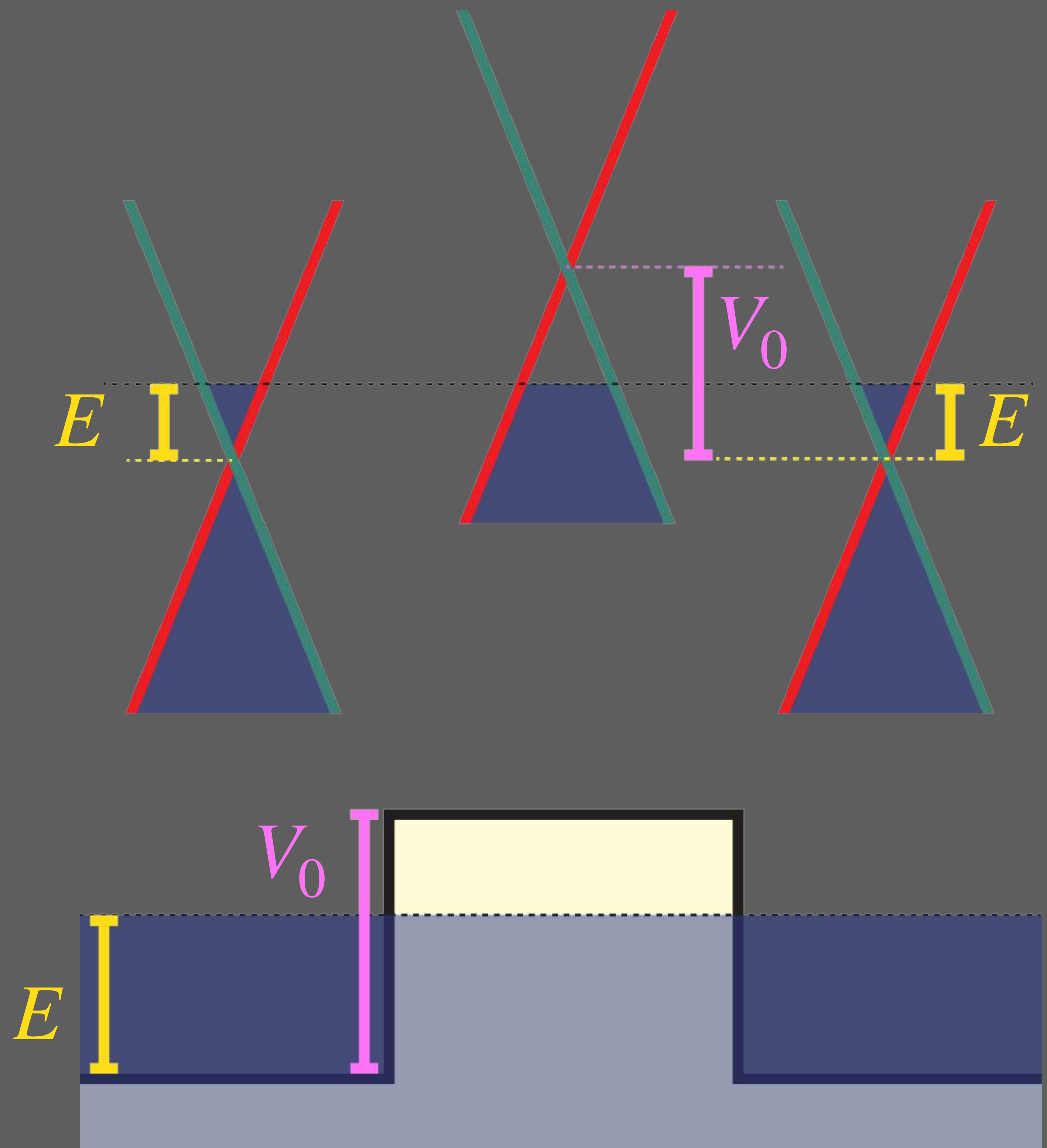
II — Electronic transport in graphene

$$E_{\pm} = \pm\, v_{\mathrm{F}} \,|\, \overrightarrow{p} \,|$$



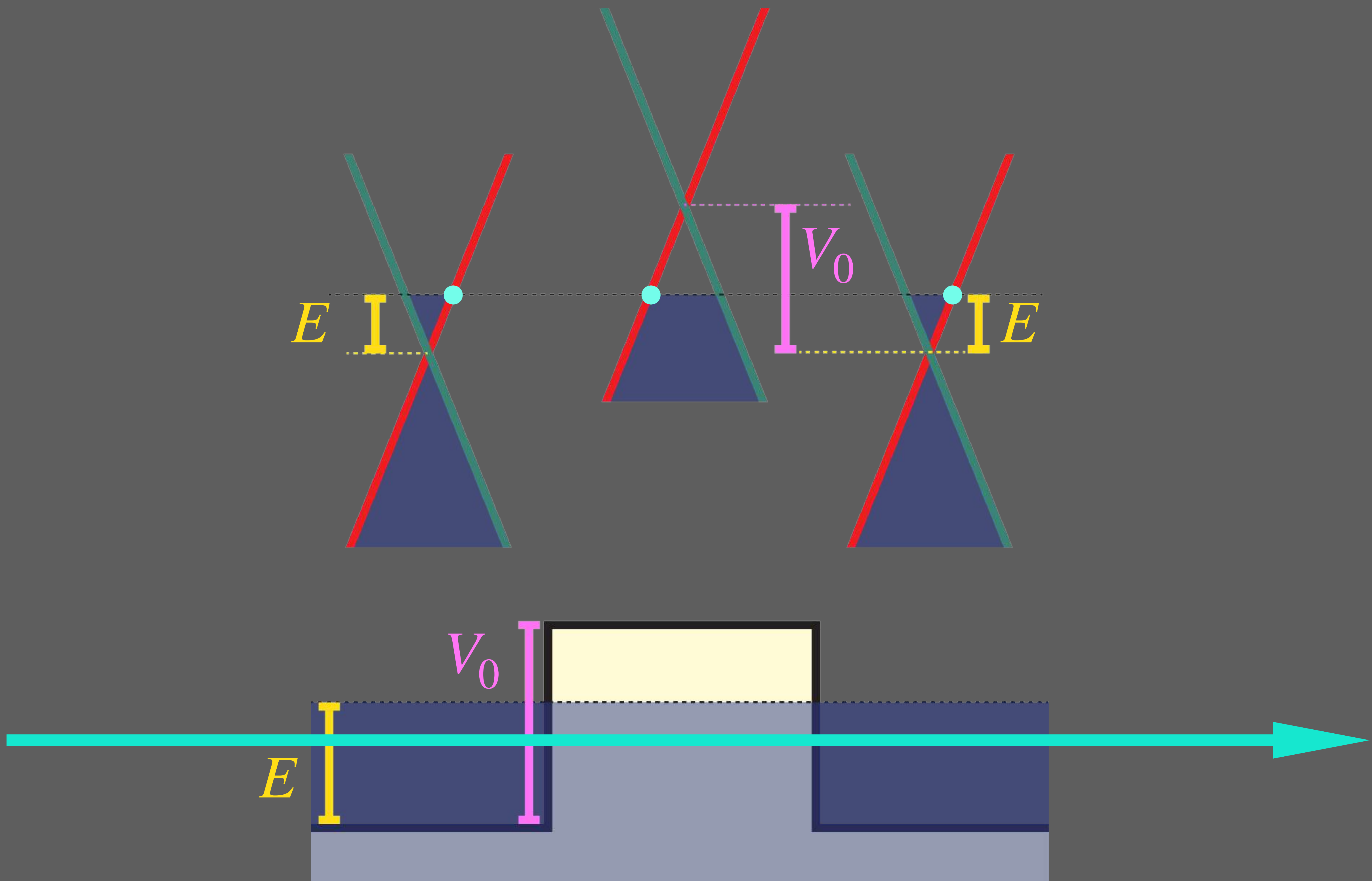
II — Electronic transport in graphene

- Behavior of electrons at a potential barrier : npn junction



II — Electronic transport in graphene

- Behavior of electrons at a potential barrier : npn junction
  - Klein tunneling

