Quantum
Mechanical &
Electromagnetic
Systems
Modelling Lab

Analysis of Electrostatically Induced Interconnect Structures in Single-Layer Graphene via a Conservative First-Principles Modeling Technique

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quest.

Outline

Motivation

Numerical method

Validation

Application: interconnect bend

Application: interconnect coupler

Conclusion

Motivation

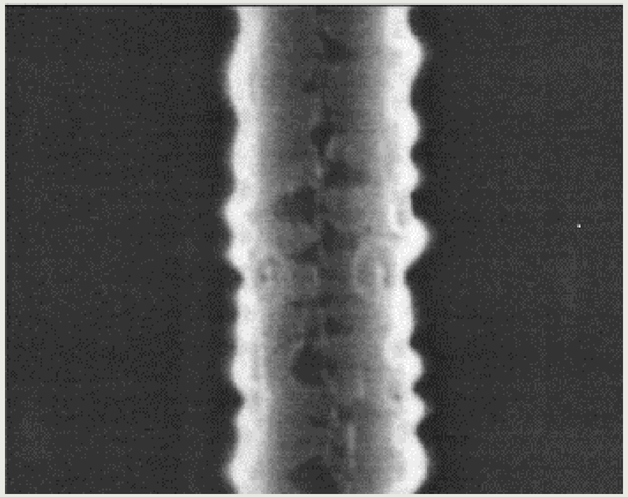
Issues related to downscaling of Cu interconnects

Classical downscaling of the IC feature size is facing many challenges

Smaller cross-sectional dimensions of Cu interconnects leads to

- Larger resistance (geometrically + increased surface scattering)
- Increased importance of electromigration

Need for novel material for local interconnects



Motivation

Carbon allotropes as alternatives for Cu

Examples: carbon nanotubes (CNT) and graphene nanoribbons (GNR)

Pros

High current carrying capabilities

No electromigration concerns

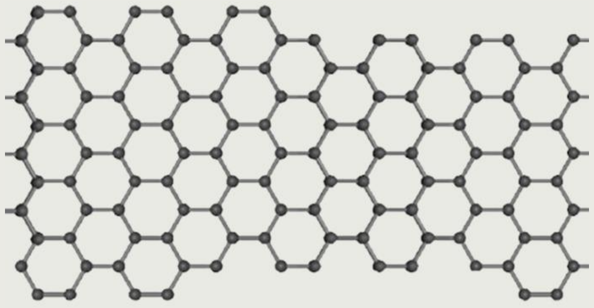
Large mean free path

Cons

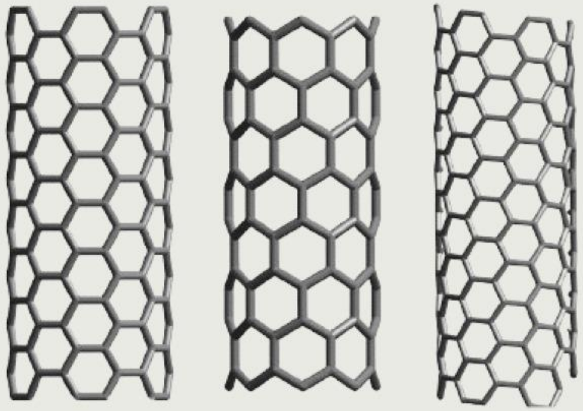
Graphene nanoribbons suffer from line edge roughness

Present growth techniques lead to a mixture of semiconducting and metallic carbon nanotubes

Solution: electrostatically induced interconnect structures in graphene



Graphene nanoribbon



Armchair Zigzag Chiral

Motivation

Electrostatically induced interconnects in graphene

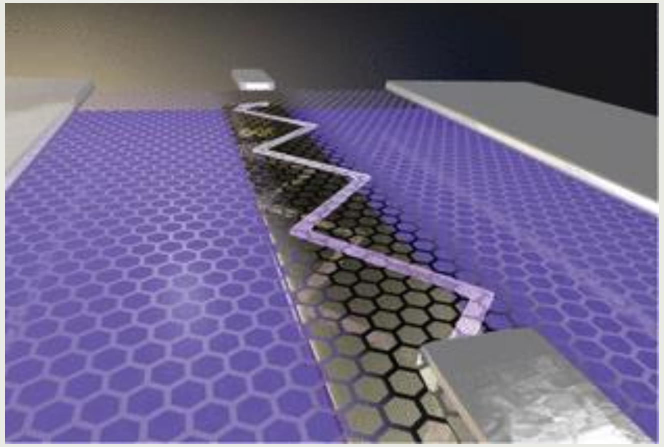
Electrons are guided by an electrostatic potential

