Analysis of Electronic Waveguide Bends in Graphene Subject to Dirac Point Fluctuations

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Objectives

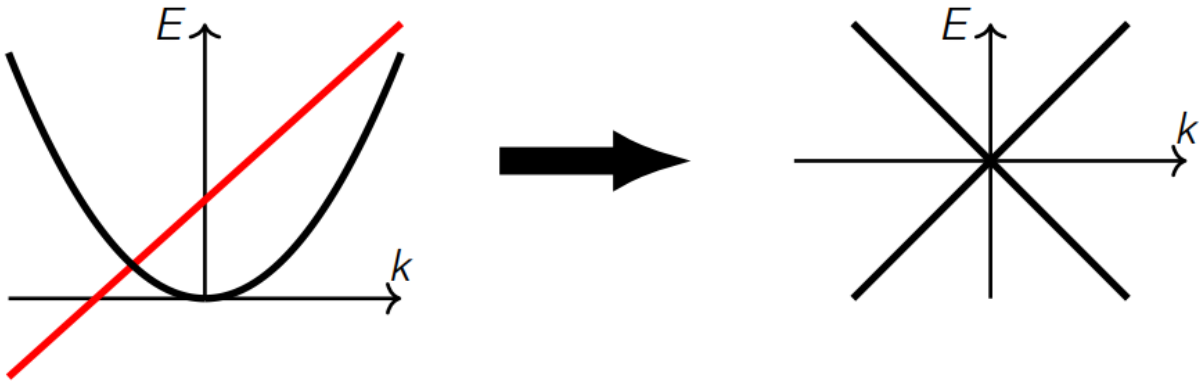
- Constructing a numerical solver for electron optics phenomena in graphene
- Studying the transmission properties of electronic waveguide bends in graphene
- Examining the effect of Dirac point fluctuations

Outline

- Electron optics in graphene
- Dirac point fluctuations
- Numerical method and setup
- Results of the simulation of a waveguide bend

Graphene and the Dirac equation

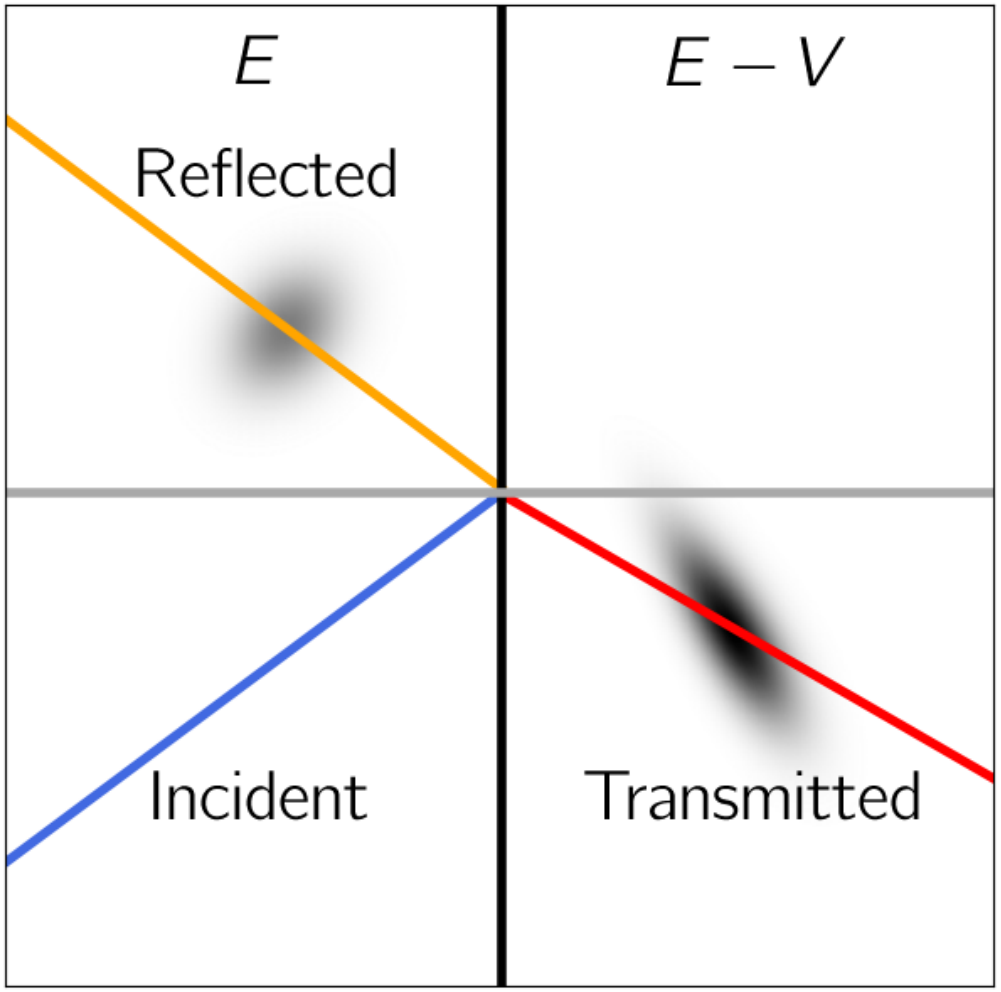
- Linear instead of parabolic dispersion relation
- Charge carriers are described by a (2+1)D massless Dirac equation
- $i\hbar \frac{\partial}{\partial t} \Psi = v_{\mathrm{F}}\, \boldsymbol{\sigma}.\hat{\boldsymbol{p}}\, \Psi + V(x,y)\Psi$
  - $\Psi = \begin{pmatrix} u \\ v \end{pmatrix}$ two component wavefunction
  - v_{F} Fermi velocity
  - $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ Pauli spin matrices
  - $\hat{\boldsymbol{p}} = (\hat{p}_x, \hat{p}_y)$ momentum operator