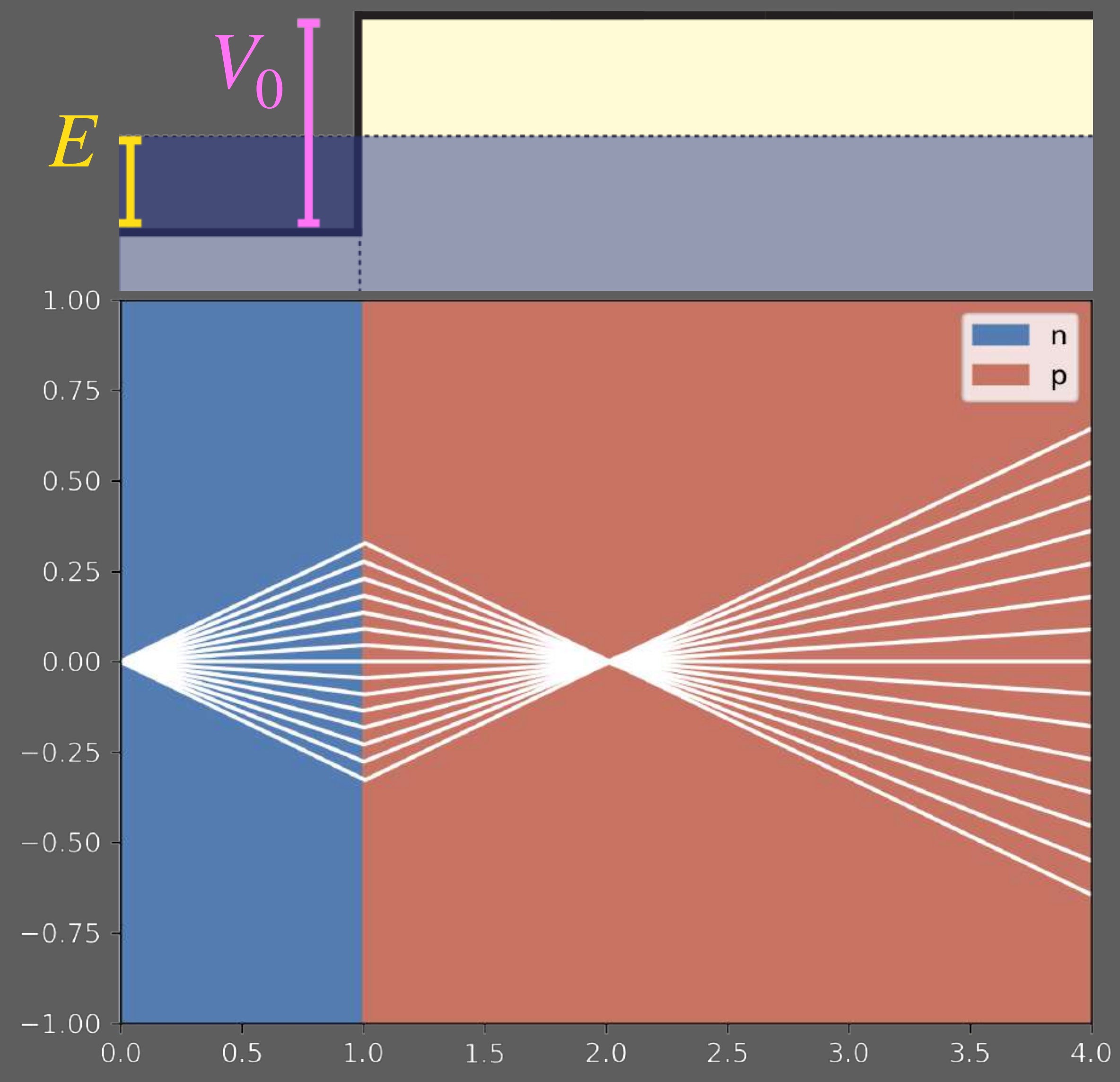


II — Electronic transport in graphene

- Veselago lensing for other angles

  Snell-Descartes law

$$n_1 \sin(\theta_1) = n_2 \sin(\theta_2)$$



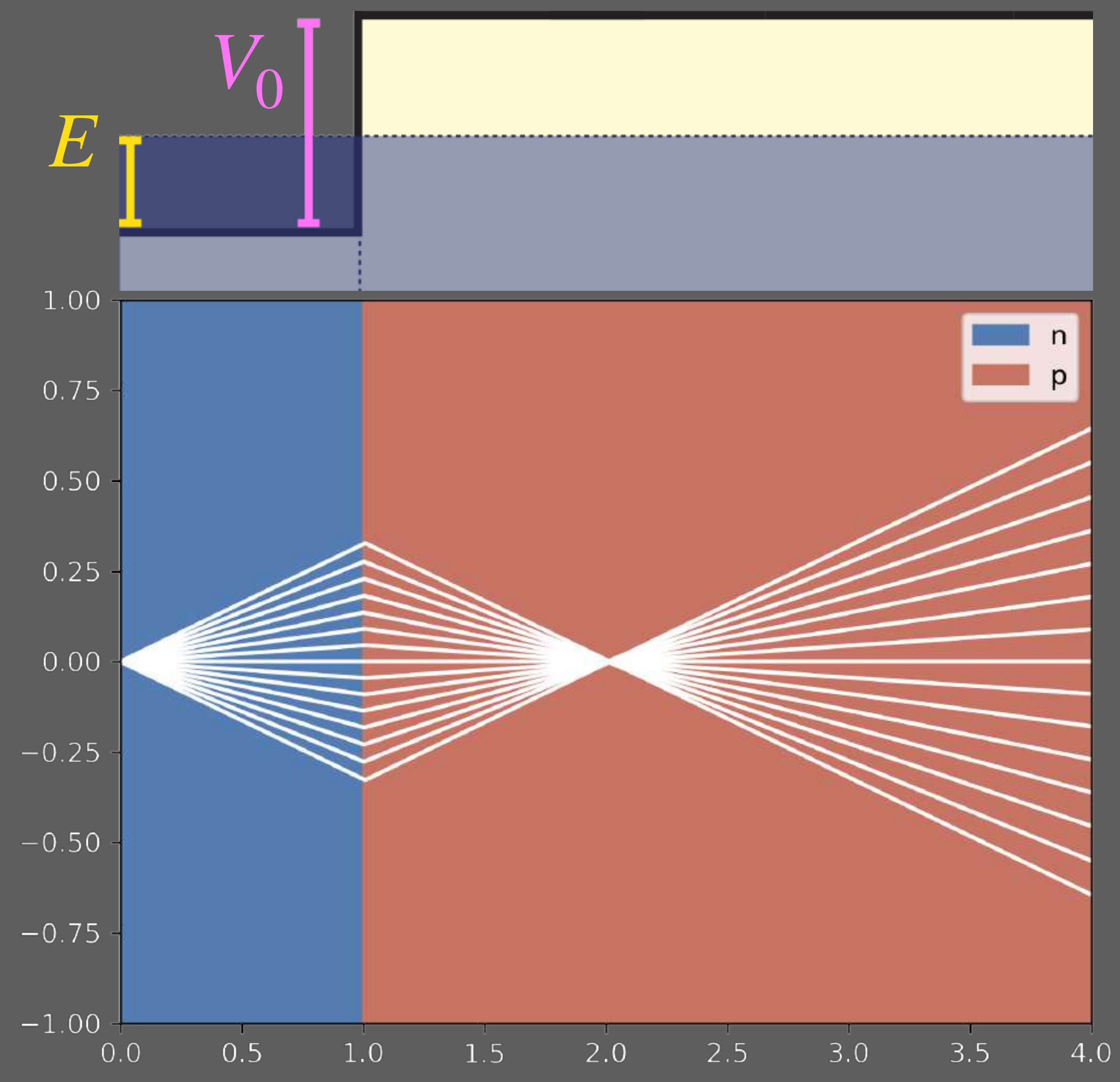
II — Electronic transport in graphene

- Veselago lensing for other angles

  Snell-Descartes law with negative refractive index

$$n_1 \sin(\theta_1) = n_2 \sin(\theta_2)$$

$$n_2 = (E - V_0)$$



I. Experimental motivations

II. Electronic transport in graphene

IIII. Classical method

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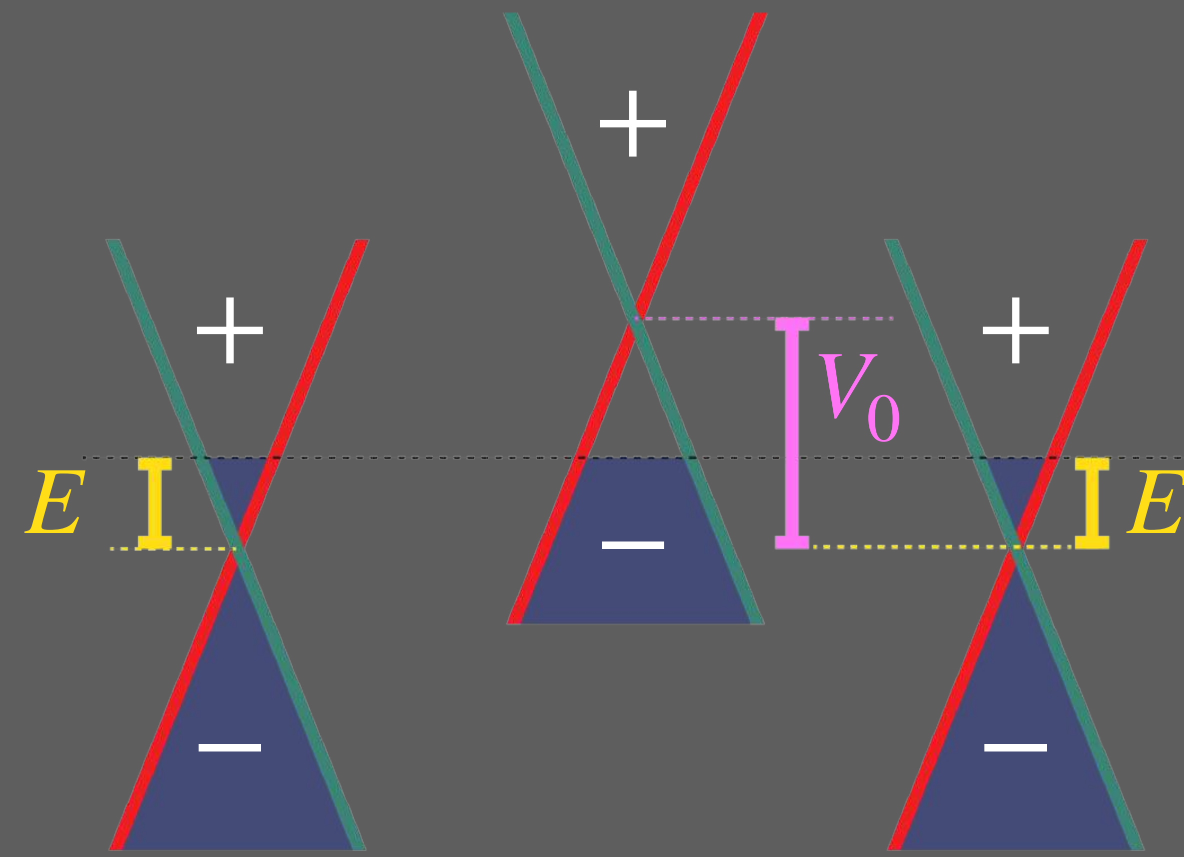
III — Classical method

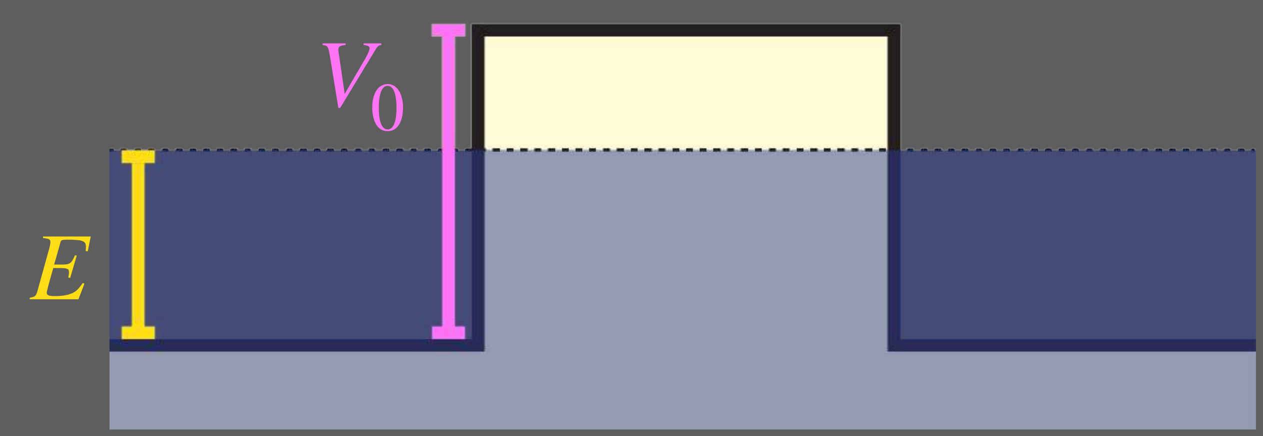
- Trajectories : Newton's equations

$$\frac{\mathrm{d}\overrightarrow{p}}{\mathrm{d}t} = -\overrightarrow{\nabla}(V(\vec{r}))$$

$$\frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = v_{\mathrm{F}}\frac{\overrightarrow{p}}{|\overrightarrow{p}|}\mathrm{sgn}(E - V(\vec{r}))$$



- v_{F} is constant



III — Classical method

- Trajectories : Newton's equations

$$\frac{\mathrm{d}\vec{p}}{\mathrm{d}t} = -\vec{\nabla}(V(\vec{r}))$$

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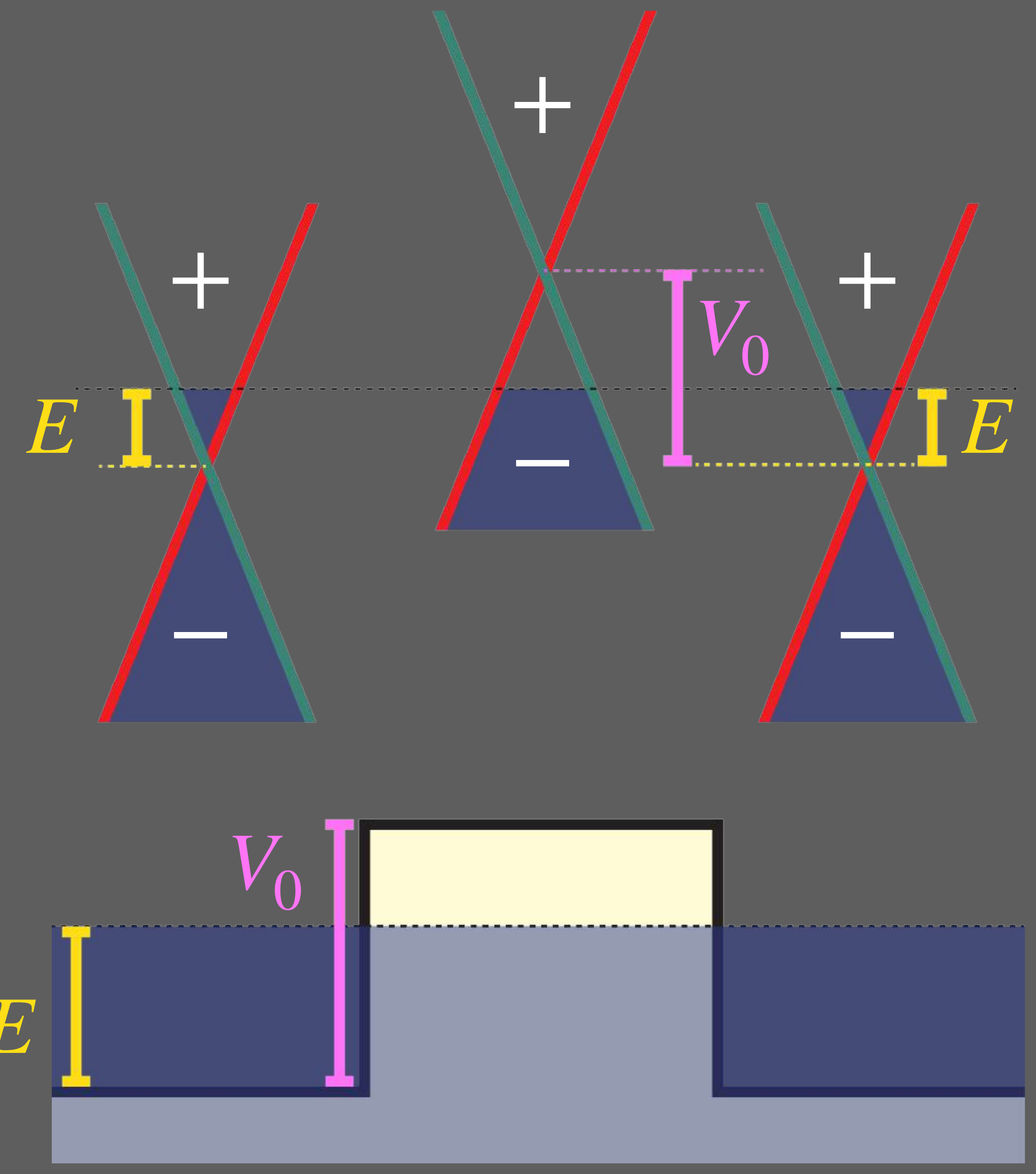
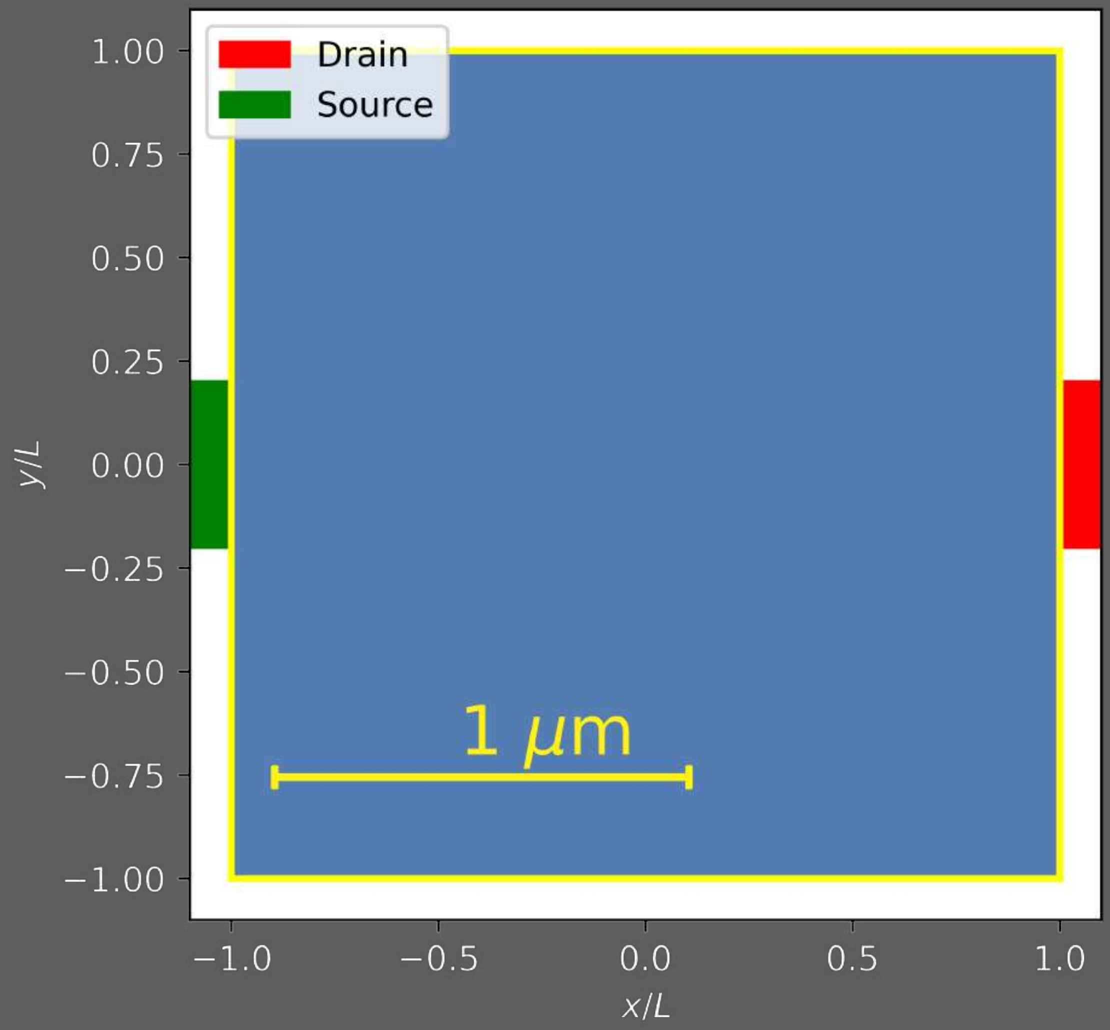
- v_{F} is constant



III — Classical method

- Monte Carlo generation of initial conditions



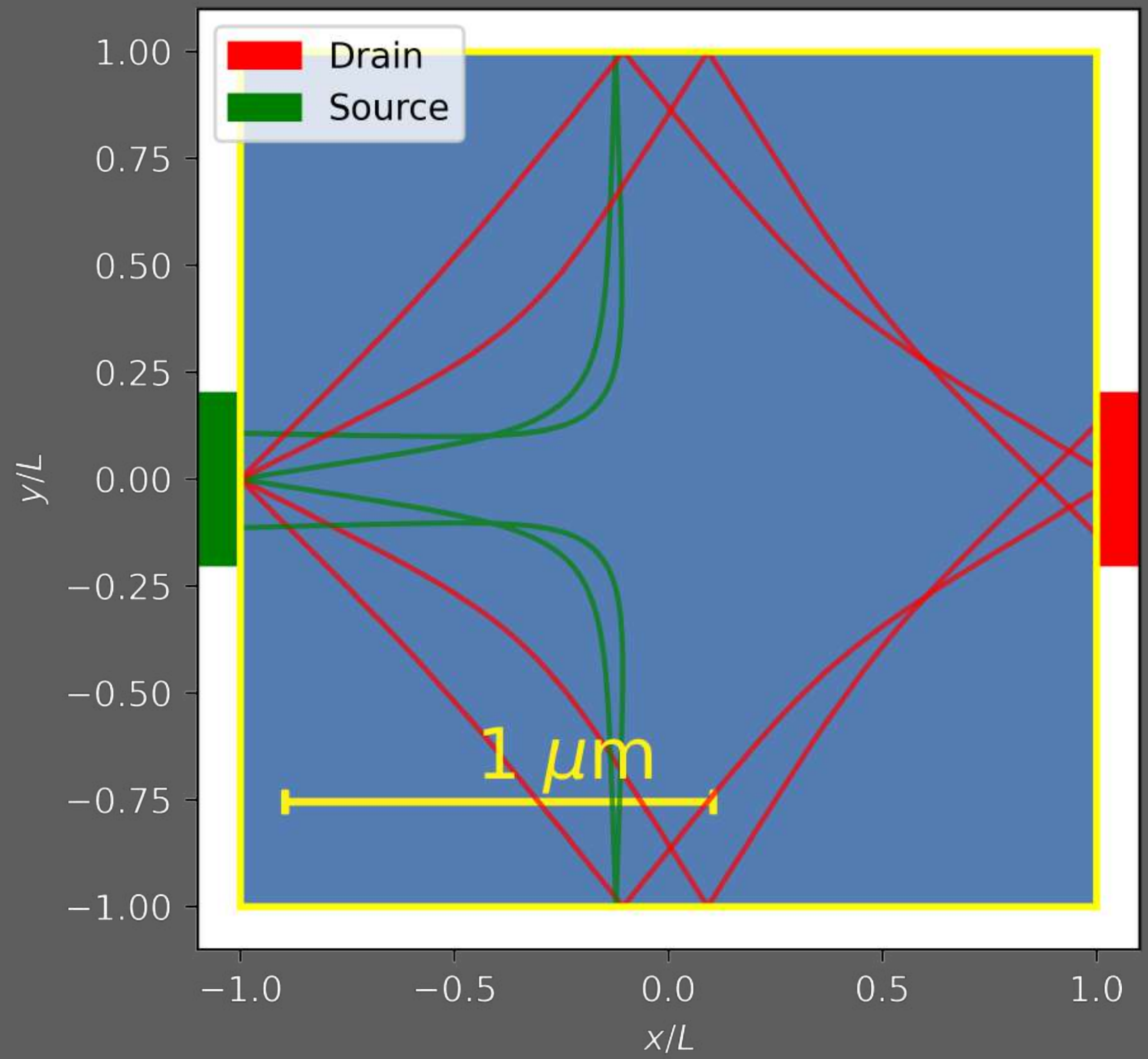
- Trajectories : Iterative procedure → Runge-Kutta method
- Studying transmission of electrons