No scattering at the boundaries

Properties can be tuned by varying shape and amplitude of the potential

Analytical solutions are scarce and understanding is insufficient at the moment

Goal: develop numerical method to analyze electrostatically induced interconnect structures in graphene



Numerical method

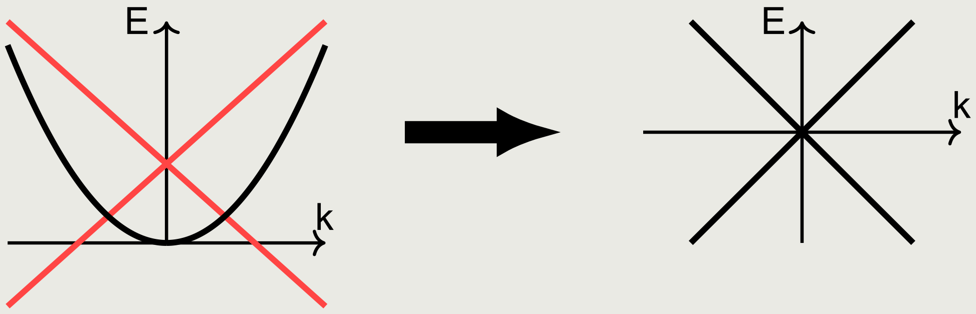
(2+1)D Dirac equation for charge carriers in graphene

Charge carriers in graphene adhere to a **linear dispersion relation**

$$i\hbar\frac{\partial}{\partial t}\Psi(x,y,t) = \left[v_F\left(\sigma_x p_x + \sigma_y p_y\right) + V(x,y)\right]\Psi(x,y,t)$$

with:

- Two component wavefunction $\Psi(x,y,t) = \begin{pmatrix} u(x,y,t) \\ v(x,y,t) \end{pmatrix}$
- Fermi velocity v_F
- Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$
- Momentum operators $p_x = -i\hbar\frac{\partial}{\partial x}$ and $p_y = -i\hbar\frac{\partial}{\partial y}$
- Potential $V(x,y)$



Probability density $|u(x,y,t)|^2 + |v(x,y,t)|^2$

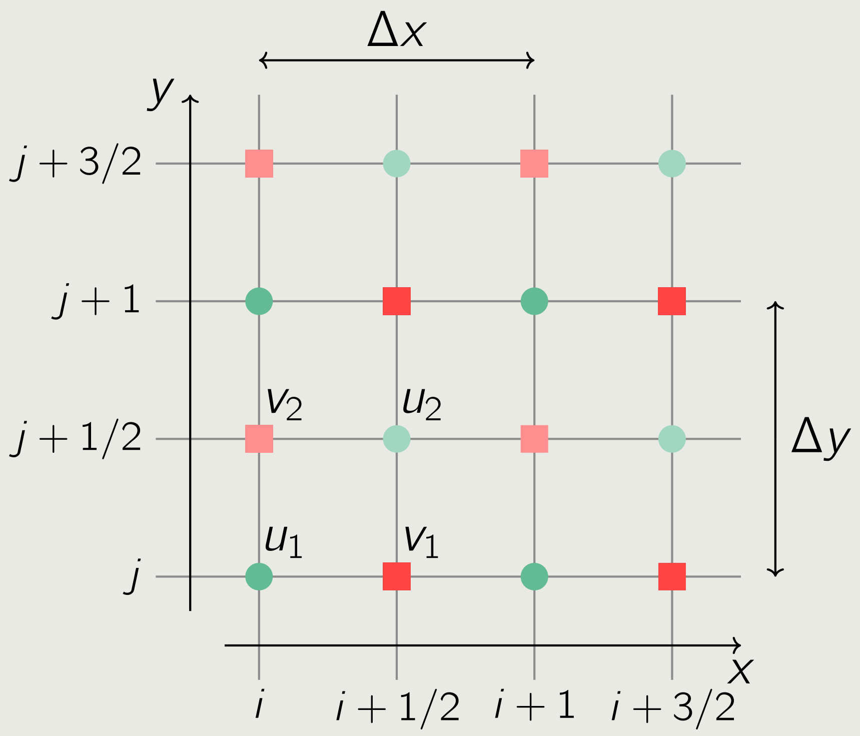
Numerical method

Spatial discretization

$$i\hbar \frac{\partial}{\partial t}\binom{u}{v} = \left[v_F\left(\sigma_x p_x + \sigma_y p_y\right) + V(x,y)\right]\binom{u}{v}$$