- Appearance of "*relativistic*" phenomena

Electron optics in graphene

- Charge carriers behave similarly as light in ordinary optics
- The kinetic energy (E-V) takes over the role of refractive index.
- Kinetic energy can be zero or negative
- Possible applications: Veselago lens, beam splitters, reflectors, transistors, waveguides…
  - High contrast leads to excellent confinement



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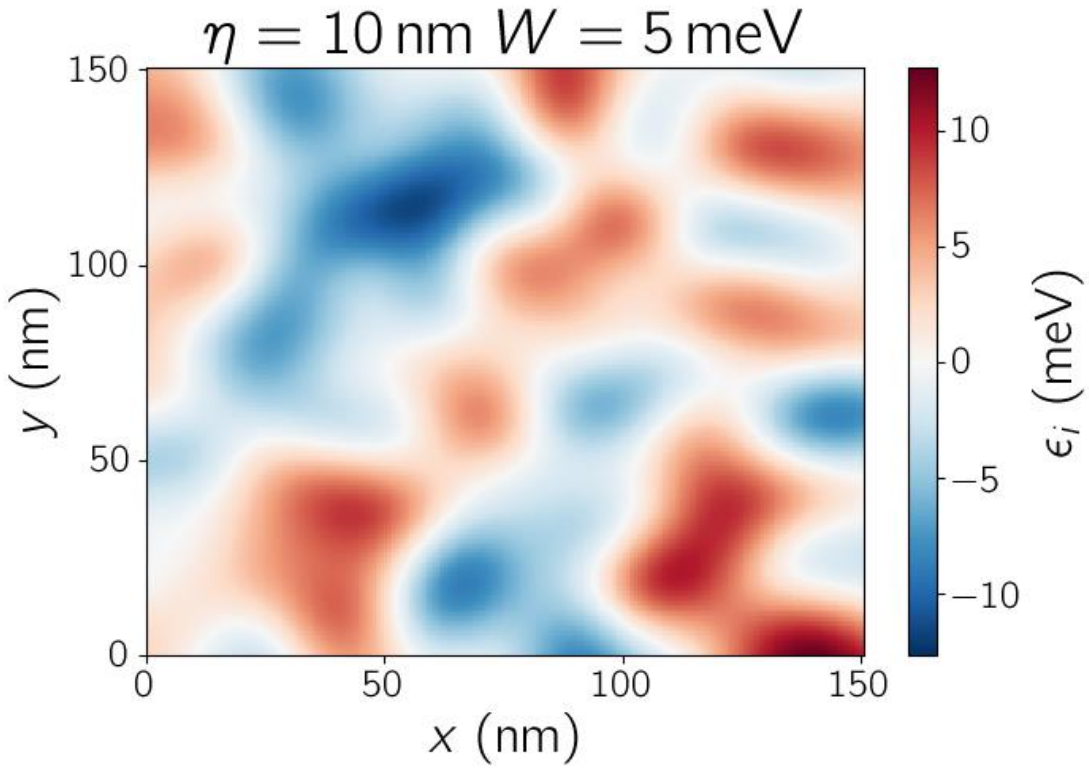
Dirac point fluctuations

- Type of disorder in graphene layers
- Local variations of the potential
- Neutral graphene corresponds to a system of electron/hole puddles
- Origin: strain, substrate inhomogeneities
- Complicates the desired confinement in waveguides

Model for Dirac point fluctuations

- Additional onsite correlated potential
- $\epsilon_i = \dfrac{\sum_j \widetilde{\epsilon_j} \exp\left(-r_{ij}^2/2\eta^2\right)}{\sqrt{\sum_j \exp(-r_{ij}^2/\eta^2)}}$
- $\widetilde{\epsilon_j}$ normal distributed with zero mean and W standard deviation
- r_{ij} distance between lattice points i and j
- η correlation length



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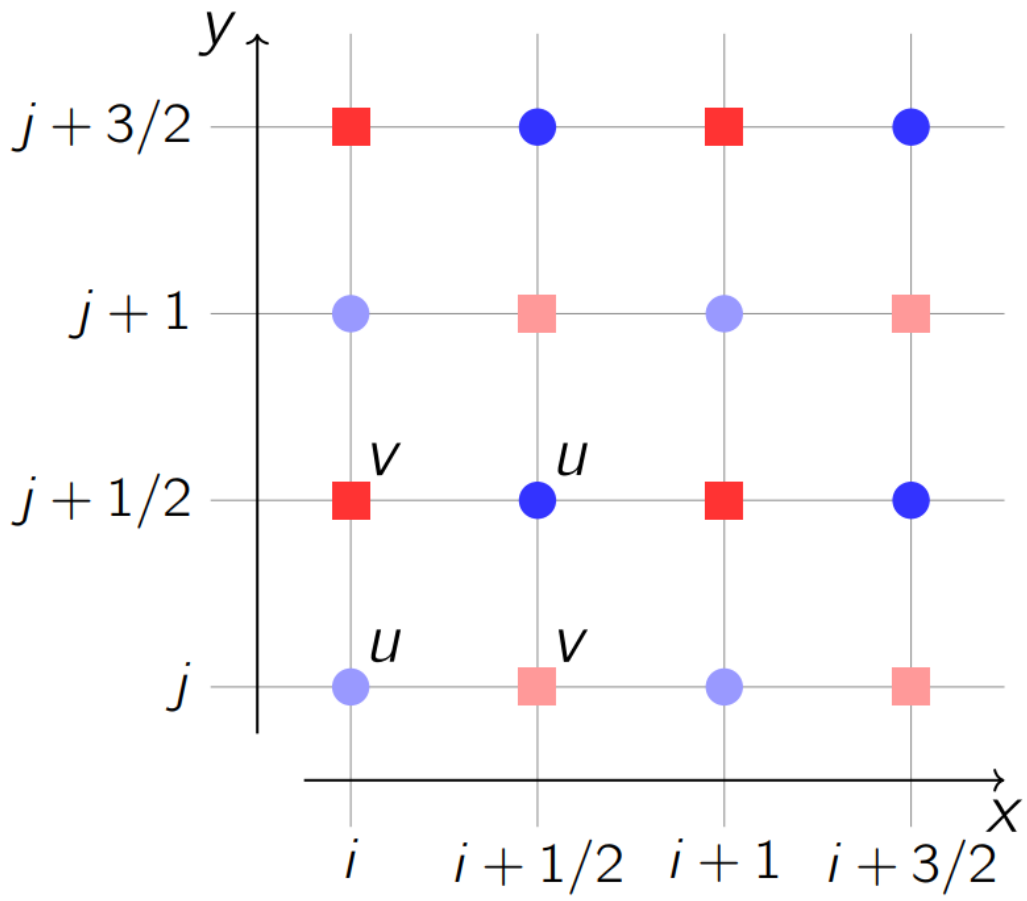
Numerical method