III — Classical method

- Conductance is linked to transmission
- Use of semiclassical transmission formula

$$G \propto \frac{2e^2}{h} T$$

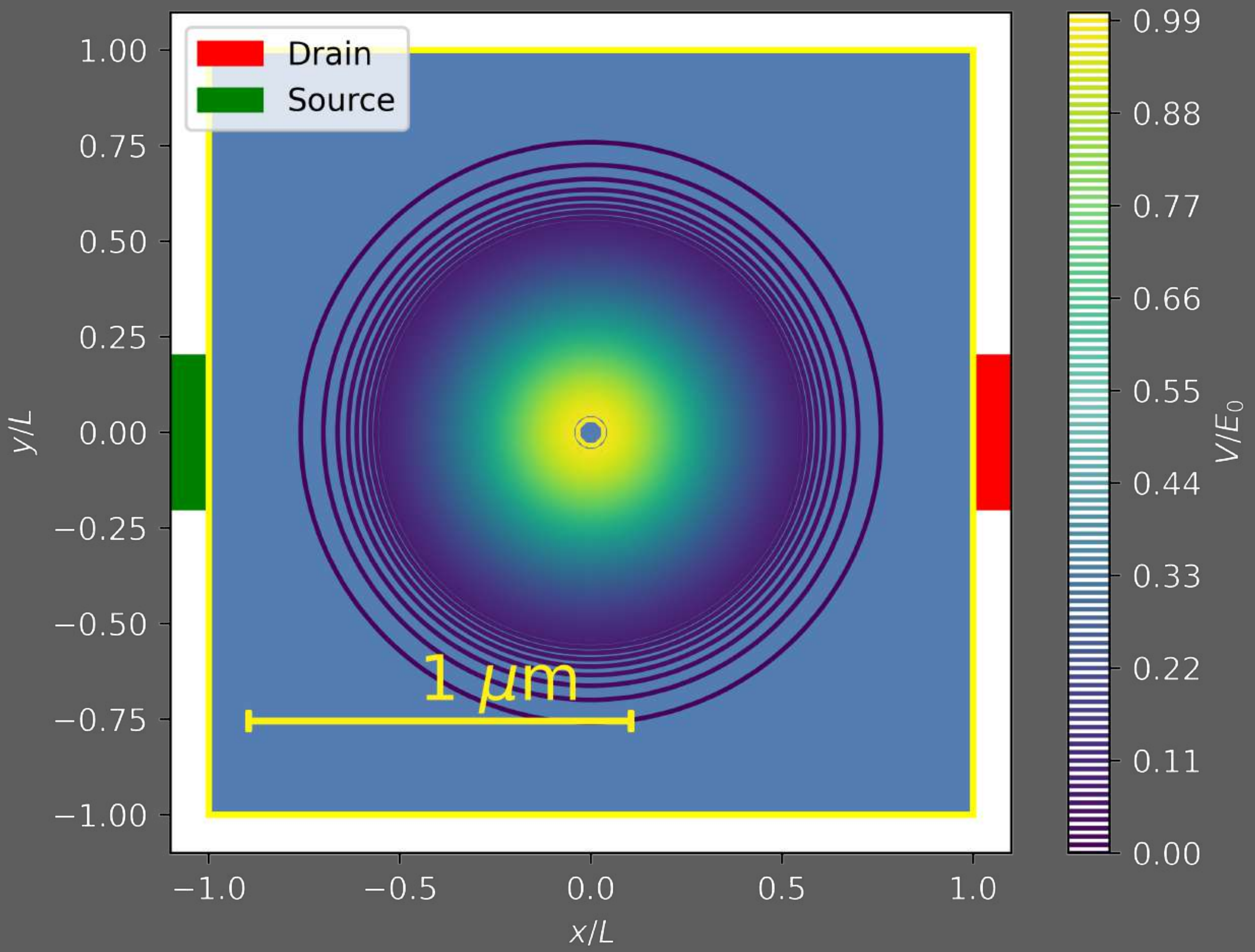
$$\text{Transmission} = \frac{\text{number of electrons in drain}}{\text{number of electrons in total}}$$



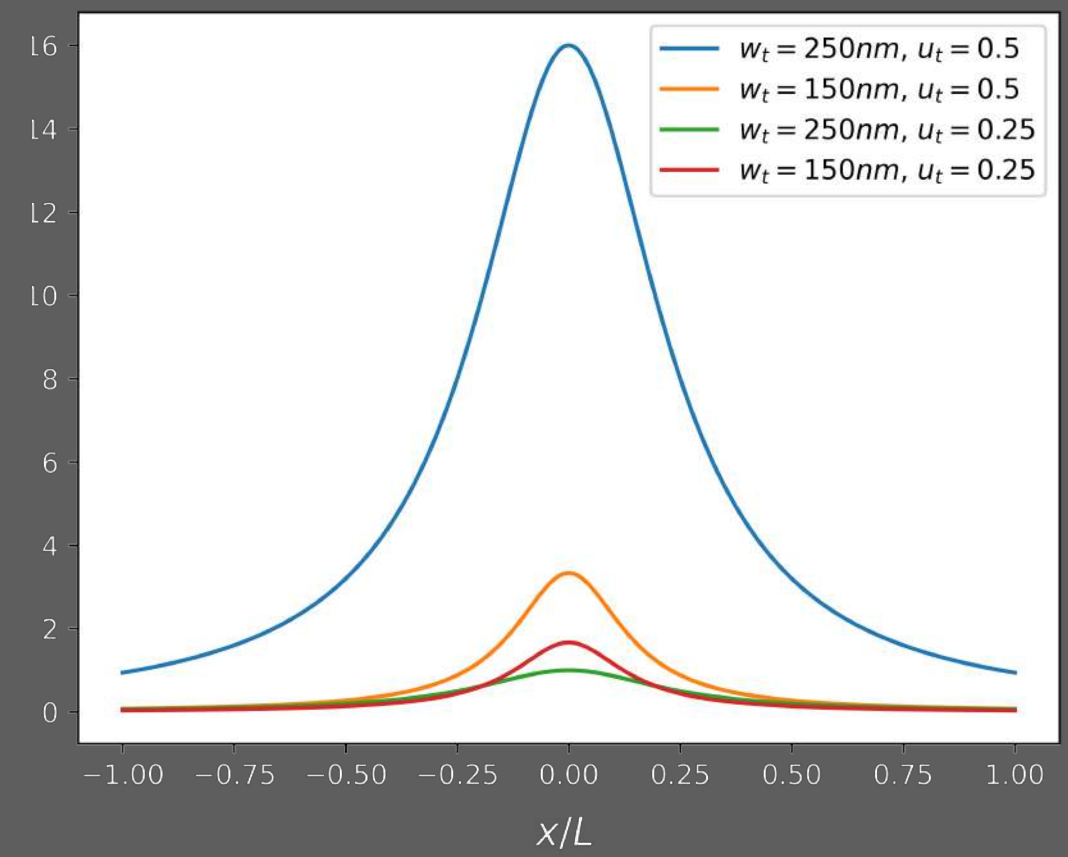
III — Classical method

- Perturbation by a Lorentzian potential

$$V(\vec{r}) = \frac{u_t E_0}{w_t^2 + |\vec{r} - \vec{r}_t|^2}$$



- Play with u_t, w_t and $\overrightarrow{r_t}$



I. Experimental motivations

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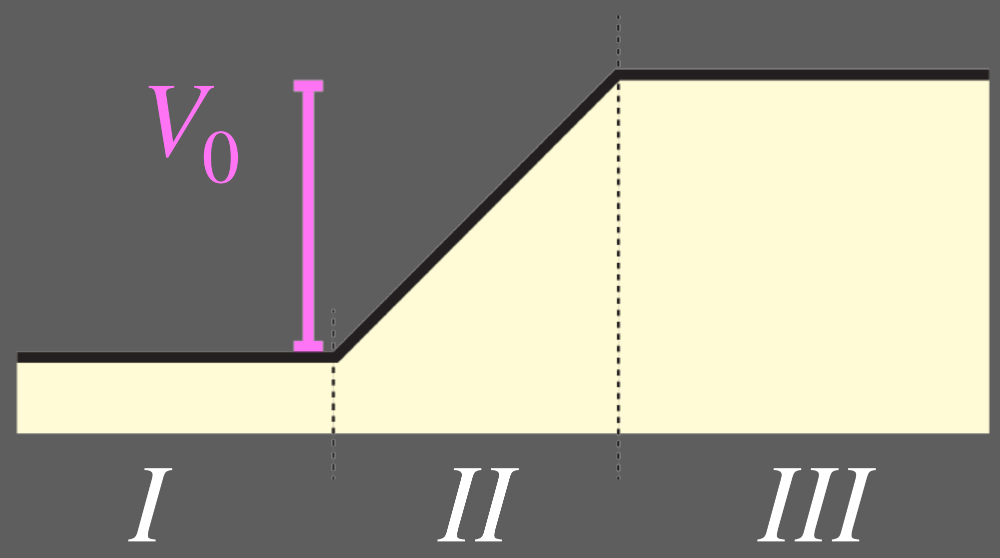
IV — Results

- Smooth potential step in a squared cavity of length L

- $V_0 = E_{\text{init}}$

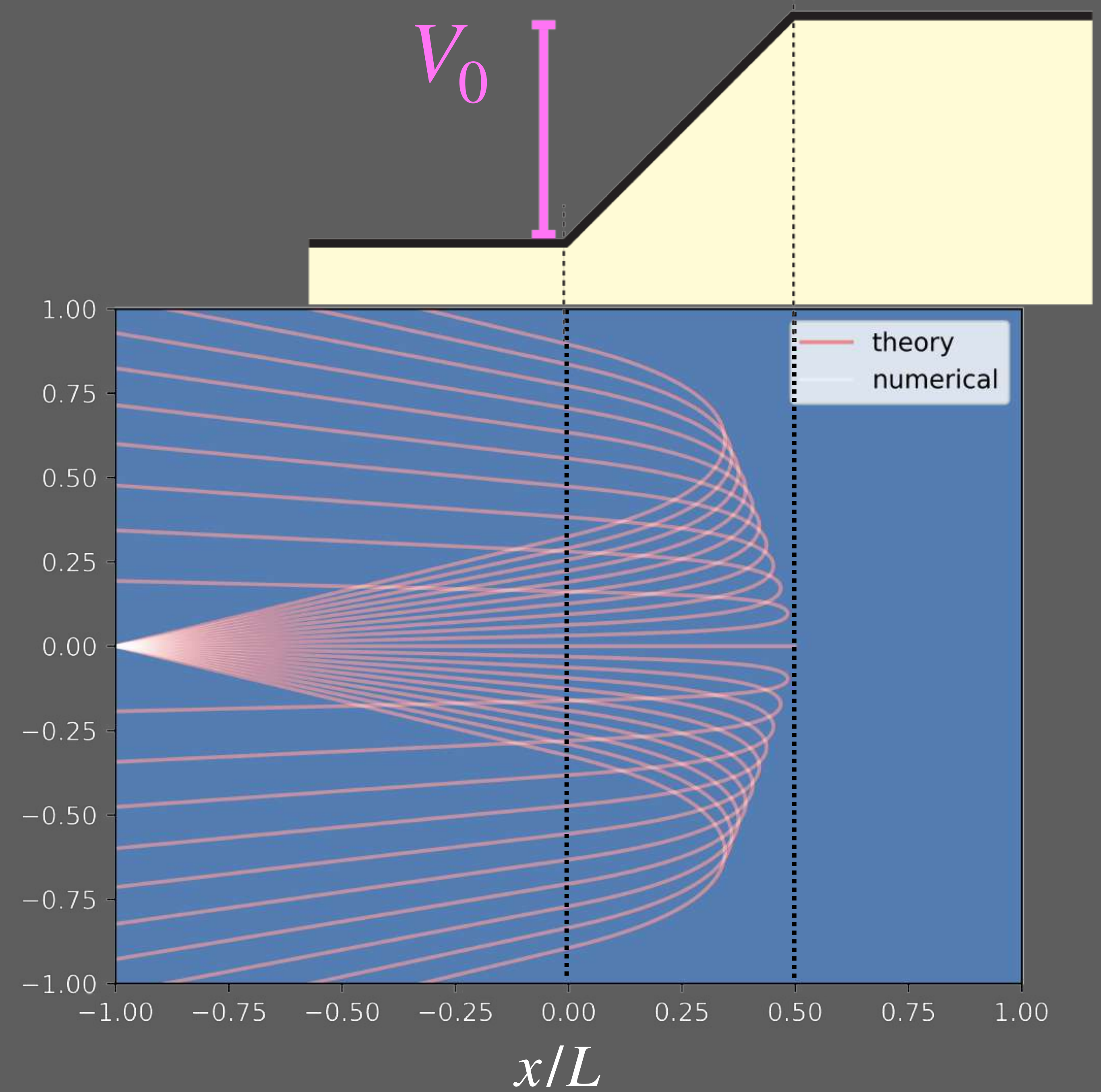


IV — Results

- Smooth potential step in a squared cavity of length L

Classical trajectories of the electrons

- $V_0 = E_{\text{init}}$



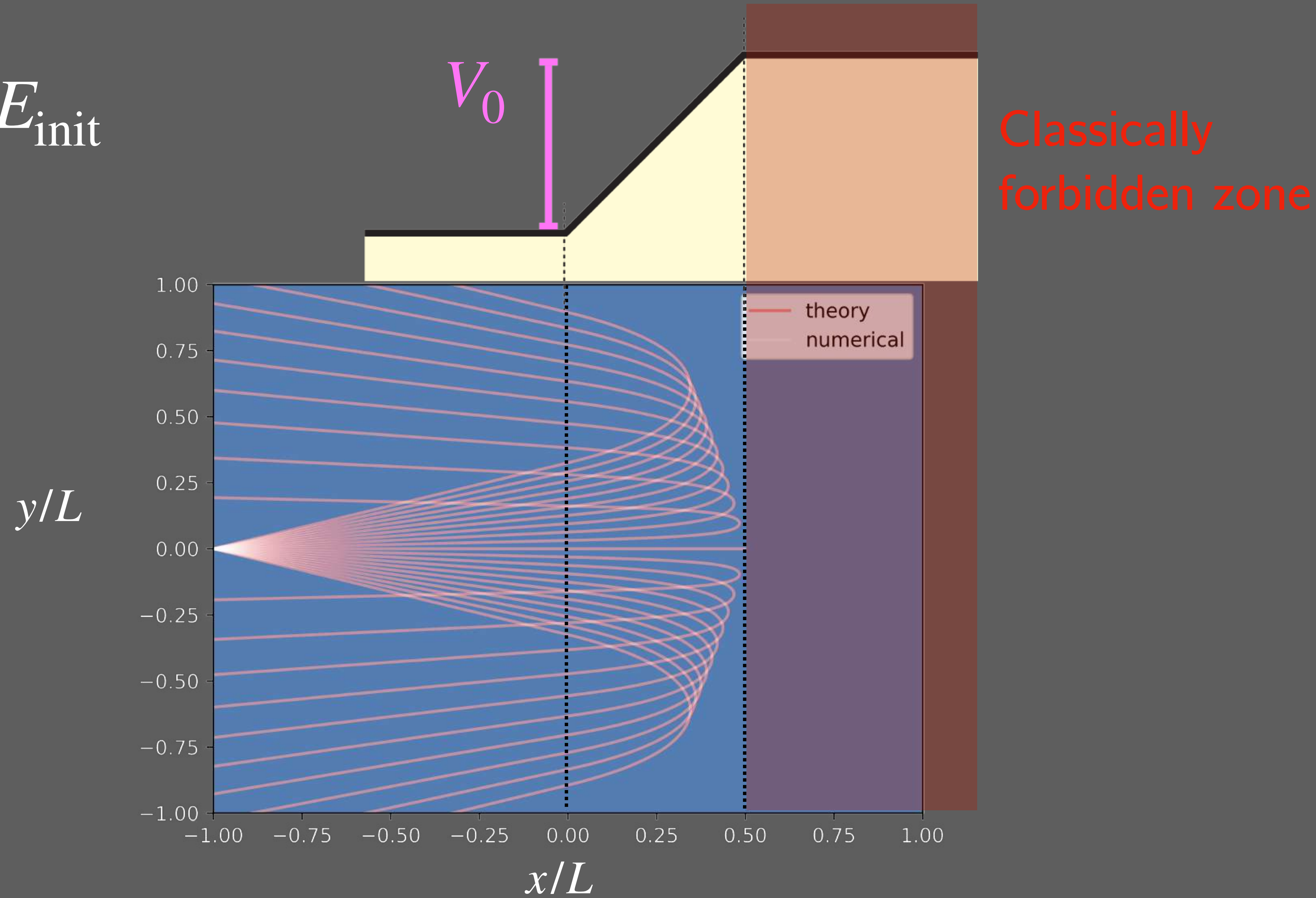
Relative error : $\approx 0.1\,\%$ over the trajectories