Staggered grid
Fourth-order central difference

$$\begin{cases} \frac{\mathrm{d}\mathbf{q}}{\mathrm{d}t} = K\mathbf{p} \\ \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -K^T\mathbf{q} \end{cases} \quad \text{with} \quad \mathbf{q} = \begin{pmatrix} \mathrm{Im}(\mathbf{u}_1) \\ \mathrm{Re}(\mathbf{u}_2) \\ \mathrm{Re}(\mathbf{v}_1) \\ \mathrm{Im}(\mathbf{v}_2) \end{pmatrix} \text{ and } \mathbf{p} = \begin{pmatrix} \mathrm{Re}(\mathbf{u}_1) \\ \mathrm{Im}(\mathbf{u}_2) \\ \mathrm{Im}(\mathbf{v}_1) \\ \mathrm{Re}(\mathbf{v}_2) \end{pmatrix}$$



Numerical method

Temporal discretization

$$\begin{cases} \frac{d\mathbf{q}}{dt} = K\mathbf{p} \\ \frac{d\mathbf{p}}{dt} = -K^T\mathbf{q} \end{cases} \quad \text{with} \quad \mathbf{q} = \begin{pmatrix} \mathrm{Im}(\mathbf{u}_1) \\ \mathrm{Re}(\mathbf{u}_2) \\ \mathrm{Re}(\mathbf{v}_1) \\ \mathrm{Im}(\mathbf{v}_2) \end{pmatrix} \text{ and } \mathbf{p} = \begin{pmatrix} \mathrm{Re}(\mathbf{u}_1) \\ \mathrm{Im}(\mathbf{u}_2) \\ \mathrm{Im}(\mathbf{v}_1) \\ \mathrm{Re}(\mathbf{v}_2) \end{pmatrix}$$

Symplectic fourth-order partitioned Runge-Kutta

Stepping from $t = n\,\Delta t$ to $t = (n+1)\,\Delta t$

$$\begin{aligned} \mathbf{Q}^{n,0} &= \mathbf{q}^n & \mathbf{P}^{n,1} &= \mathbf{p}^n \\ \mathbf{Q}^{n,1} &= \mathbf{Q}^{n,0} + \Delta t\, B_1\, K\, \mathbf{P}^{n,1} & \mathbf{P}^{n,2} &= \mathbf{P}^{n,1} - \Delta t\, b_1\, K^T\, \mathbf{Q}^{n,1} \\ \mathbf{Q}^{n,2} &= \mathbf{Q}^{n,1} + \Delta t\, B_2\, K\, \mathbf{P}^{n,2} & \mathbf{P}^{n,3} &= \mathbf{P}^{n,2} - \Delta t\, b_2\, K^T\, \mathbf{Q}^{n,2} \\ &\vdots & &\vdots \\ \mathbf{q}^{n+1} &= \mathbf{Q}^{n,s} & \mathbf{p}^{n+1} &= \mathbf{P}^{n,s+1} \end{aligned}$$