- Fourth-order accurate time-domain solver for the (2+1)D Dirac equation

- Spatial discretization
  - Staggered grid [1]
  - Fourth-order central difference

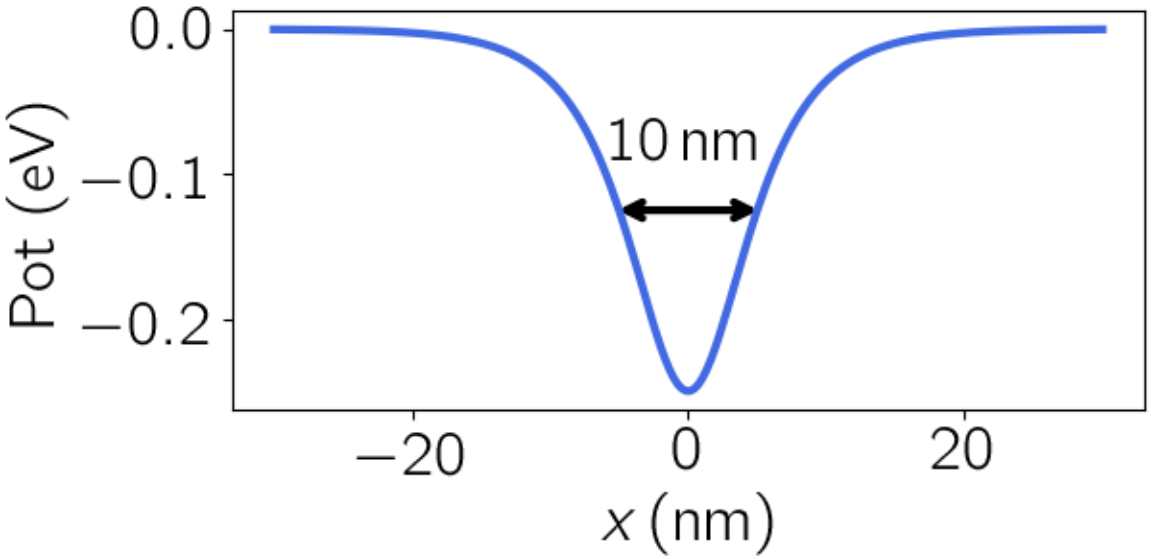
- Novel timestepping scheme
  - Partitioned Runge-Kutta method instead of standard Runge-Kutta
  - Fourth-order accurate
  - Lower memory consumption owing to fully in-place update scheme
  - Conservation of mass and energy