IV — Results

- Smooth potential step in a squared cavity of length L

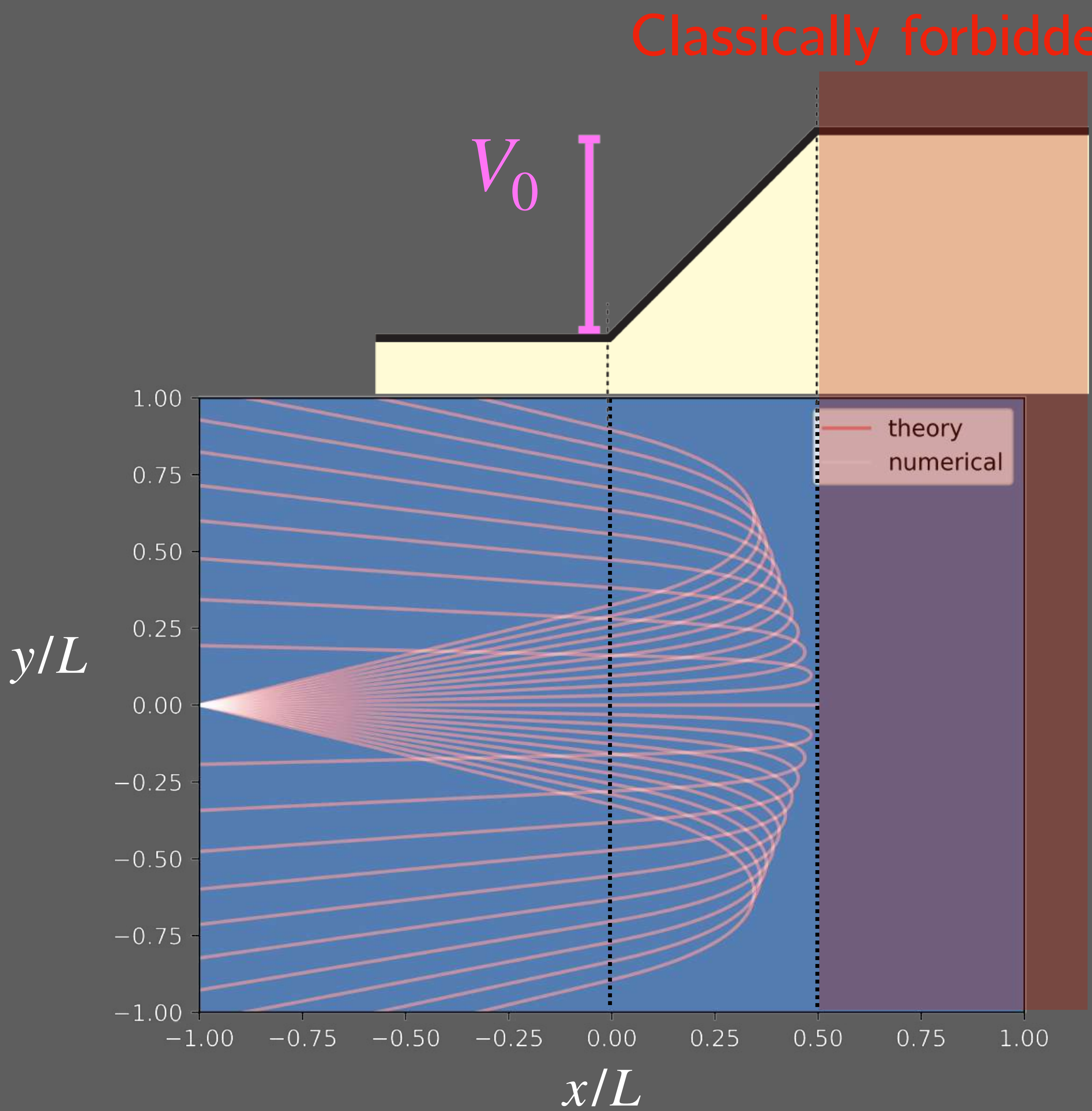
- $V_0 = E_{\text{init}}$

Classical trajectories of the electrons

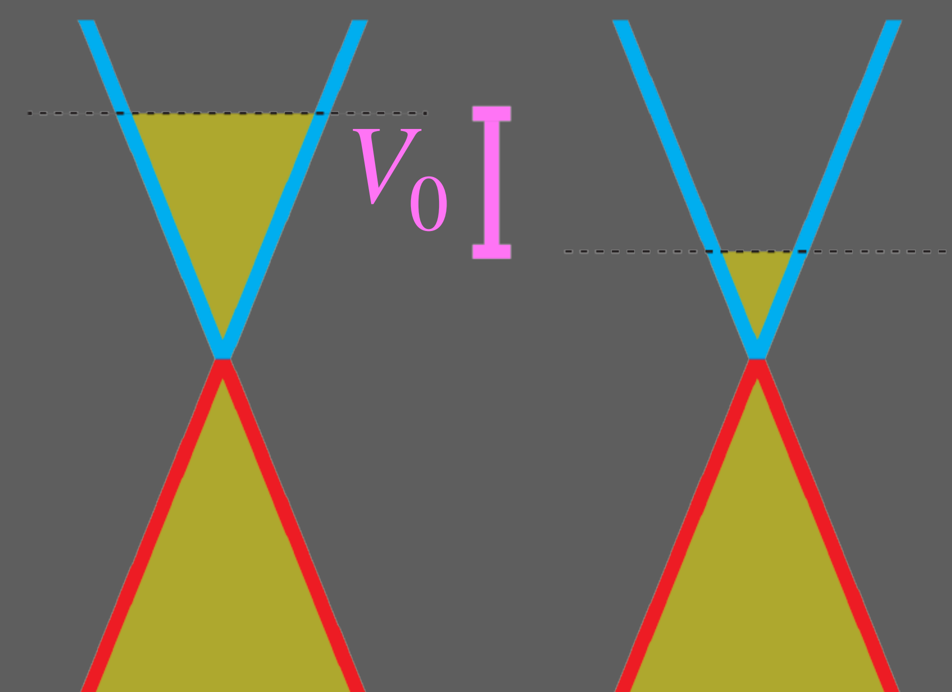


IV — Results

- No Klein tunneling



$$\frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = v_{\mathrm{F}} \frac{\vec{p}}{|\vec{p}|} \mathrm{sgn}(E - U(\vec{r}))$$