with b_i and B_i well-chosen constants

Pros

Explicit update scheme

Low memory consumption due to fully in-place update scheme

Excellent long-term properties as total **mass and energy are conserved**

Validation

Comparison with analytical solution

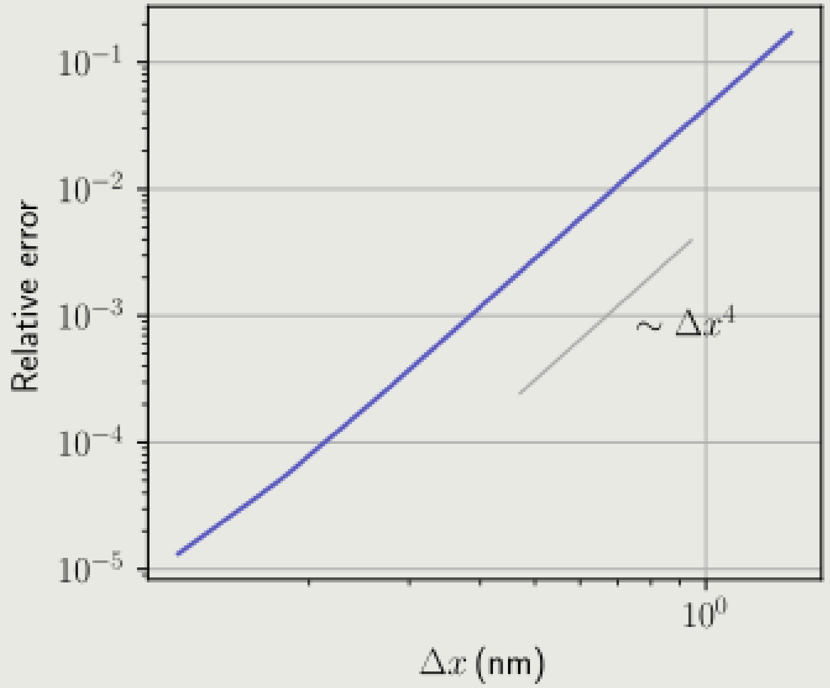
Initial wavefunction

$$\Psi(x,y,t=0) = N\begin{pmatrix}1\\1\end{pmatrix} e^{ik_x x} e^{-x^2/(4\sigma_x^2)} e^{-y^2/(4\sigma_y^2)}$$

Parameters

- k_x: 0.75 nm^{-1}
- σ_x: 5.3 nm
- σ_y: 5.3 nm
- $V(x,y)$: 0 eV
- Total duration: 29 fs

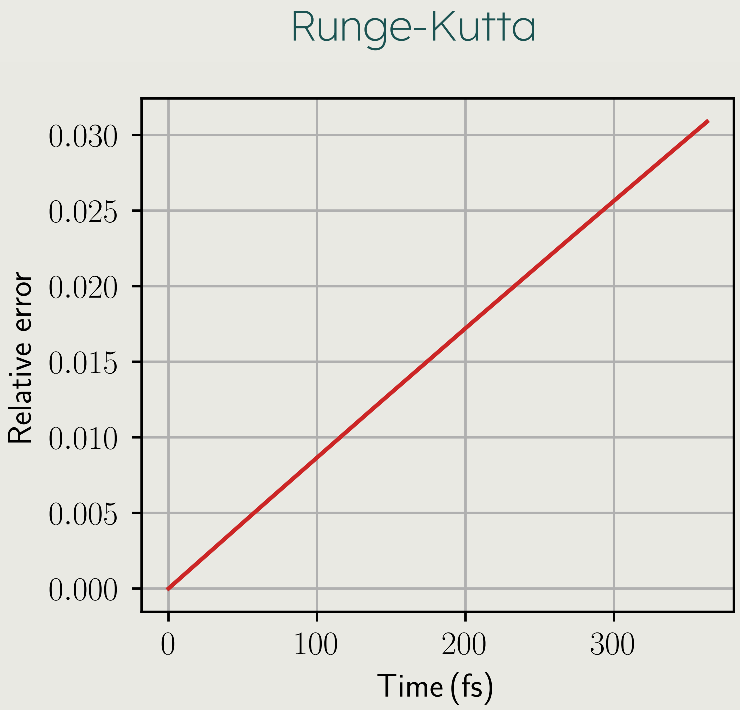
Analytical solution available!