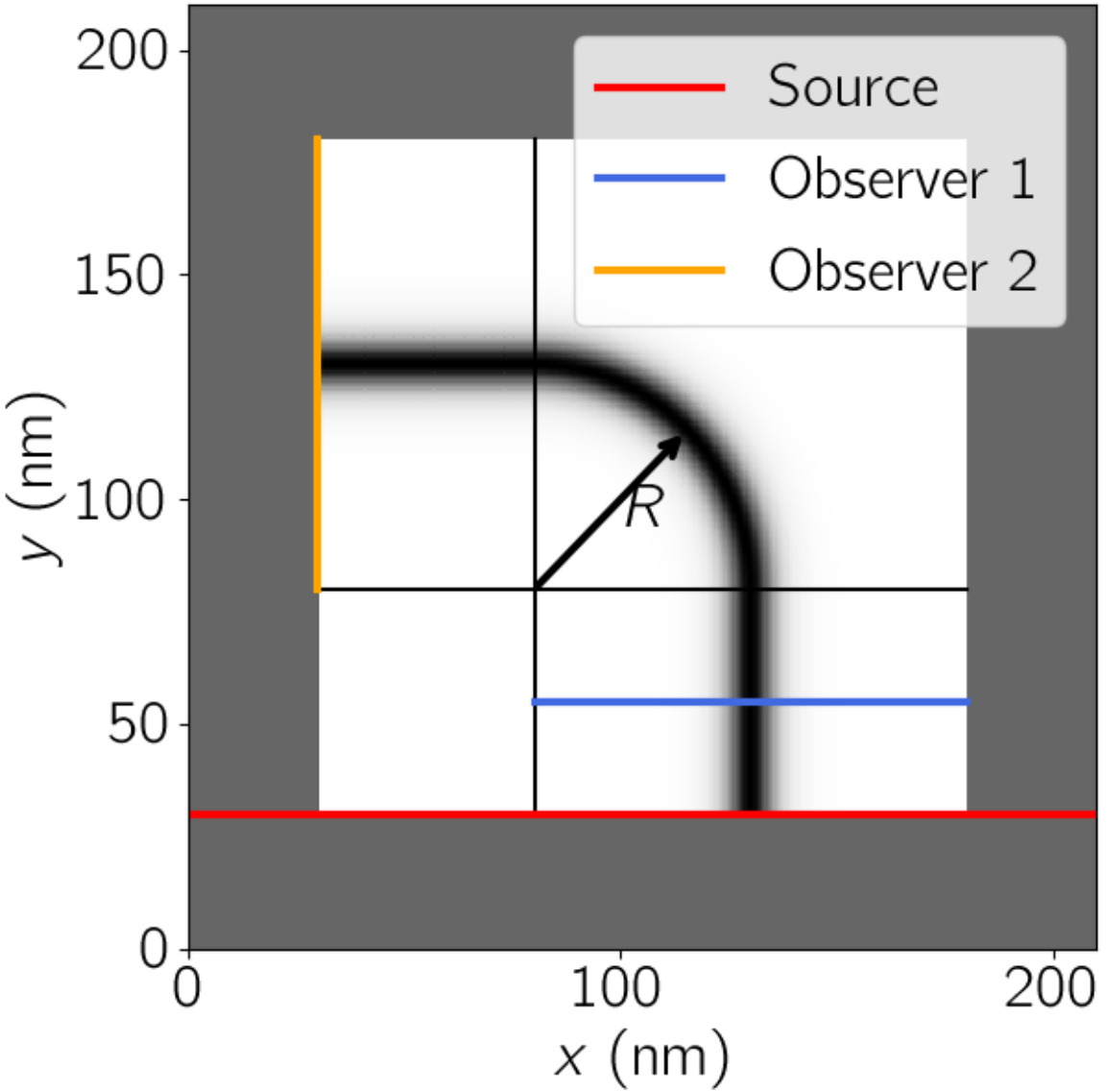


[1] R. Hammer, W. Pötz, A. Arnold, “Single-cone real-space finite difference scheme for the time-dependent Dirac equation,” *Journal of Computational Physics*, vol. 265, pp. 50-70, 2014.

Setup

- Absorbing boundaries
- Total Field Scattered Field approach for the source
- Smooth potential supporting a single mode





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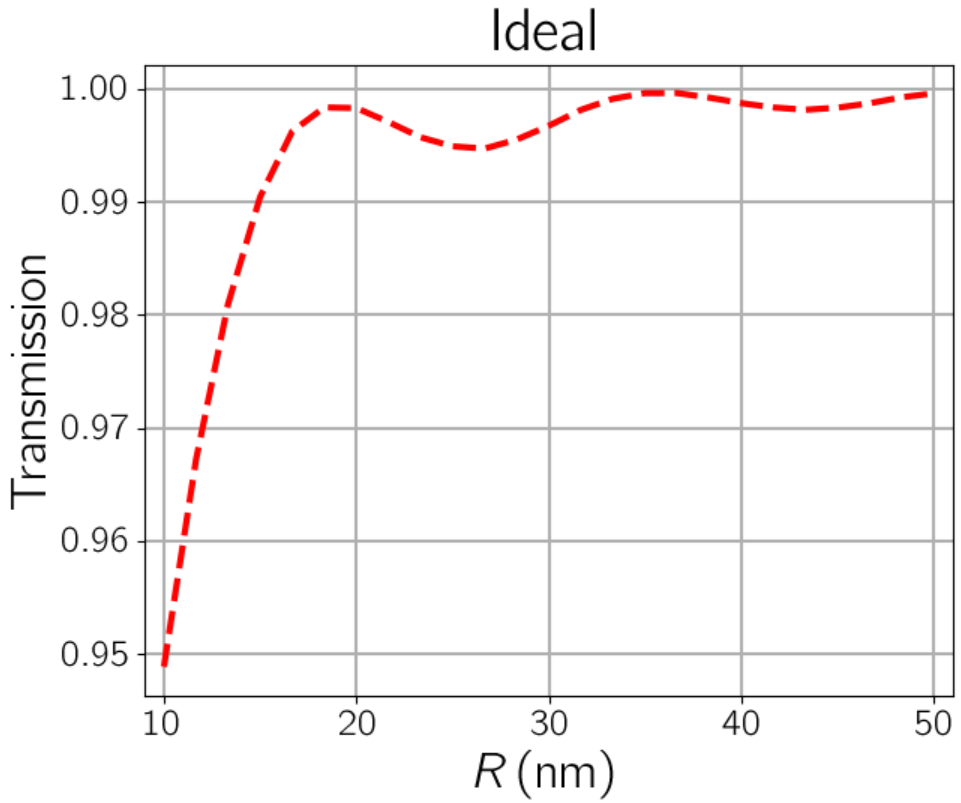
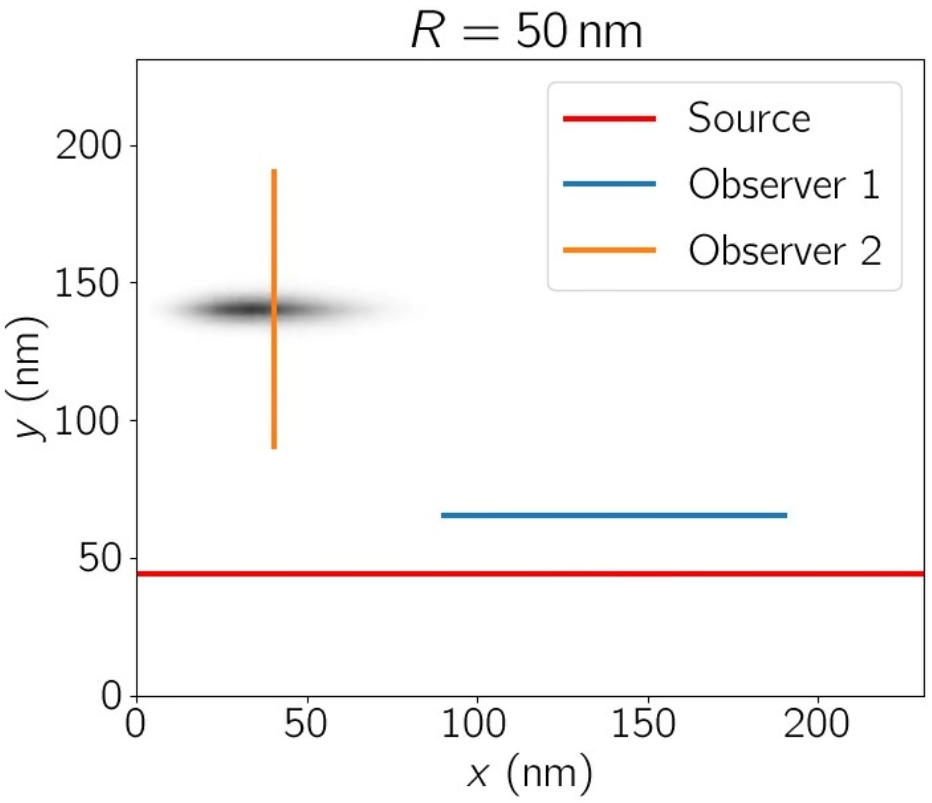
Results for the electronic waveguide bend