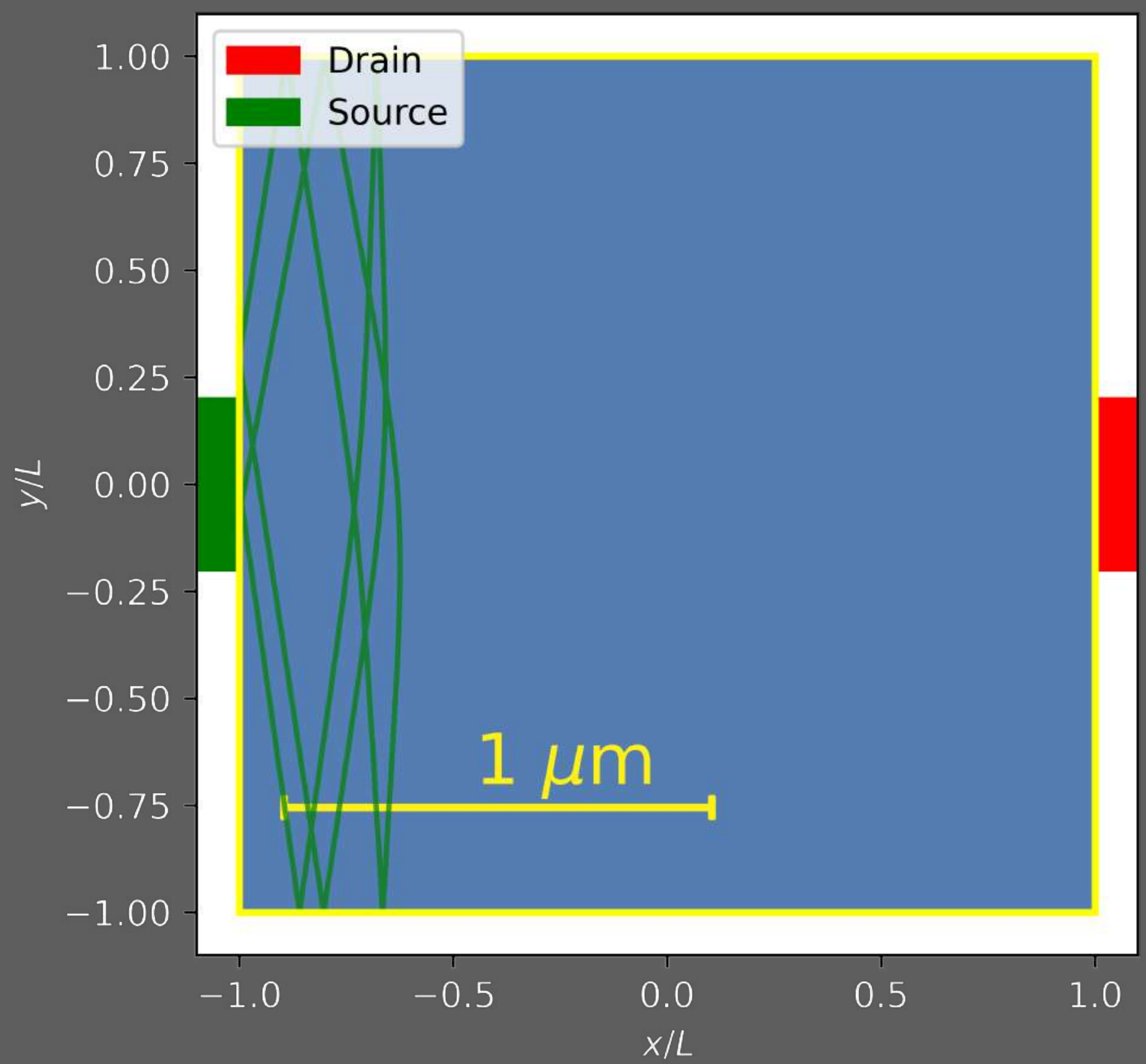


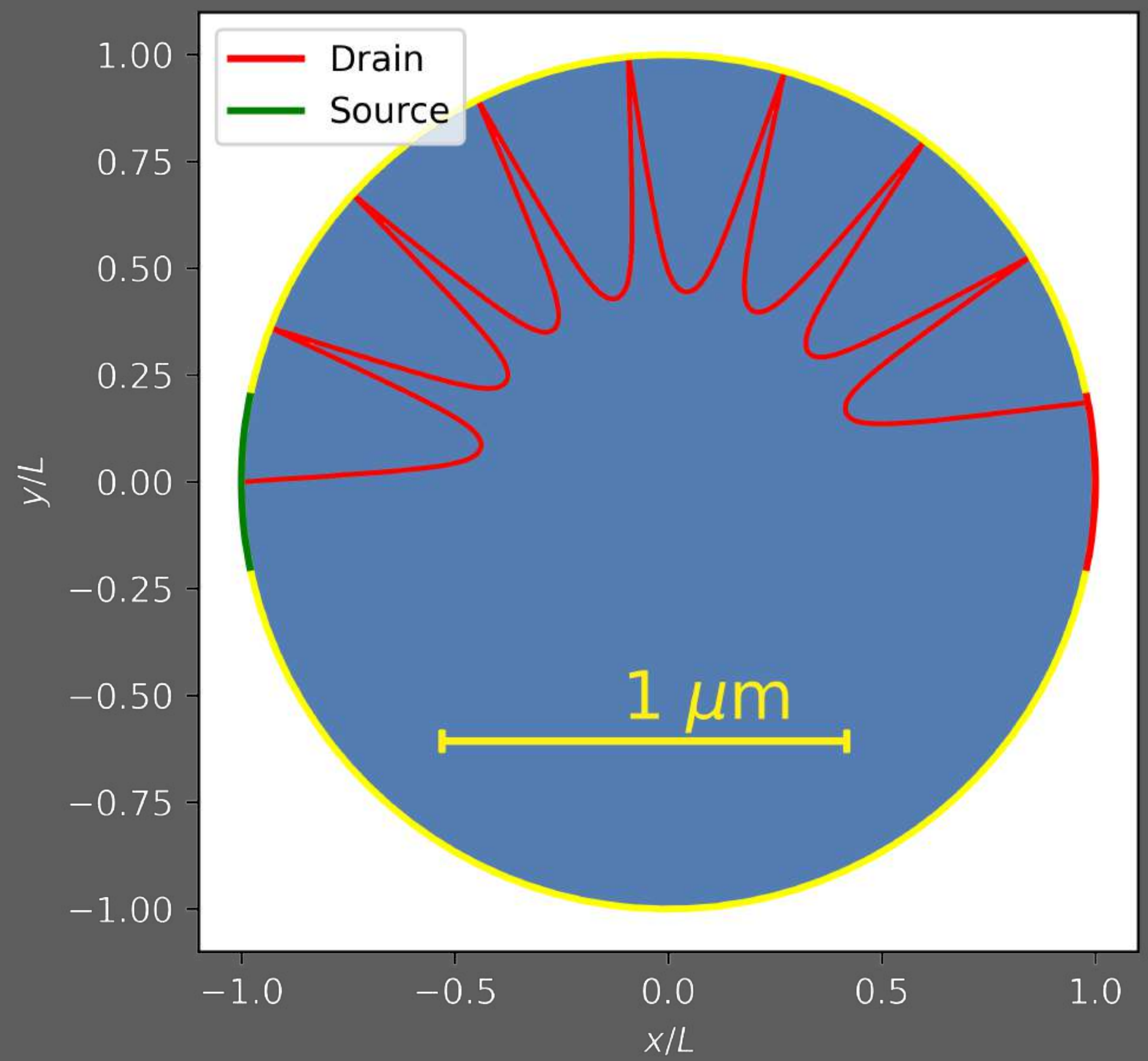
$$V_0 < E_{\mathrm{init}}$$

IV — Results

- Challenge :
  Trapped trajectories

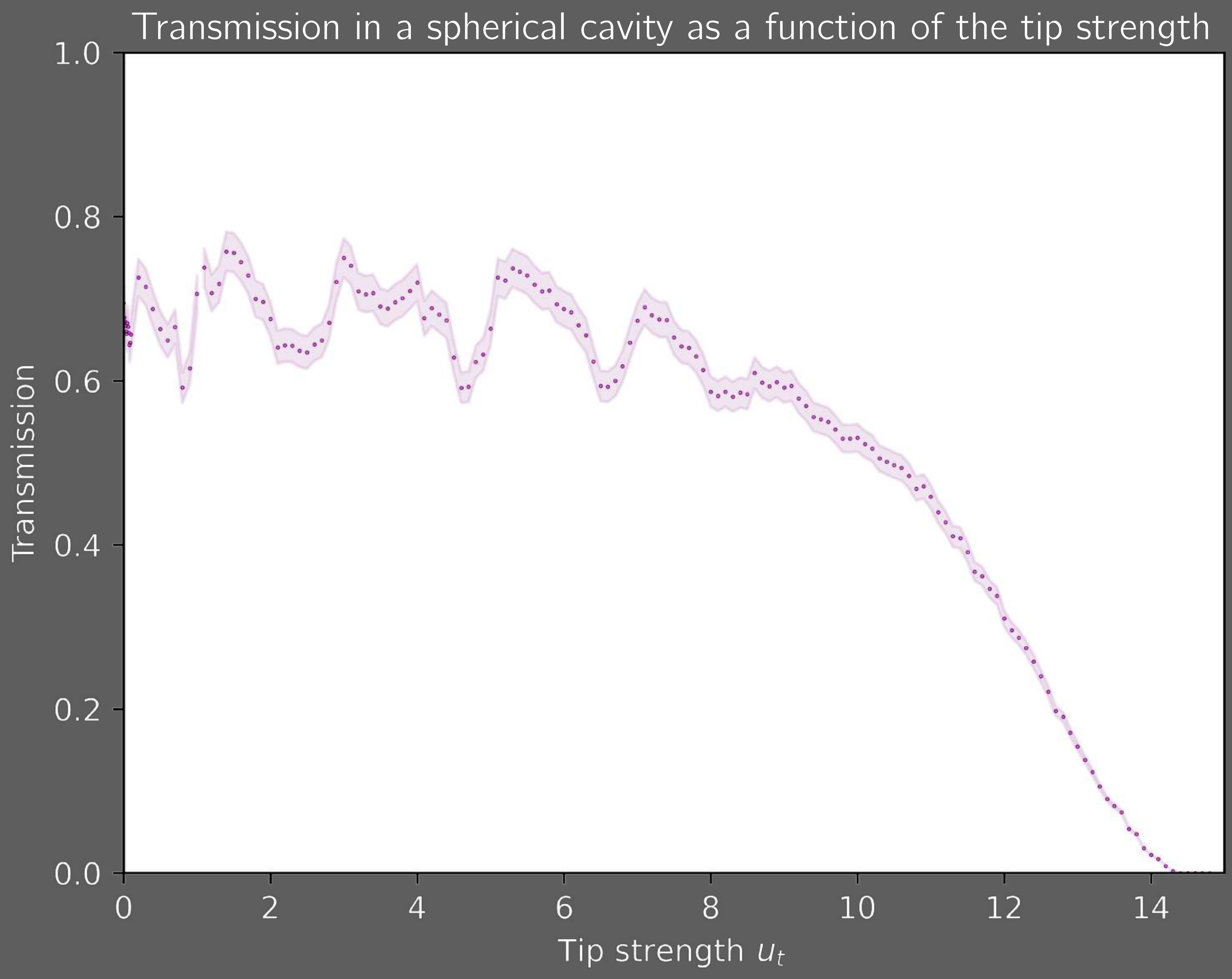
- Solution :
  Spherical cavity





IV — Results

Transmission in a spherical cavity



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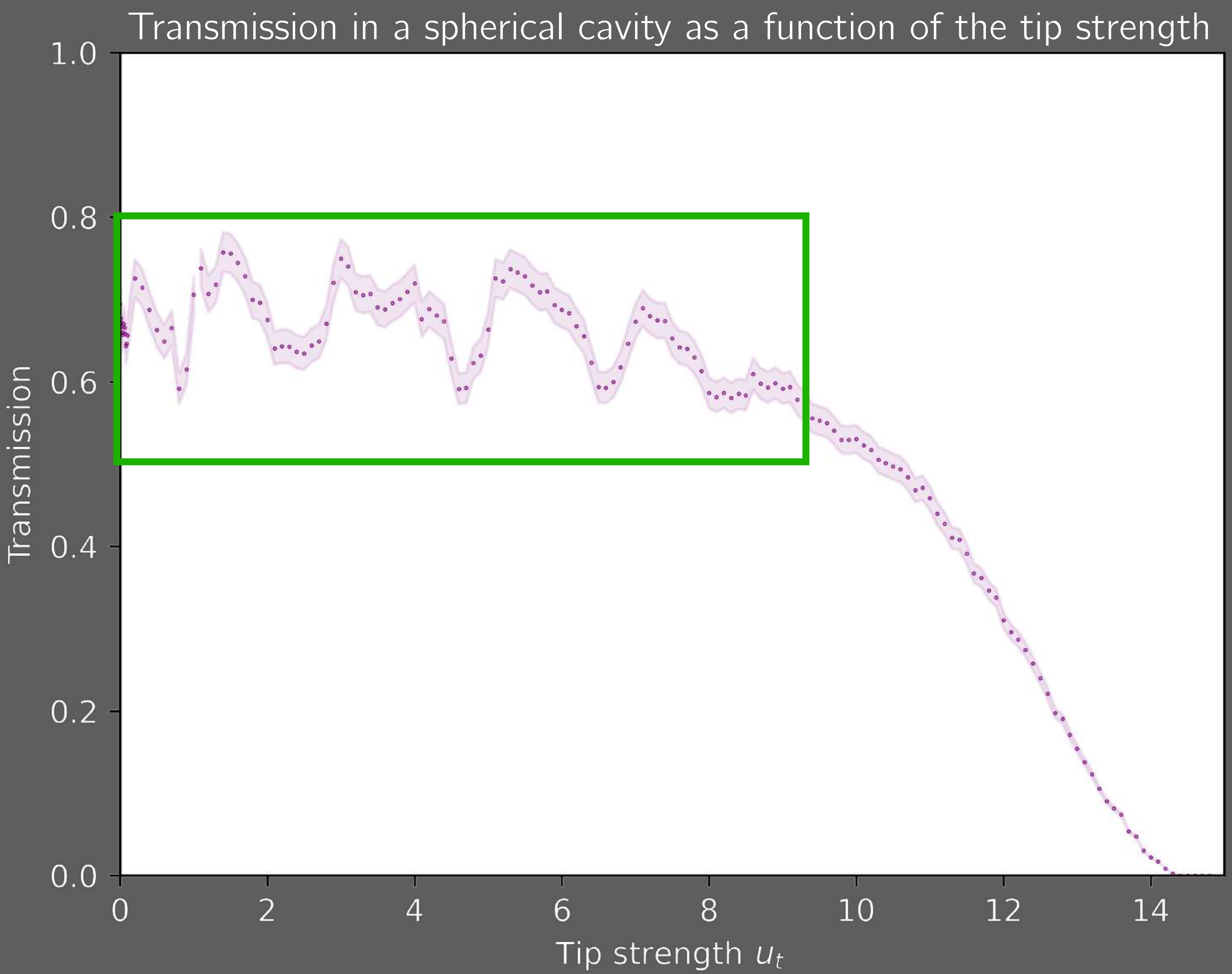

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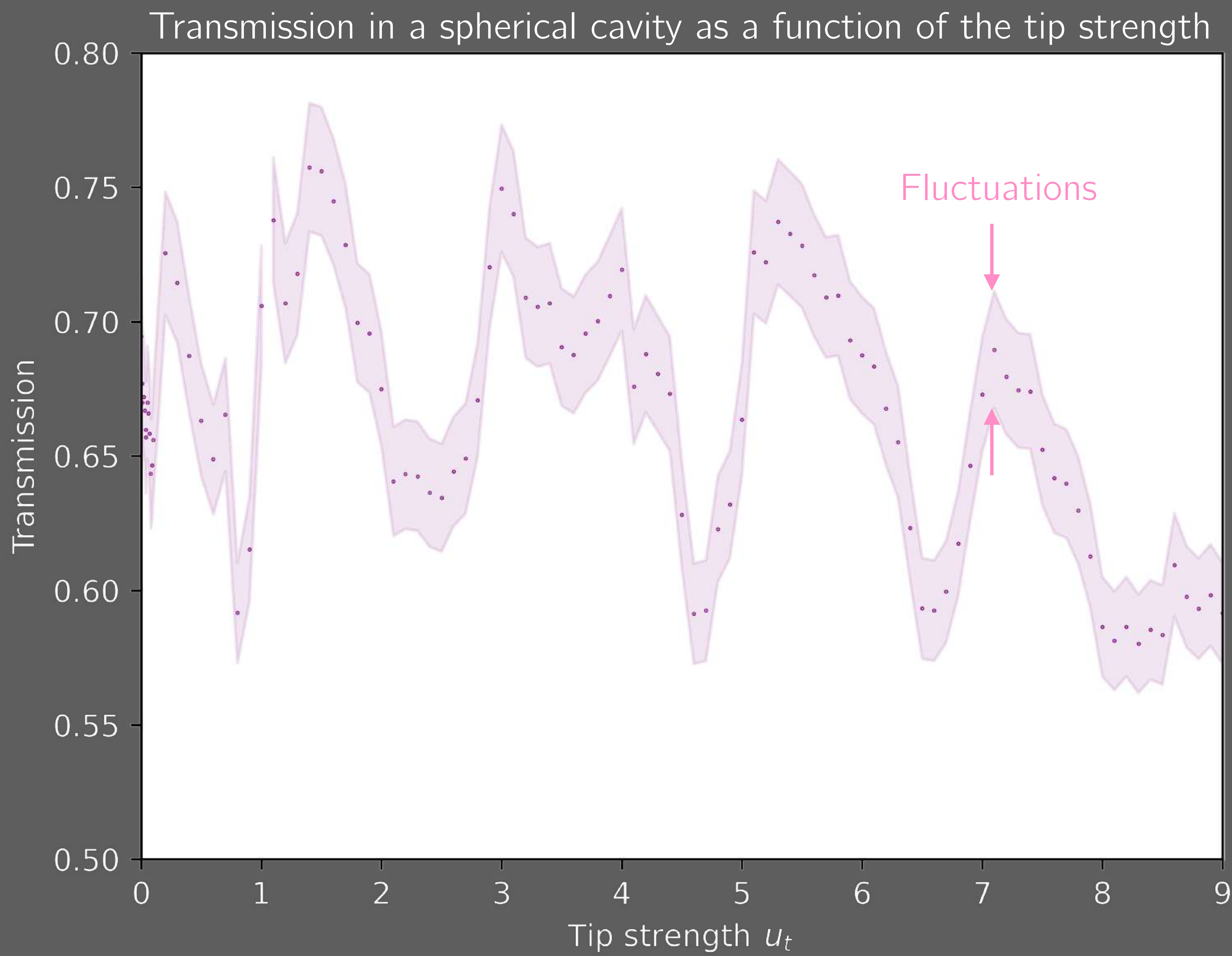
Transmission in a spherical cavity



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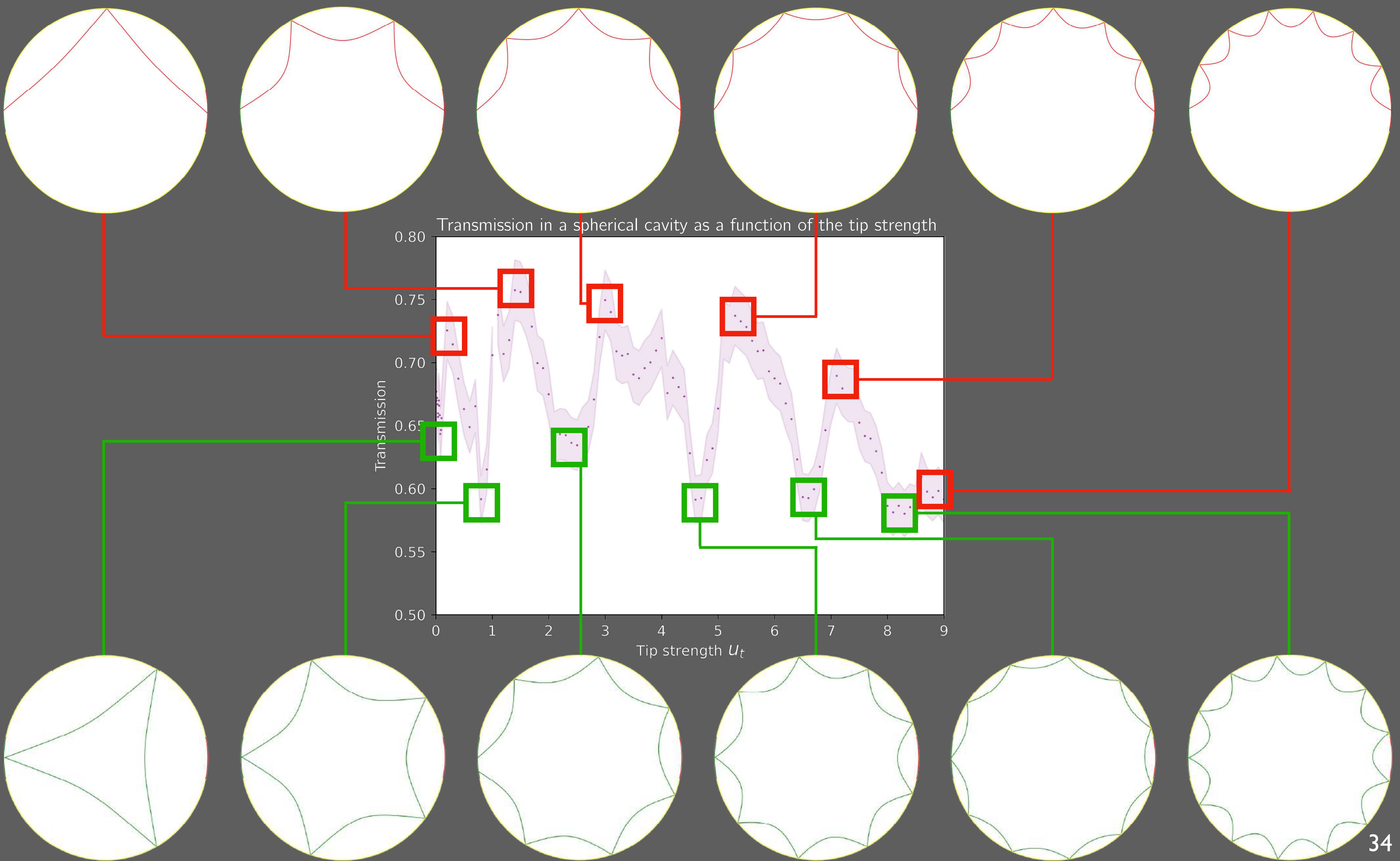
Transmission in a spherical cavity