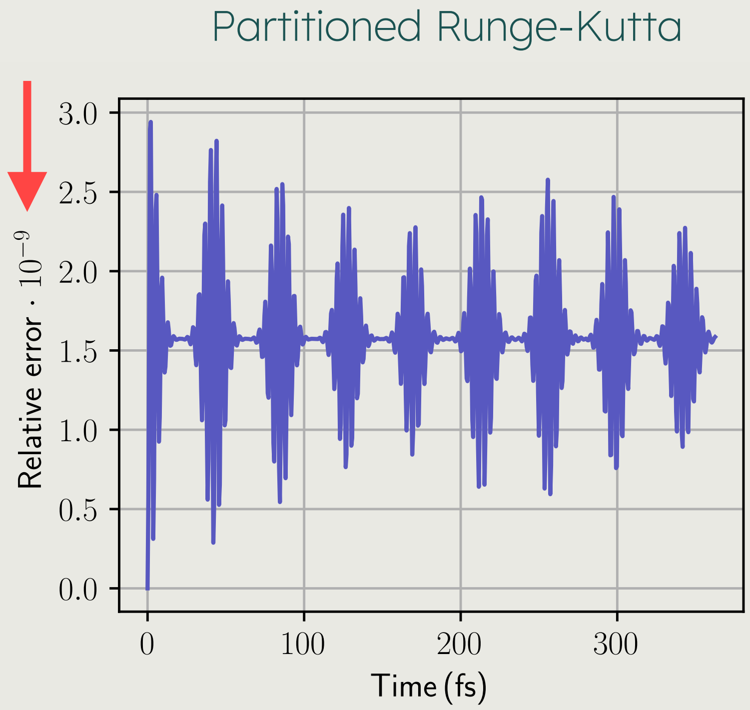


→ Constructed numerical method is fourth-order accurate

Validation

Conservation of mass





→ **Constructed numerical method is conservative**

Application: interconnect bend

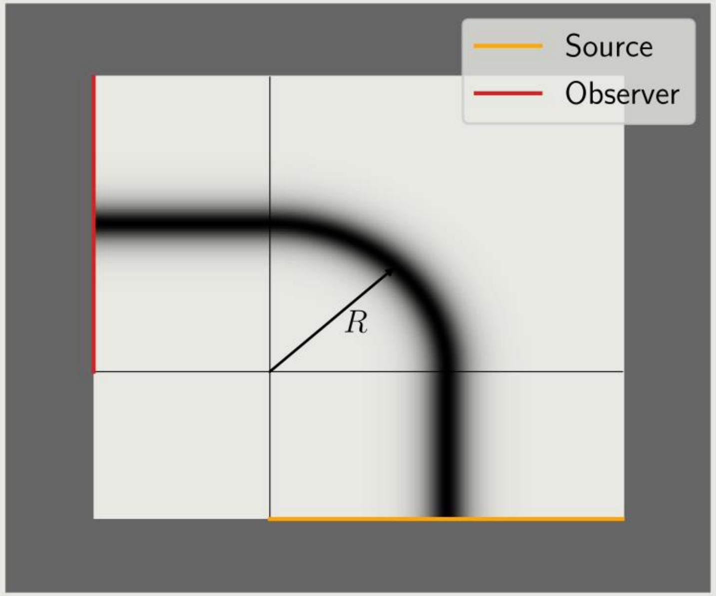
Simulation setup

Hyperbolic secant potential $V(x, y) = -\frac{V_0}{\cosh(\beta x)}$ with $\beta = \frac{2 \operatorname{arccosh}(2)}{W}$ and W the full width at half maximum

Simulation domain terminated by absorbing boundary conditions

Time dependence of incoming mode $e^{-iEt/\hbar}$ modulated with additional gaussian $1/\sqrt{2\pi\sigma_t} e^{(t-t_0)^2/(2\sigma_t)^2}$

Calculating transmission by means of Fast Fourier Transform

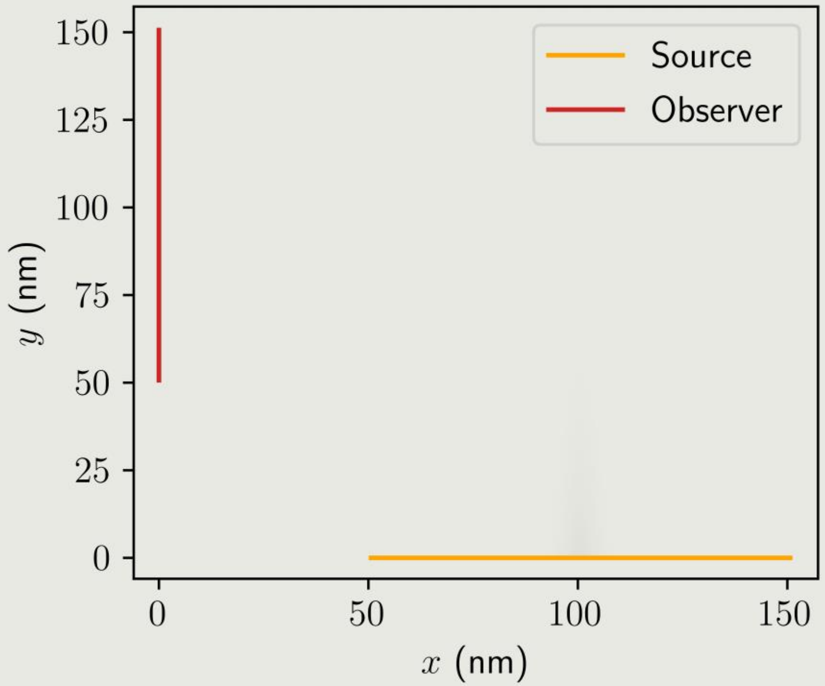


Application: interconnect bend

Snapshots

Parameters

- Potential width W: 8 nm
- Potential depth V_0: 0.25 eV
- Energy E: 0 eV
- Radius R: 50 nm