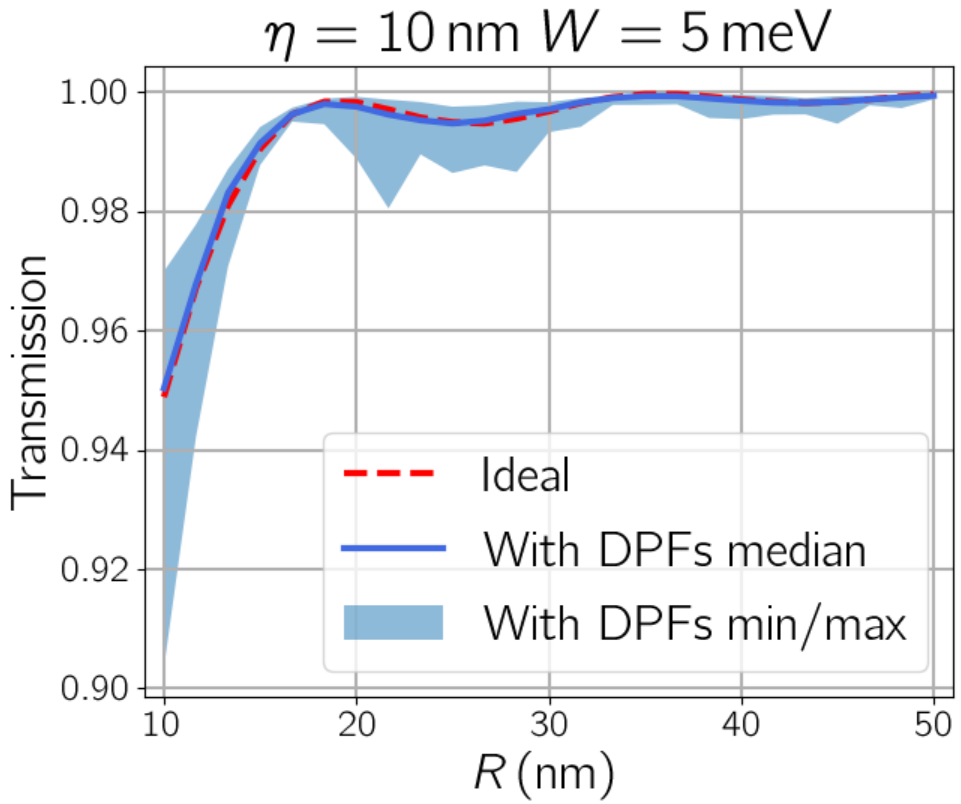
- Ideal situation
  - Mode adaptation losses
  - Low losses, even for very small radii