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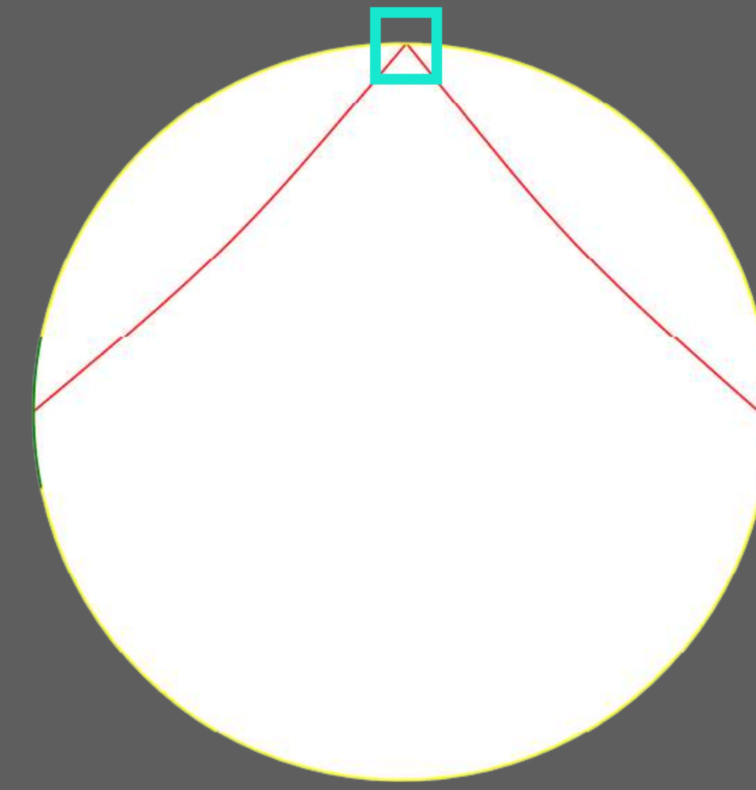
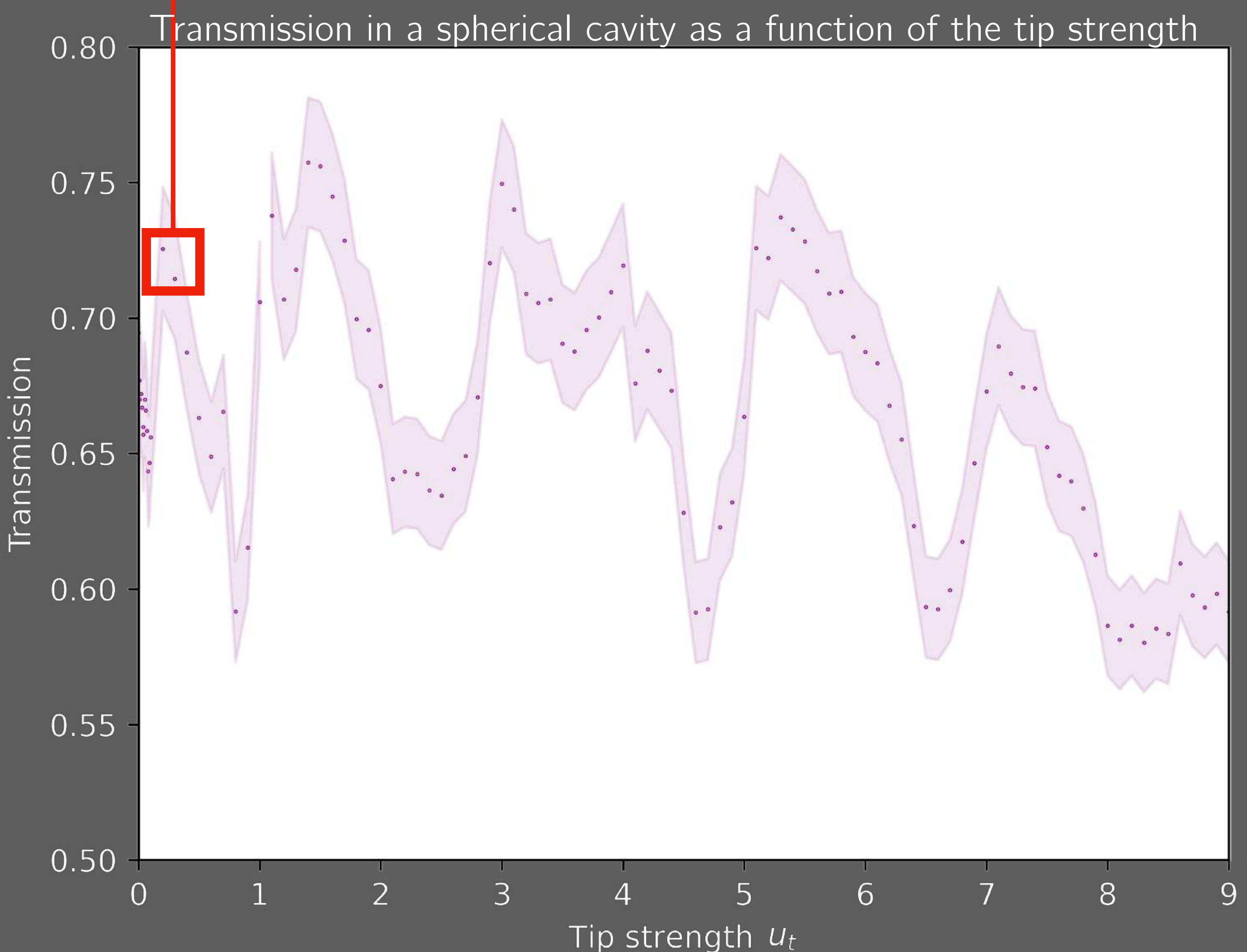
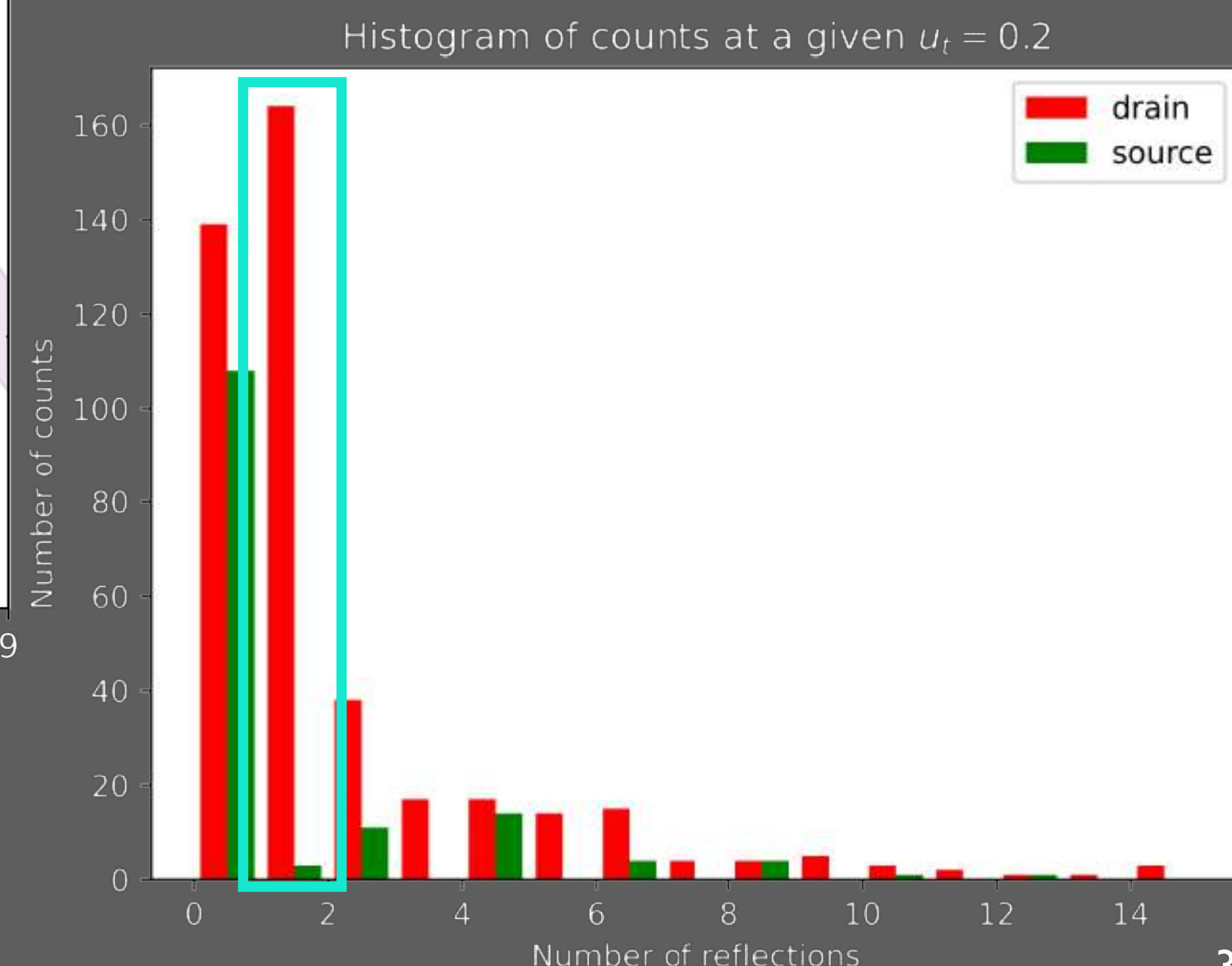
Transmission in a spherical cavity







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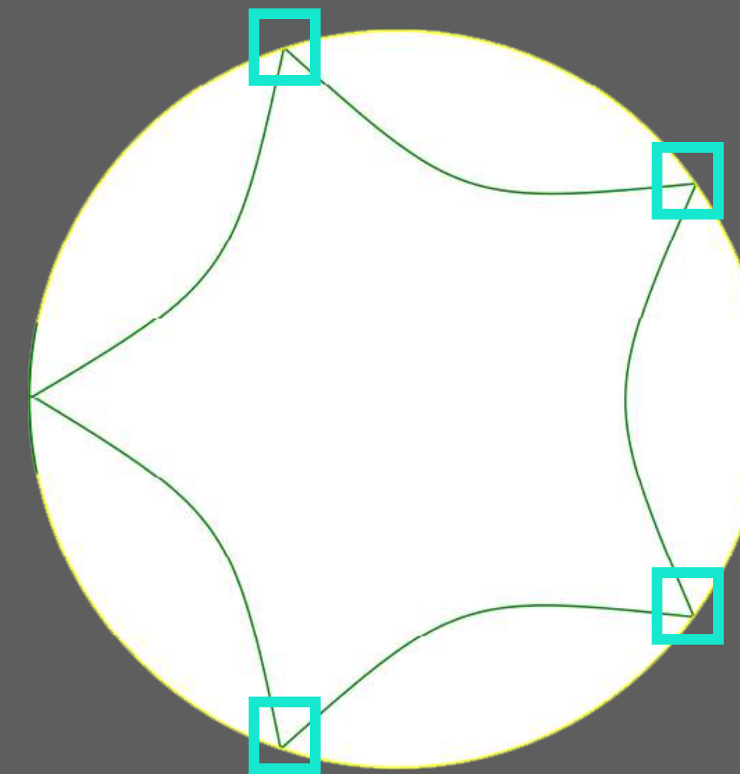
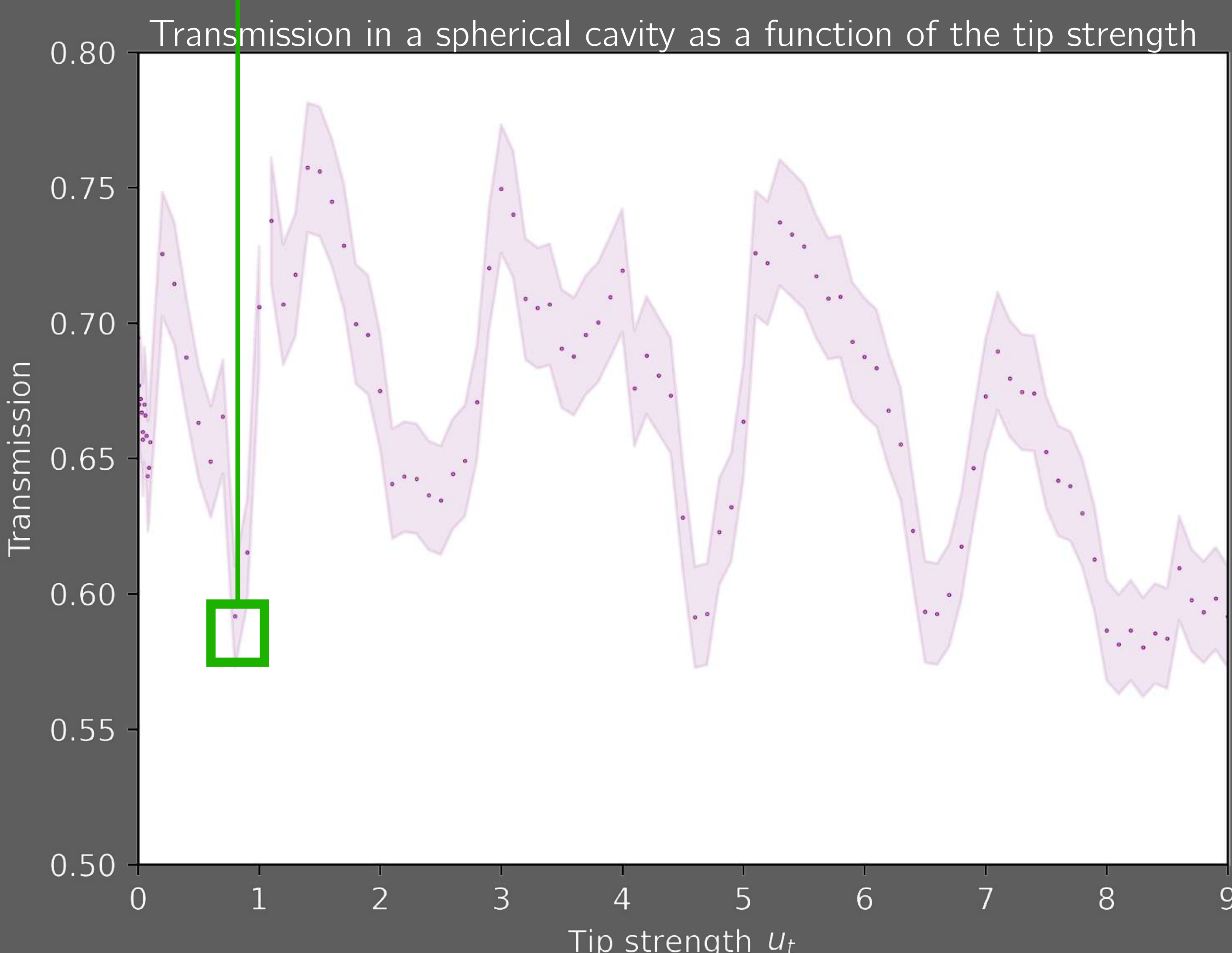
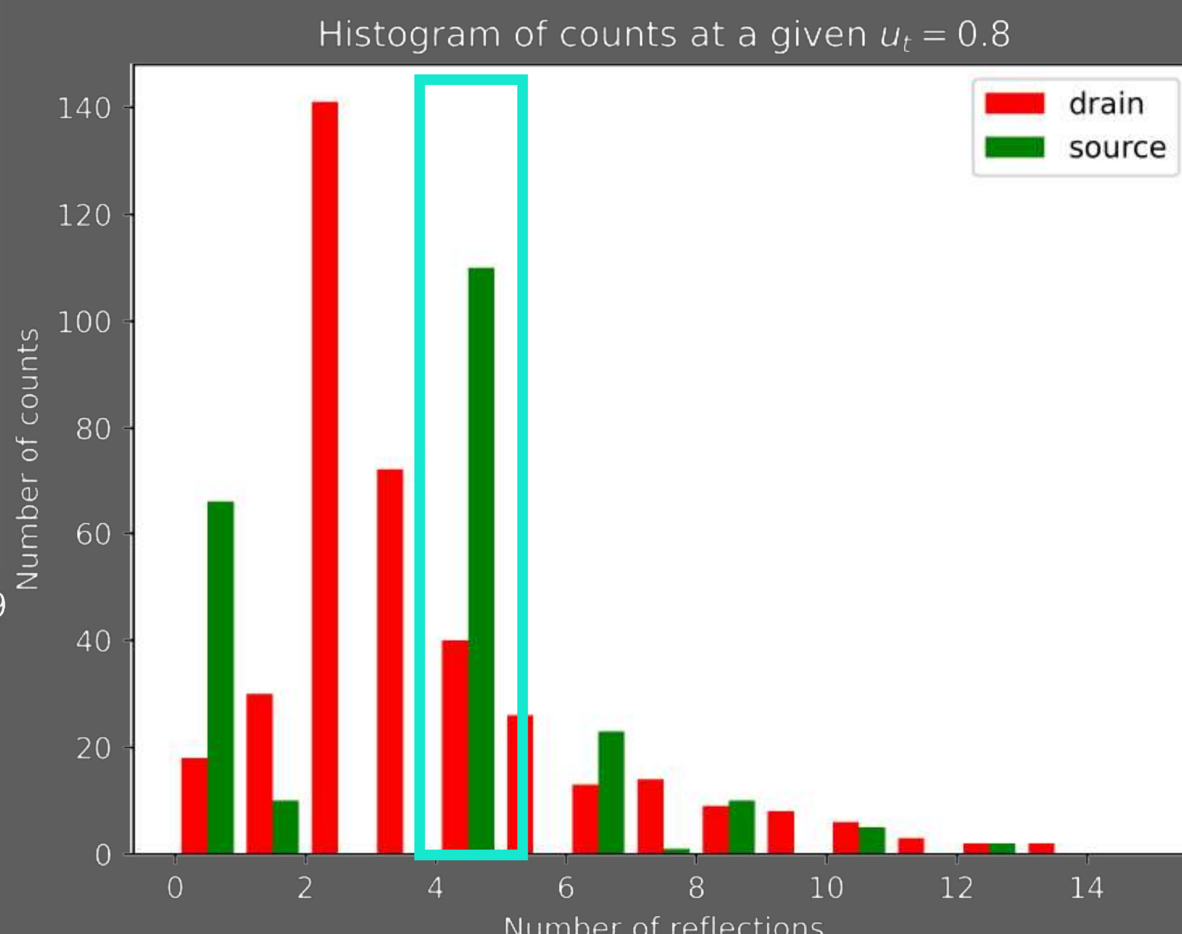