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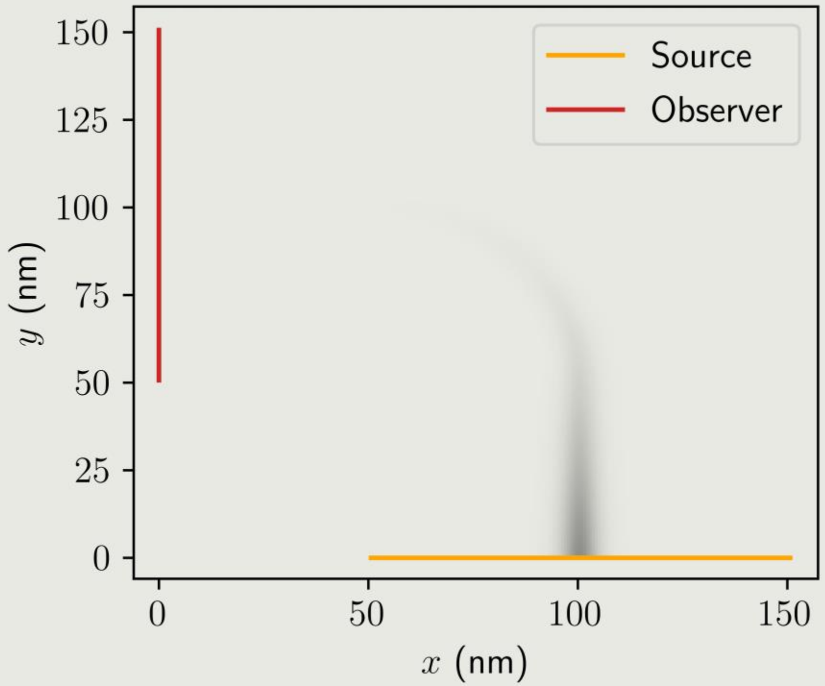

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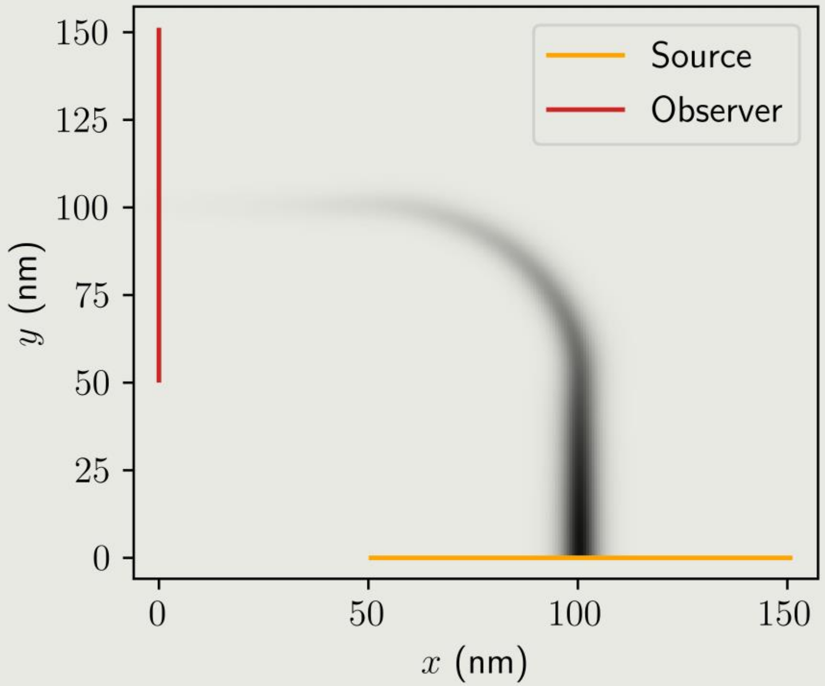