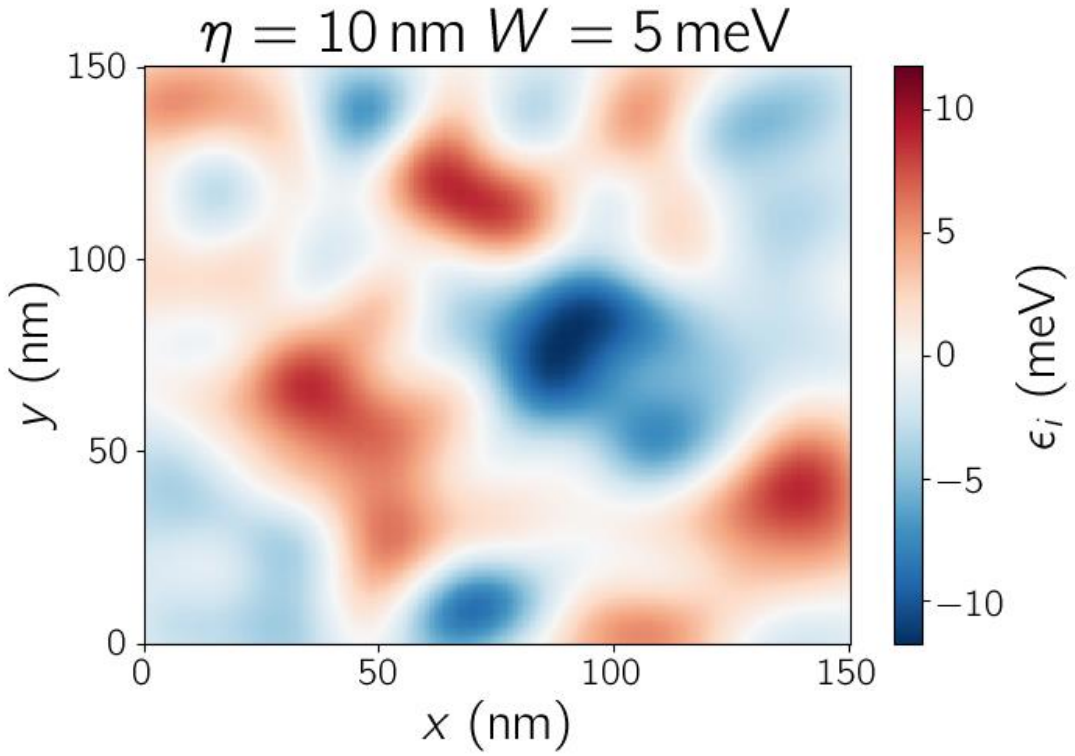




Results for the electronic waveguide bend

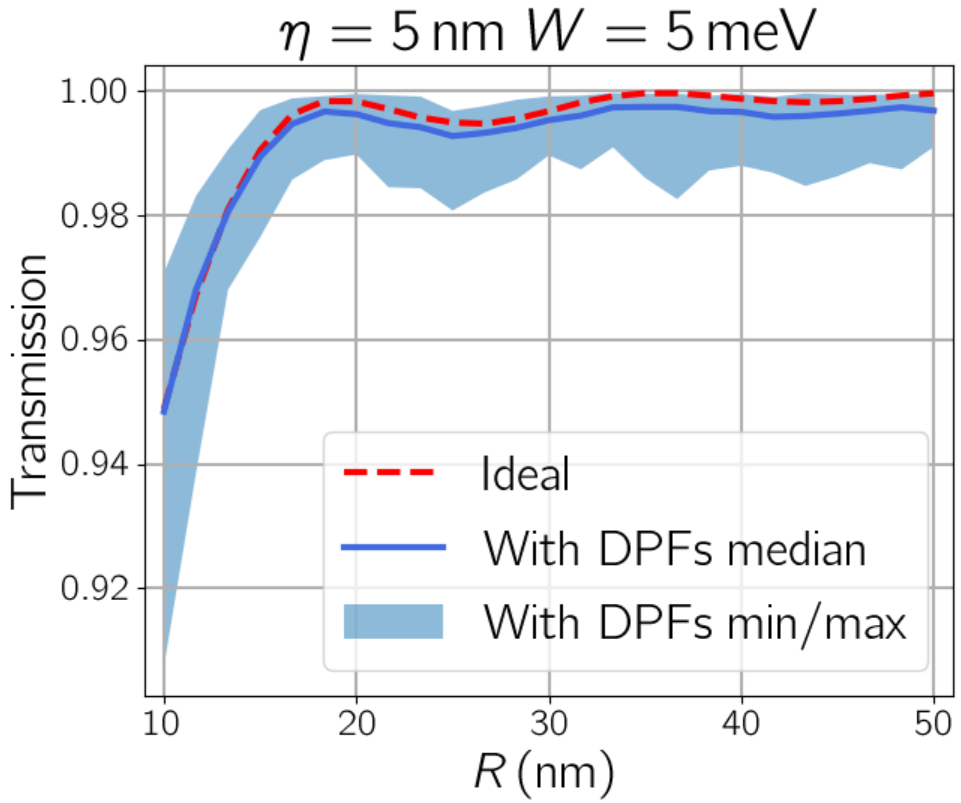
- With Dirac point fluctuations (DPFs)
  - Higher transmission than ideal situation is possible