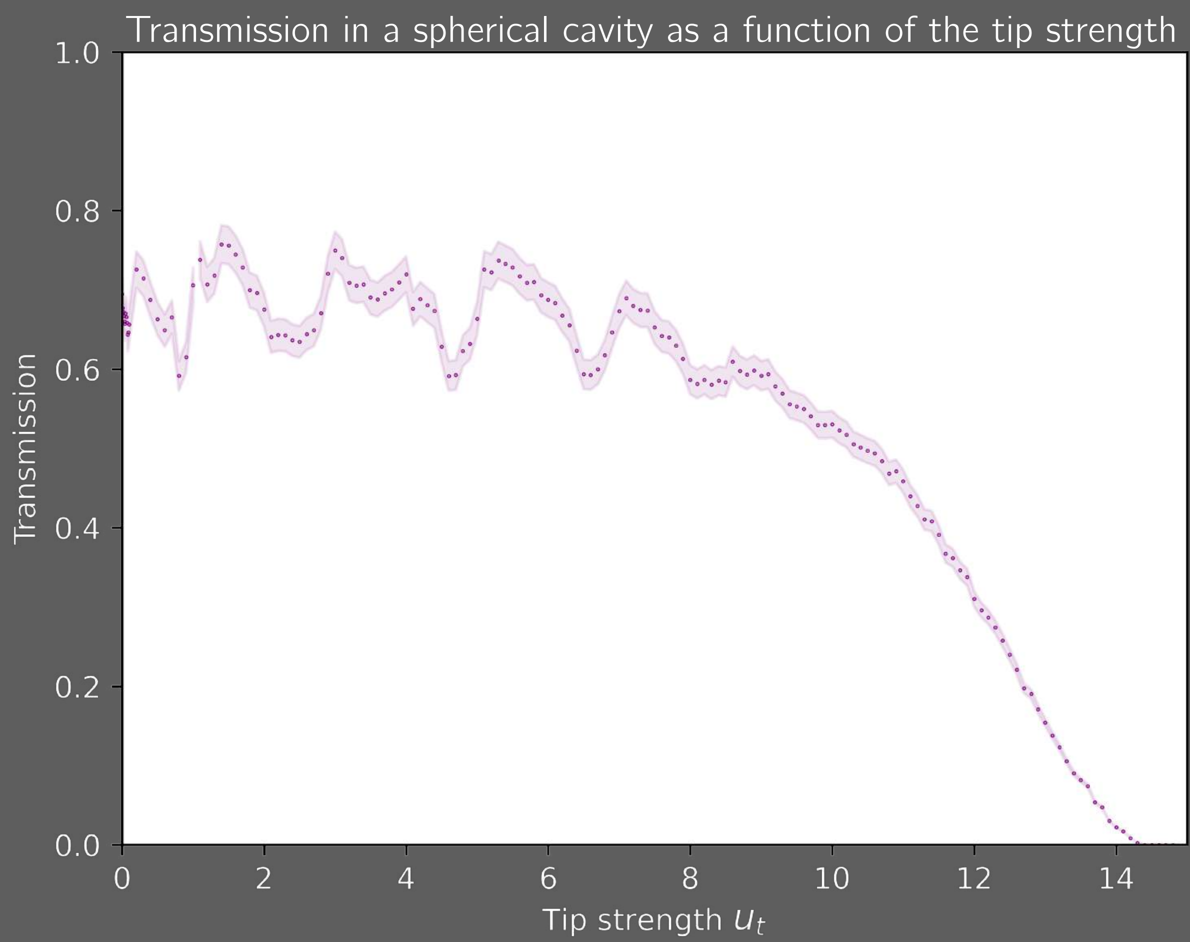




IV — Results

Comparison with semiconductor heterostructures

Graphene



GaAs

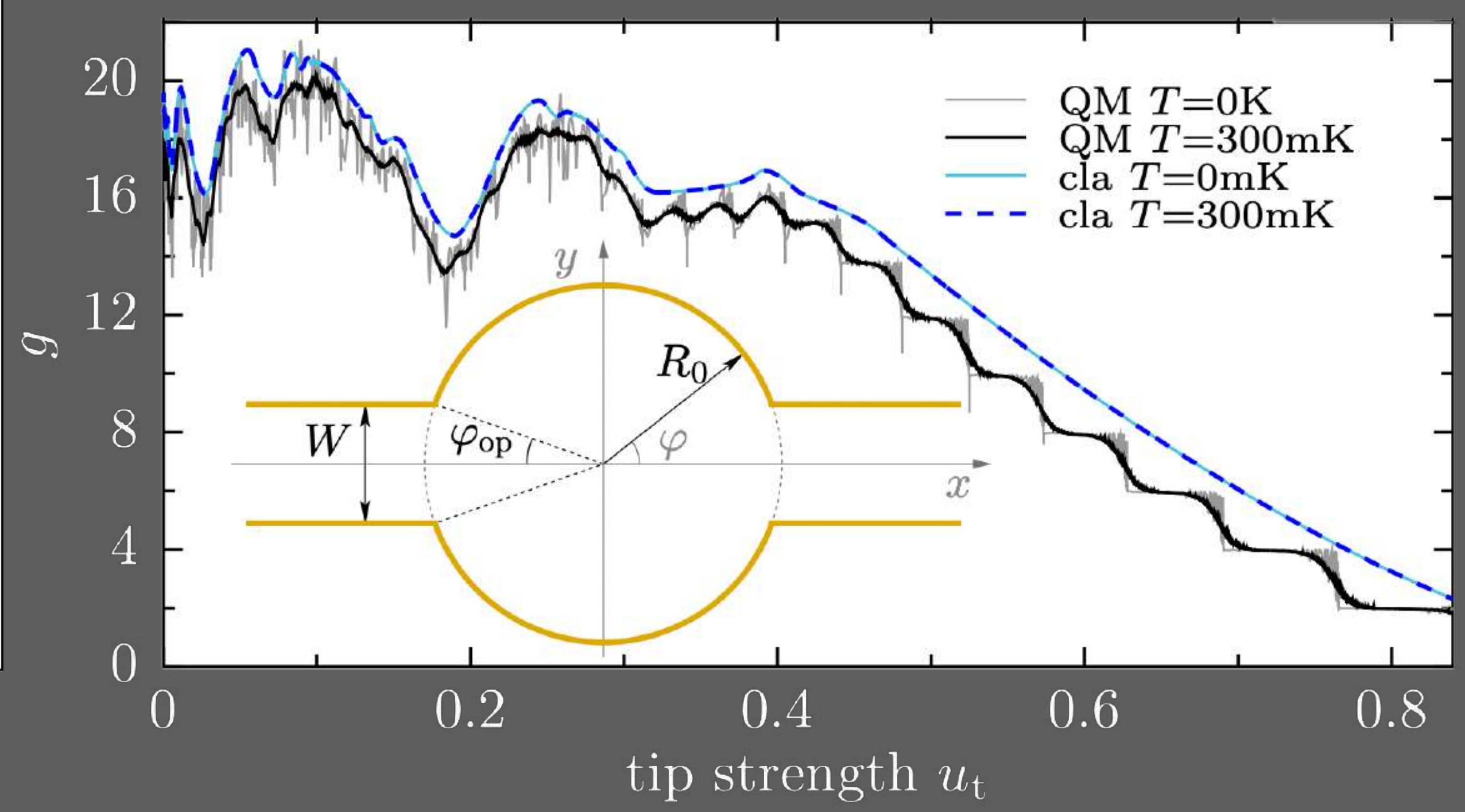


Image source : Right : C. Pöltl, Phys. Rev. B 94 (2016).

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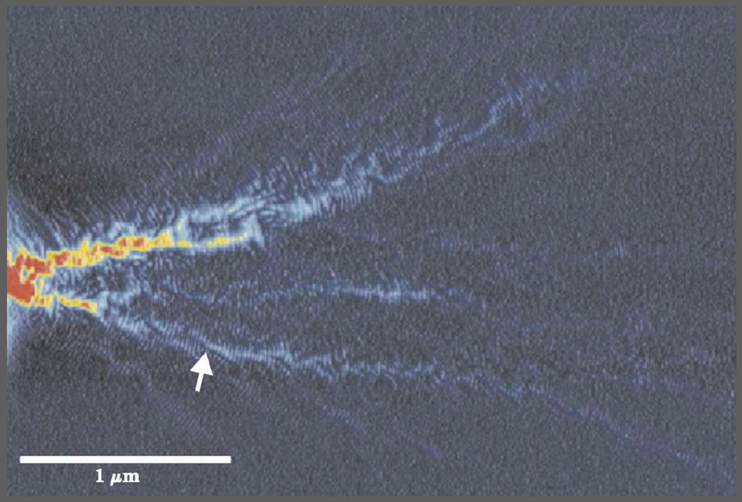
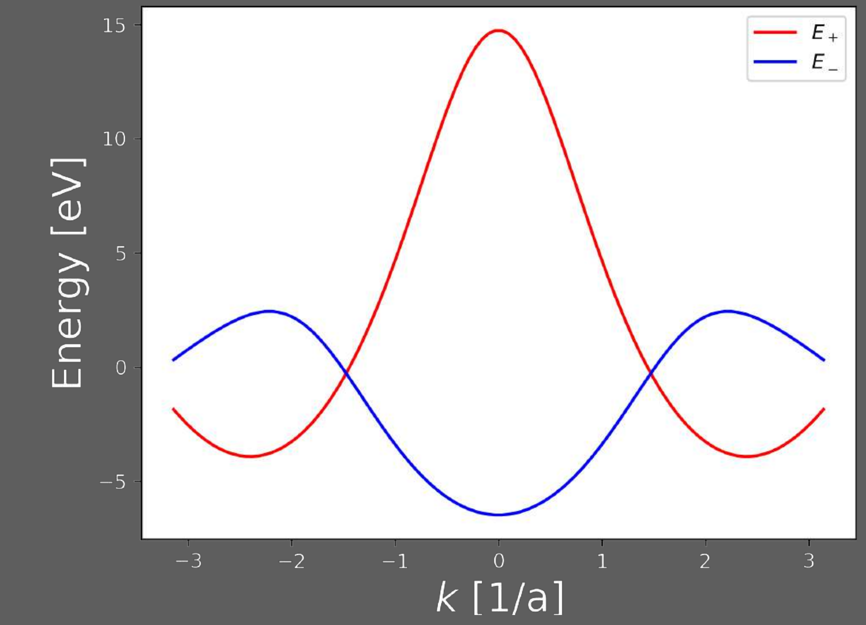
V — Conclusion and outlook

What have we seen ?

- SGM : imaging electron flow
- Interesting aspects of graphene : linear dispersion relation
- Classical trajectories of electrons in graphene : similarities with semiconductor heterostrucutres





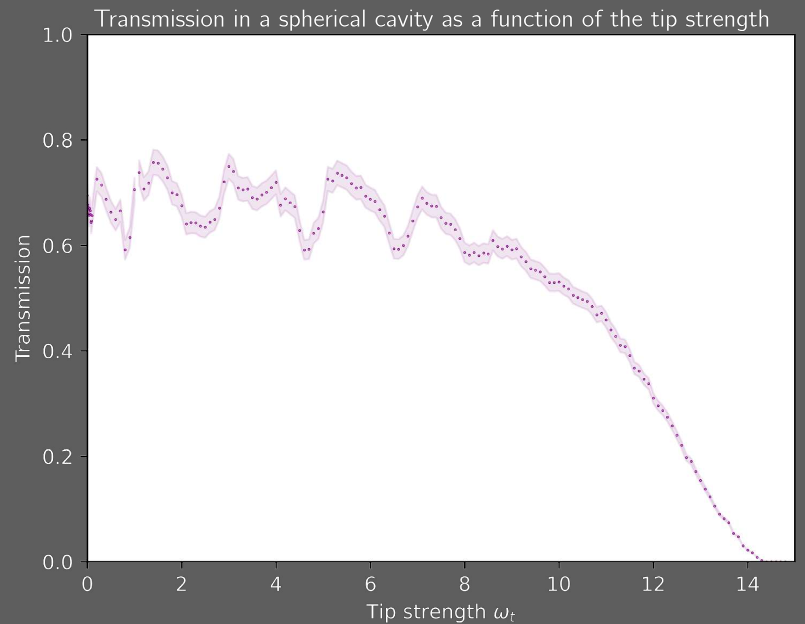
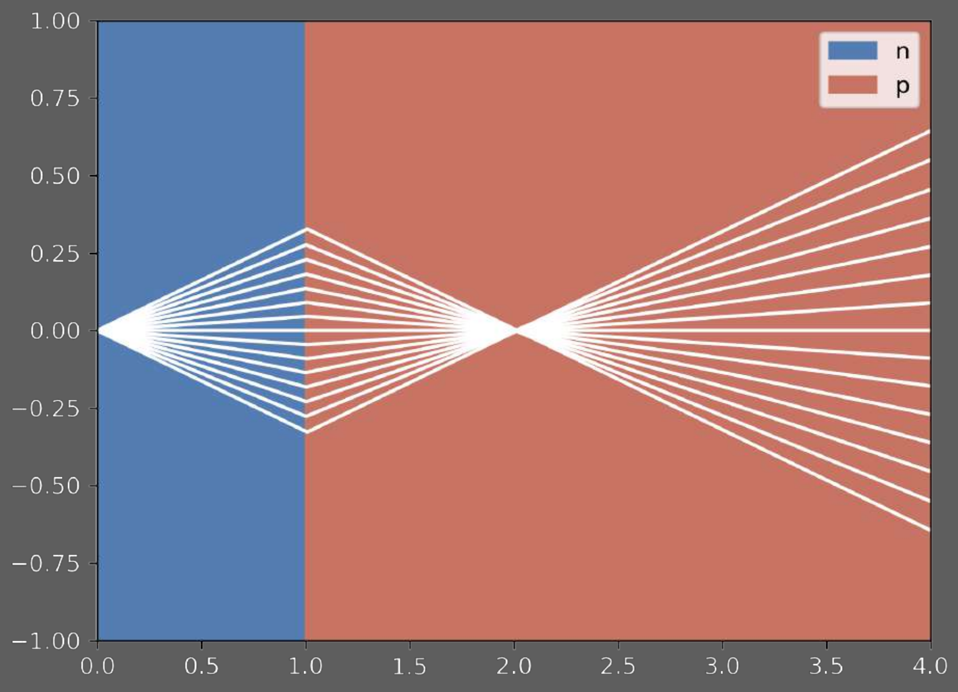


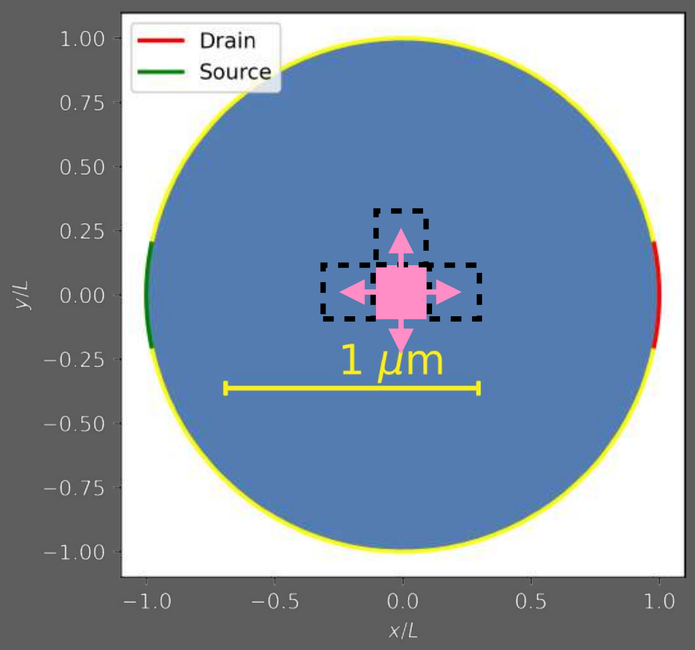
Image source : Top : M. Topinka, Physics Today 56 (2003).

V — Outlook and beyond

What is next ?

- More advanced semi-classical theory to explain Veselago lensing
- Geometry impact
- SGM map
- Quantum simulation





Appendix

- Tight binding
  - Only take p_z orbitals

$$\Psi_{\pm}(\overrightarrow{k},\vec{r}) = c_{\pm,\mathrm{A}}\Phi_{\mathrm{A}}(\overrightarrow{k},\vec{r}) + c_{\pm,\mathrm{B}}\Phi_{\mathrm{B}}(\overrightarrow{k},\vec{r})$$

$$E_{\pm}(\overrightarrow{k}) = \frac{\langle \Psi_{\pm} | H | \Psi_{\pm} \rangle}{\langle \Psi_{\pm} | \Psi_{\pm} \rangle}$$

  - Secular equation

$$\det(H - E_{\pm}S) = 0$$

$$S = \begin{pmatrix} 1 & s_0 f(\overrightarrow{k}) \\ s_0 f(\overrightarrow{k}) & 1 \end{pmatrix}$$

$$S_{i,j} = \langle \Phi_i | \Phi_j \rangle$$

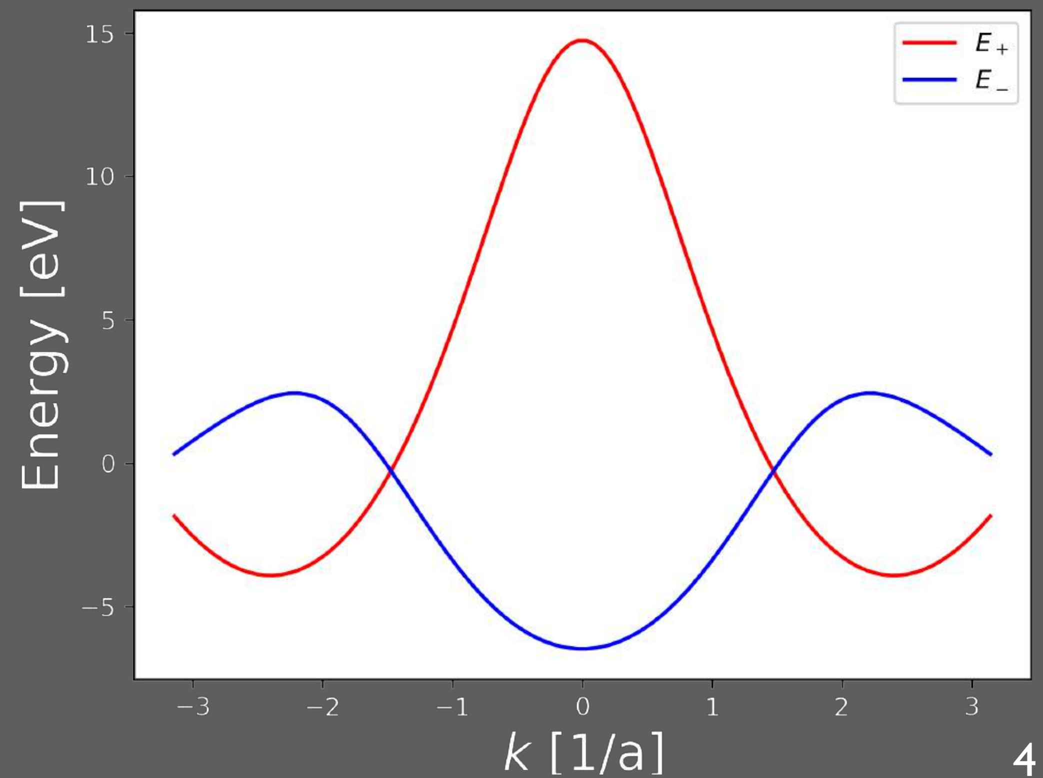
$i, j = A, B$

$$E_{\pm} = \frac{\gamma_0 s_0 f^2(k) + \varepsilon_{2p} \pm f(k)(\gamma_0 + s_0 \varepsilon_{2p})}{(1 - s_0^2 f^2(k))}$$