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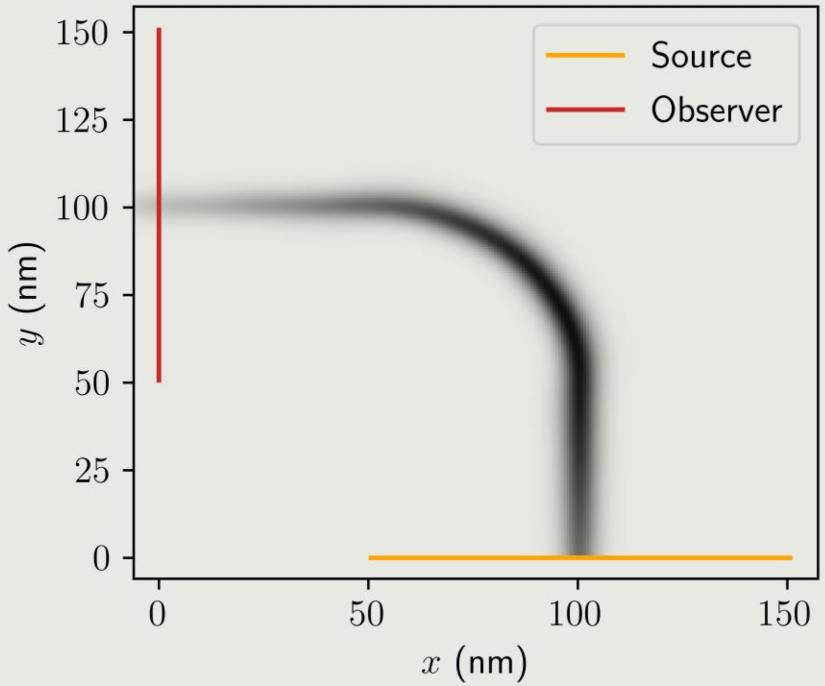

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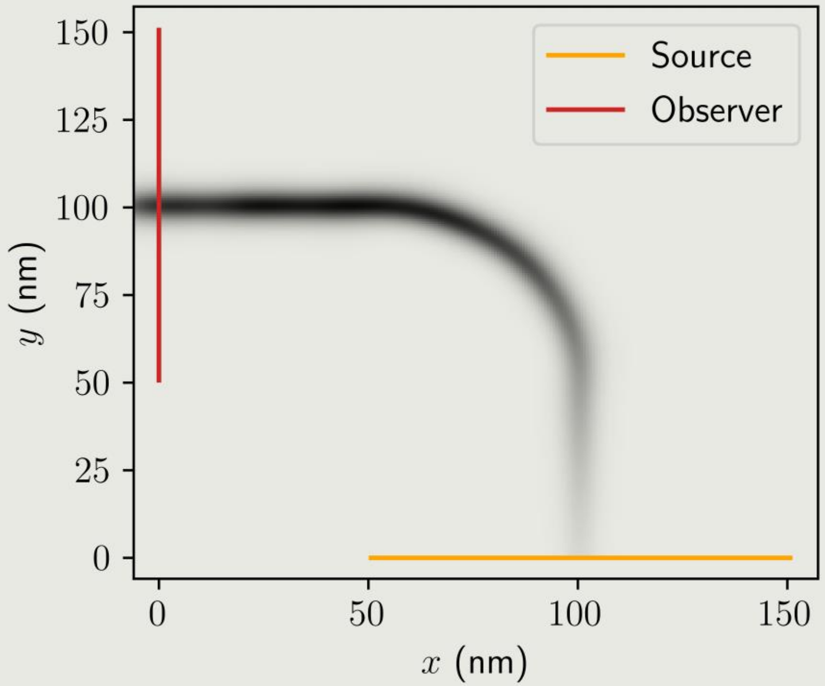

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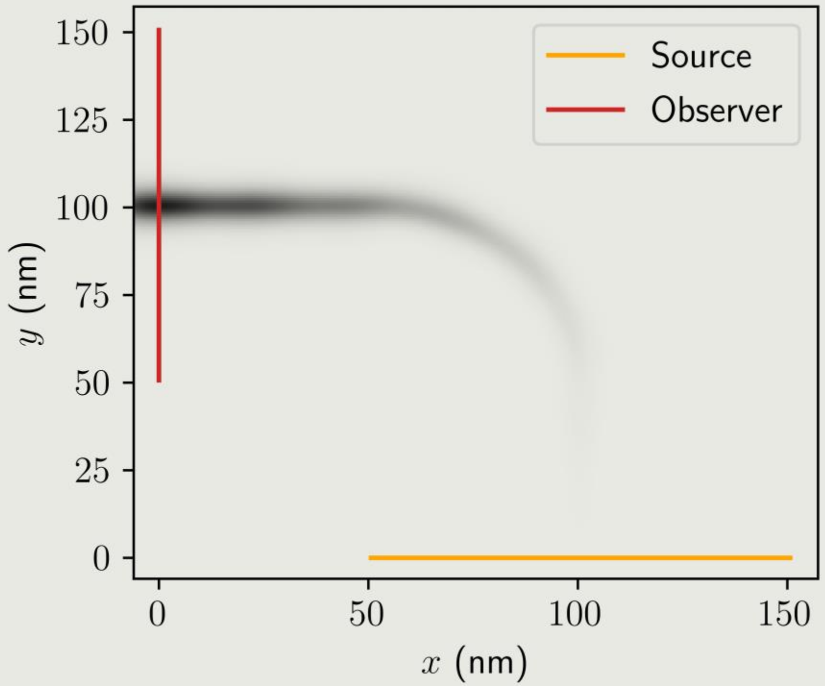