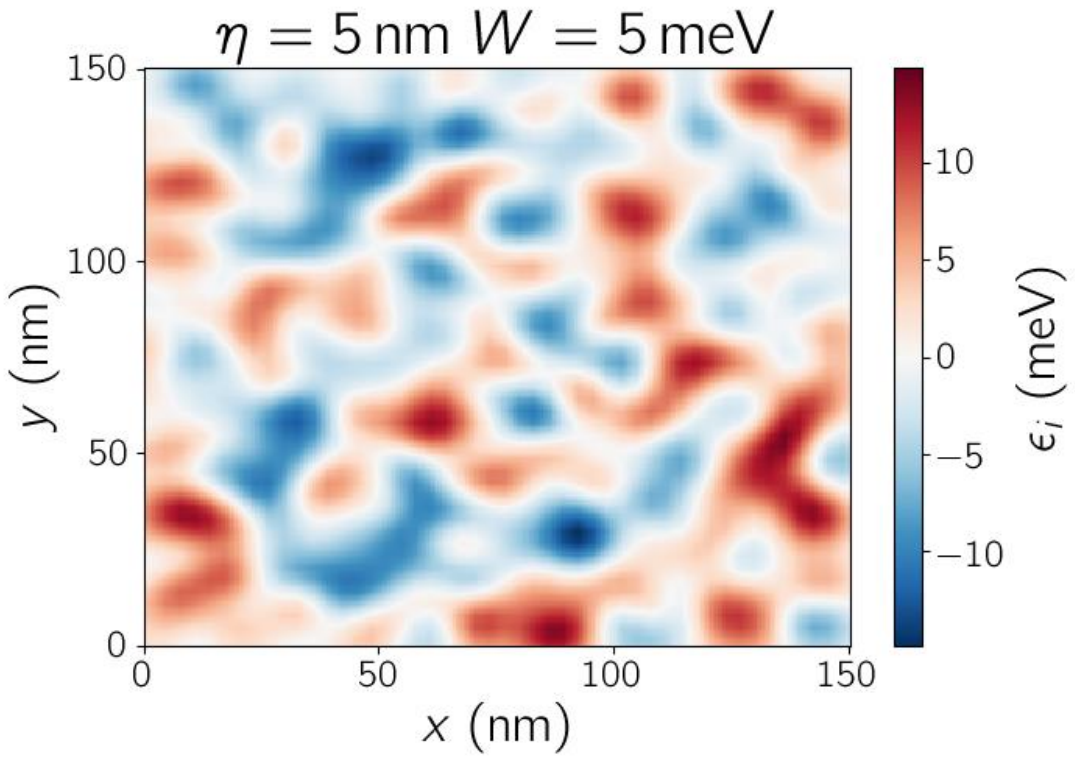




Results for the electronic waveguide bend

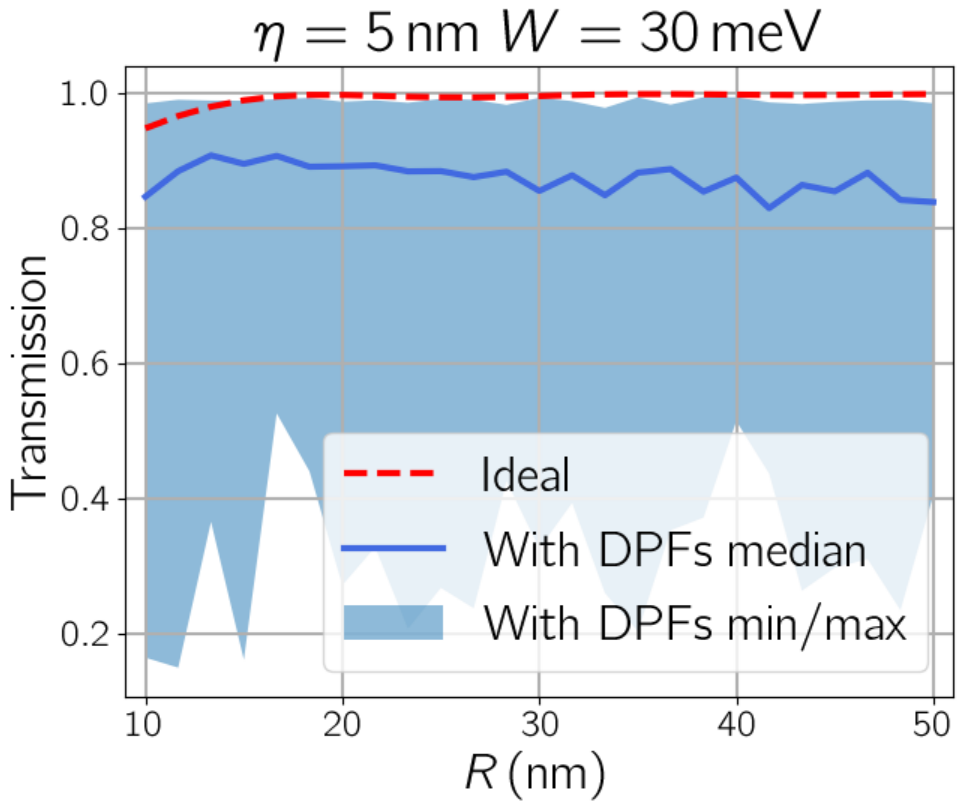
- With Dirac point fluctuations (DPFs)
  - Decreasing the correlation length η increases the deviation