ε_{2p} : energy of $2p_z$ orbitals

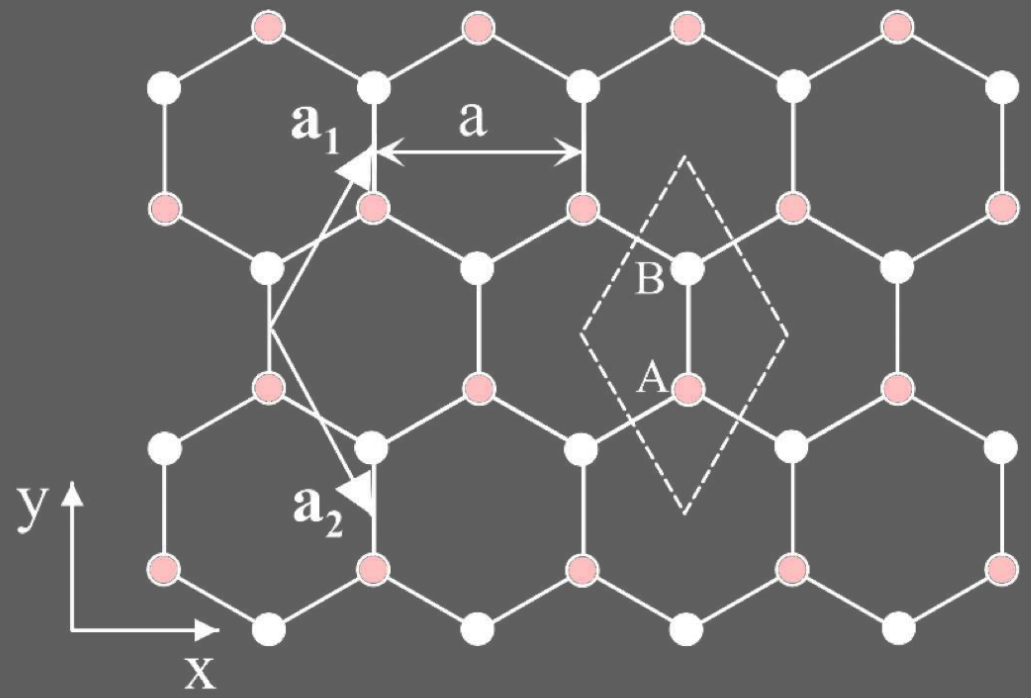
γ_0 : coupling between A and B (hopping)

s_0 : overlap between AA or BB



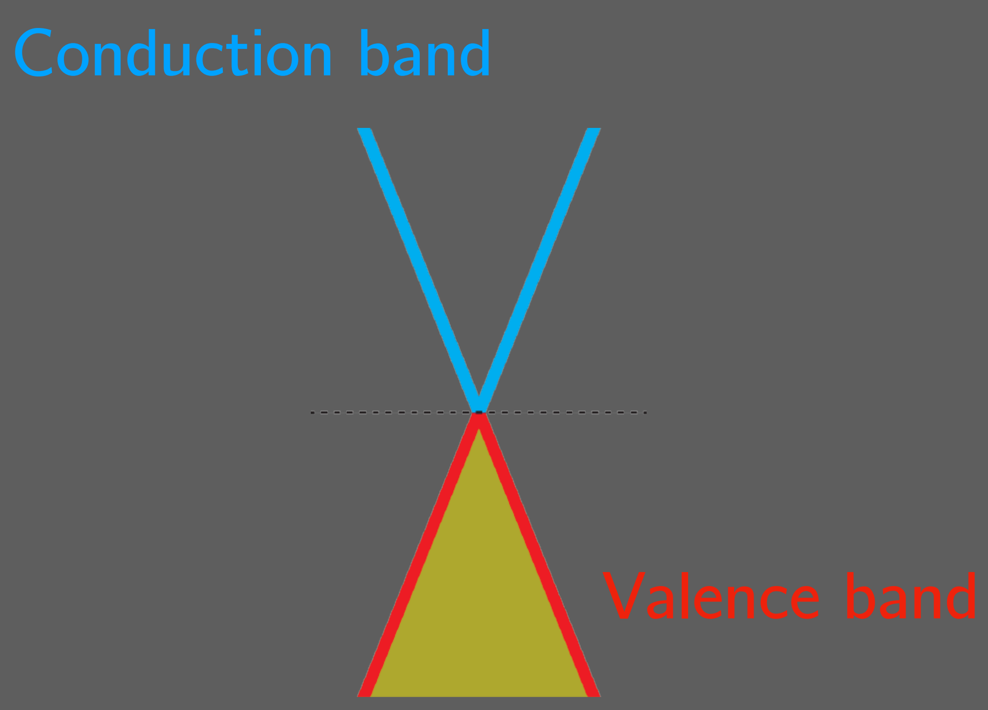
Appendix

- Explanation of Klein tunneling and Veselago lensing



Pseudo spin up : atoms A

Pseudo spin down : atoms B



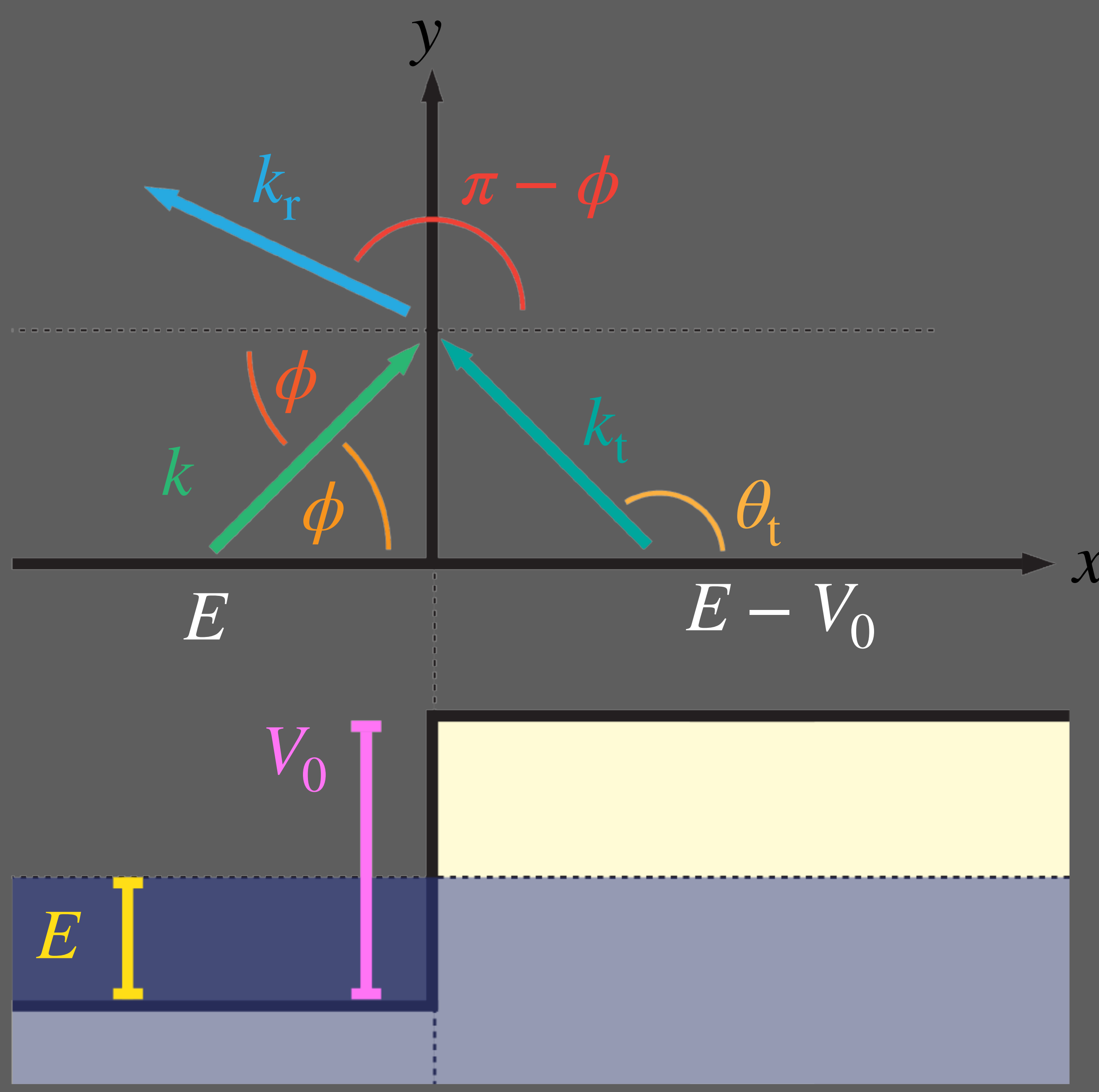
CB : $\overrightarrow{\sigma} \parallel \overrightarrow{p}$

VB : $\overrightarrow{\sigma} \nparallel \overrightarrow{p}$

Appendix

- Explanation of Klein tunneling and Veselago lensing

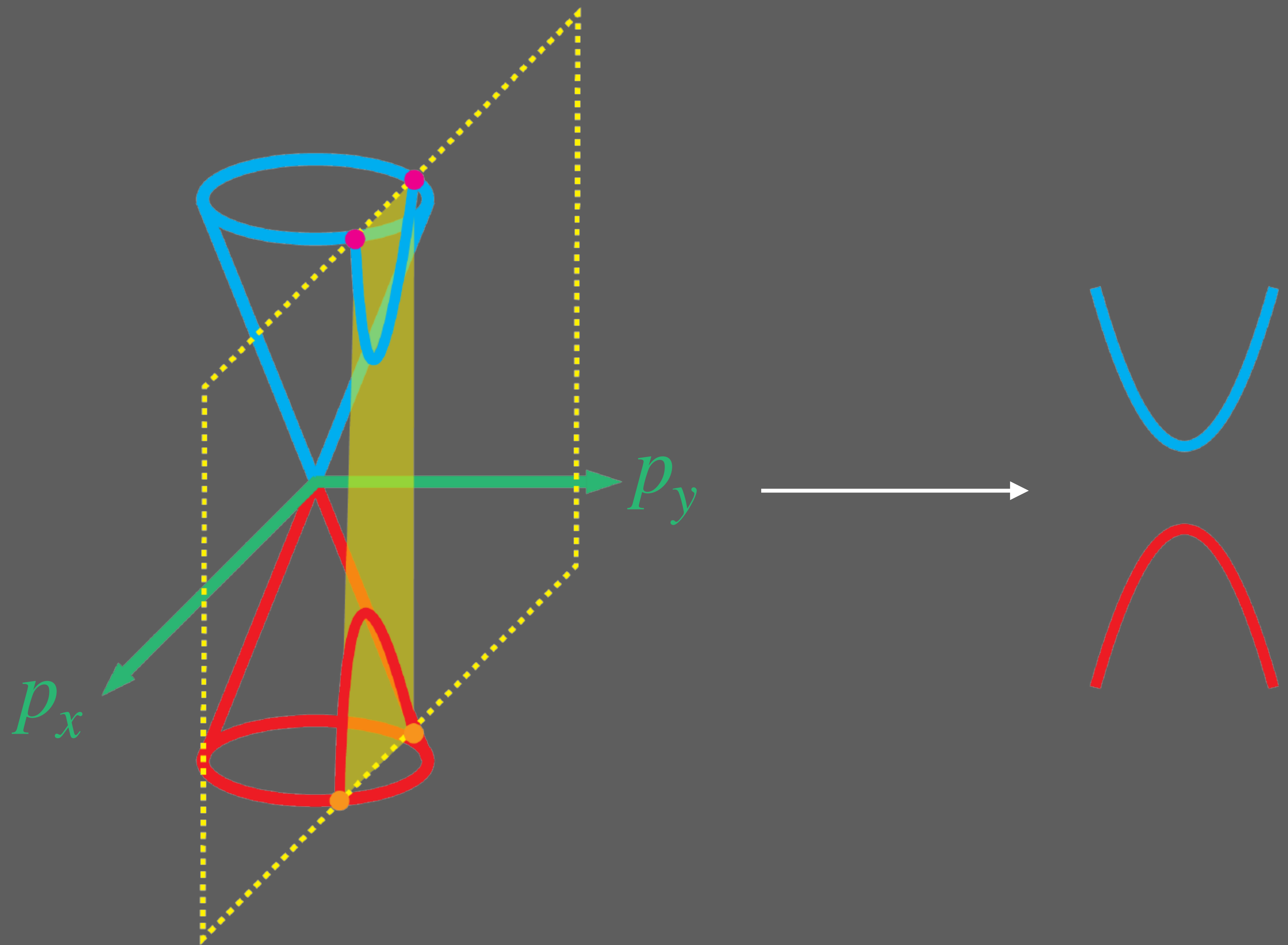
Pseudo spin conservation $[\hat{H}, \hat{\sigma}] = 0$



For $\theta_t = \pi$: no retrodiffusion : Klein tunnelling

Appendix

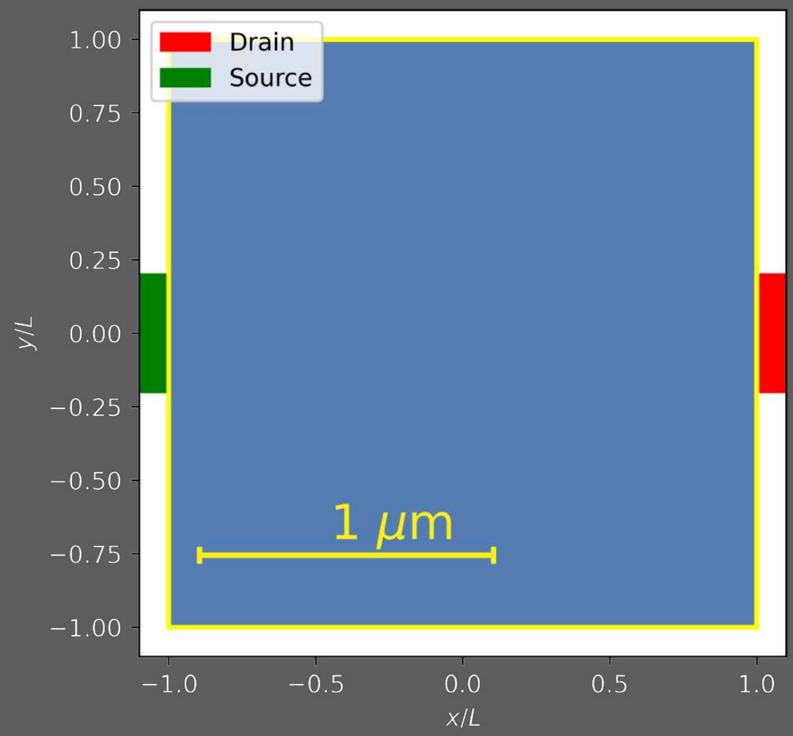
- Why can't we explain np junctions classically ?



Tunneling only possible if $p_x = p_y = 0$

Appendix

- Scaling in the numerical scheme



  - Length of the cavity : L
    - Our simulation : $L = 1\ \mu\text{m}$
  - Energy first transverse mode : $E_0 = \hbar v_F \pi / L$
    - Our simulation : $E_0 \approx 5$ meV corresponding to $T \approx 60$ K

Appendix

- Gaussian and Lorentzian