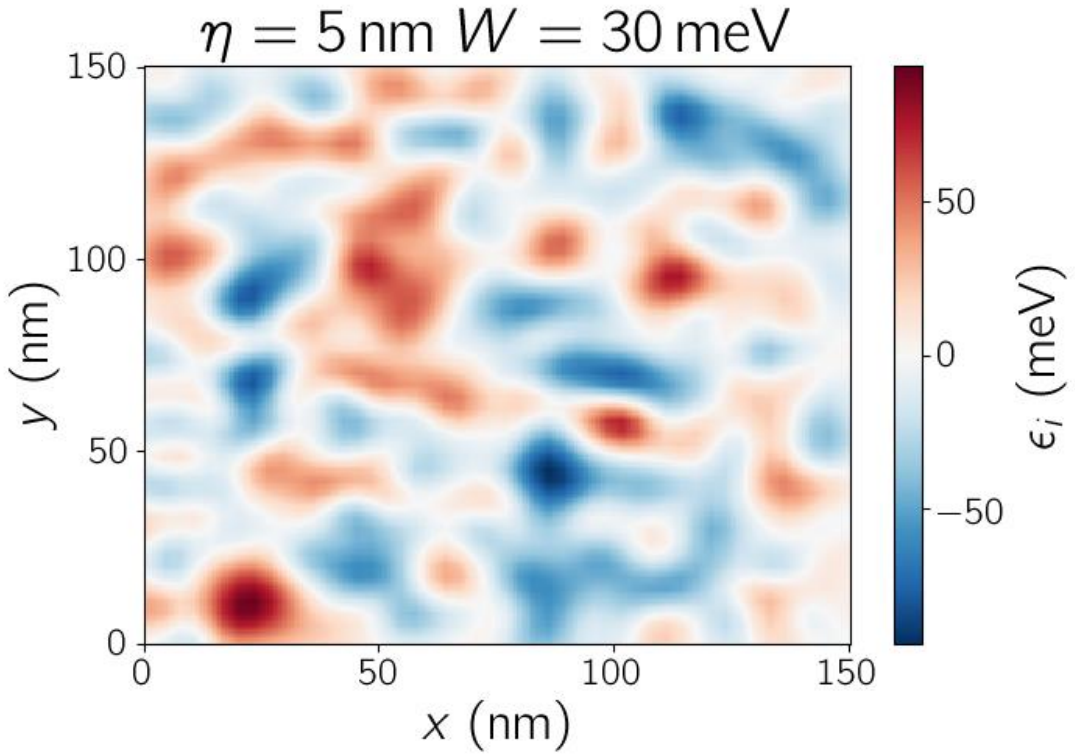




Results for the electronic waveguide bend

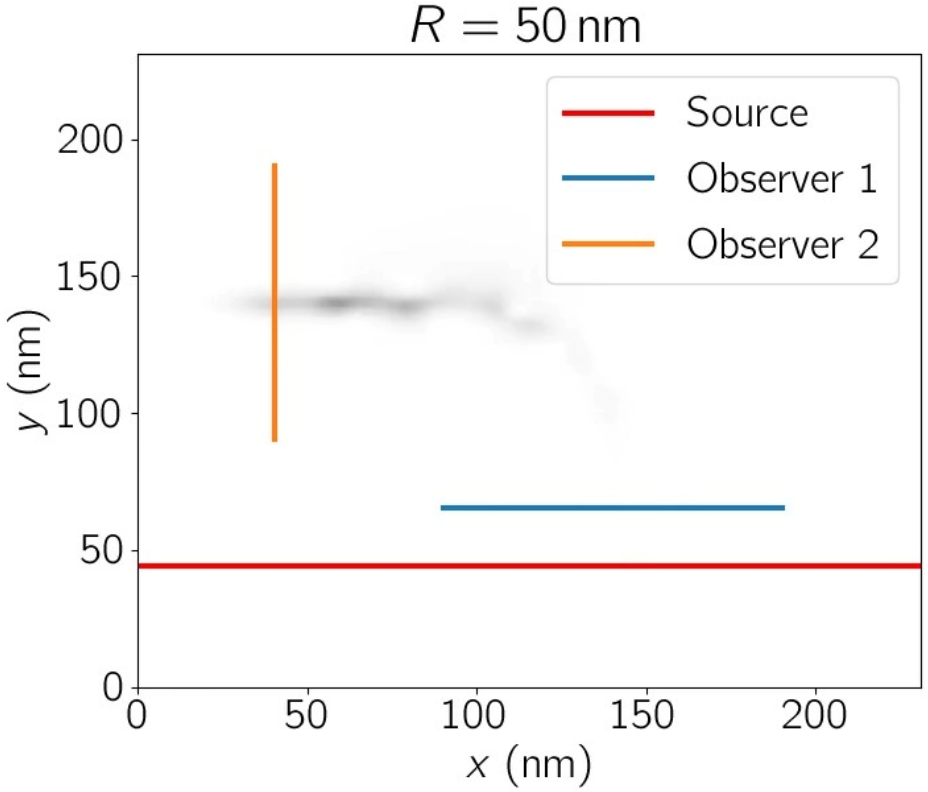
- With Dirac point fluctuations (DPFs)
  - Increasing the standard deviation W increases the deviation

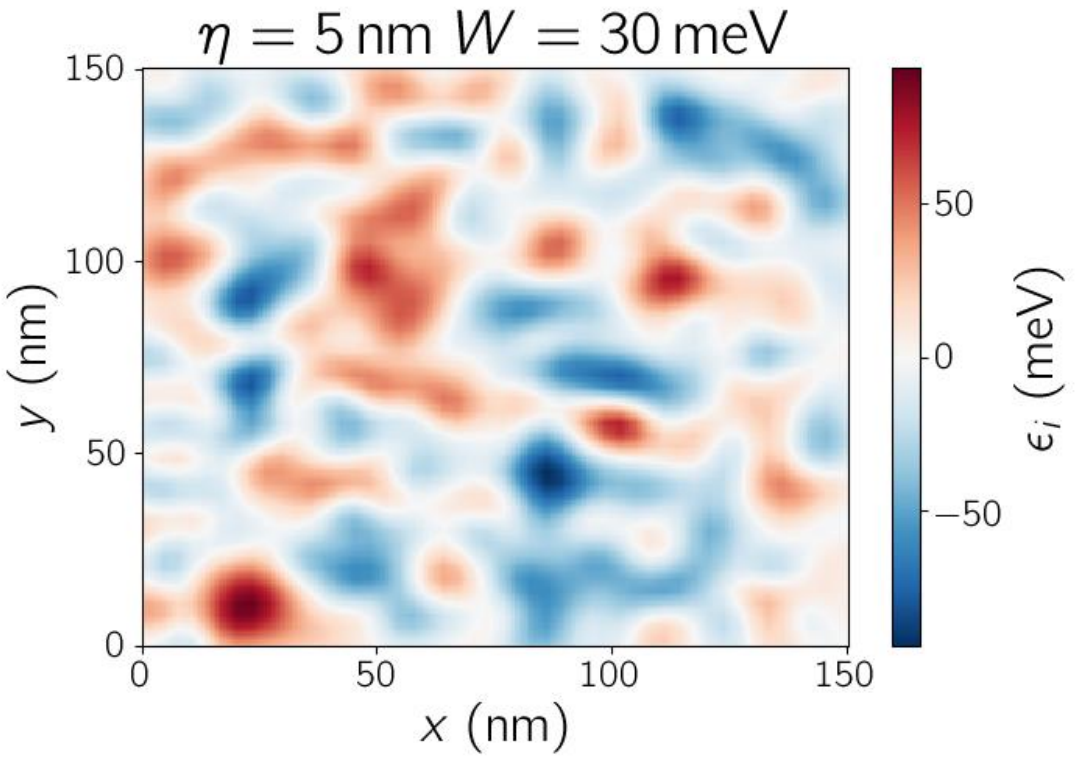




Results for the electronic waveguide bend

- With Dirac point fluctuations (DPFs)
  - Example with Transmission $= 0.40$





Conclusion

- Constructed numerical solver capable of simulating electron optics phenomena and applications in graphene
- Electronic waveguide bends can be obtained that exhibit excellent transmission properties
- Dirac point fluctuations must be considered when studying electron optics phenomena in graphene