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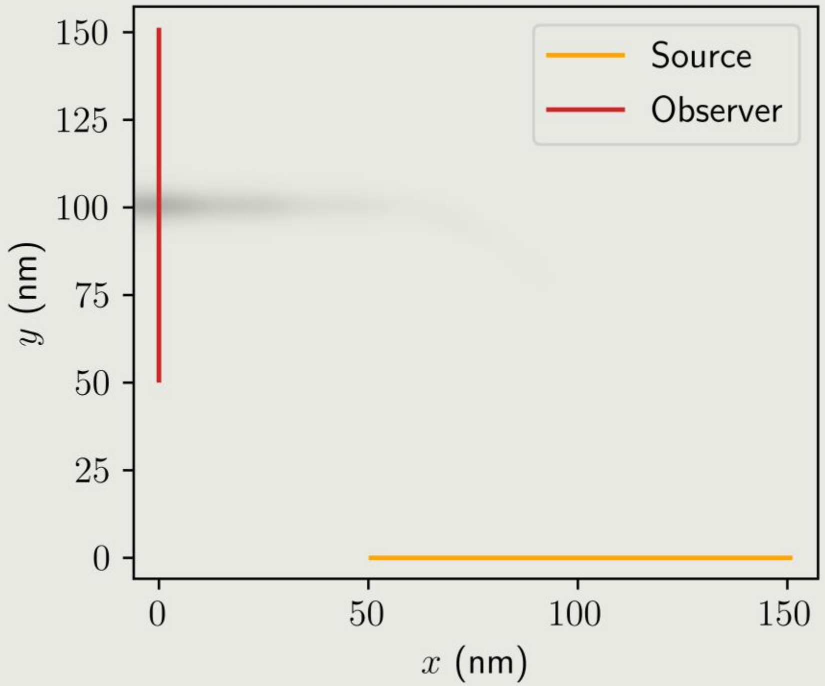

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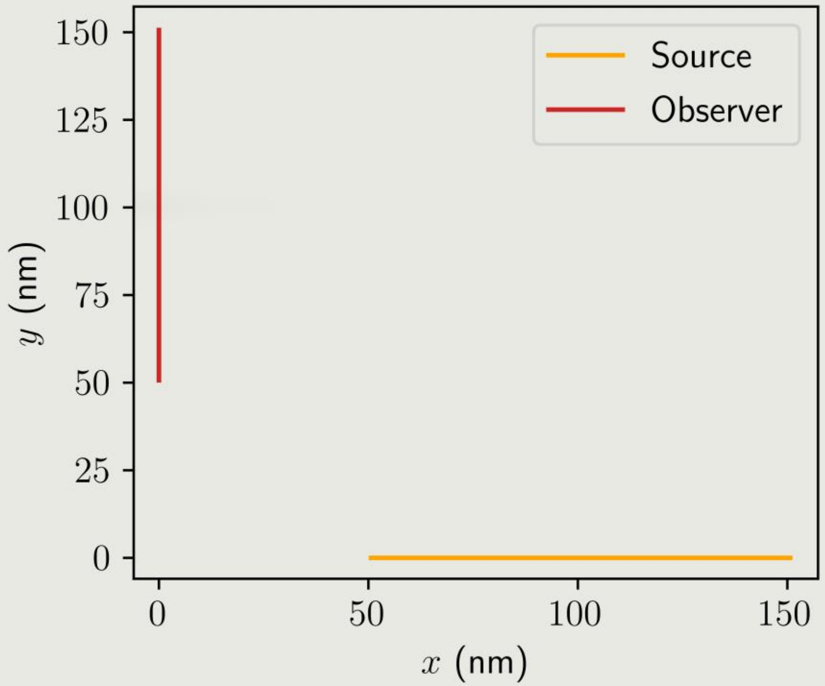


Application: interconnect bend

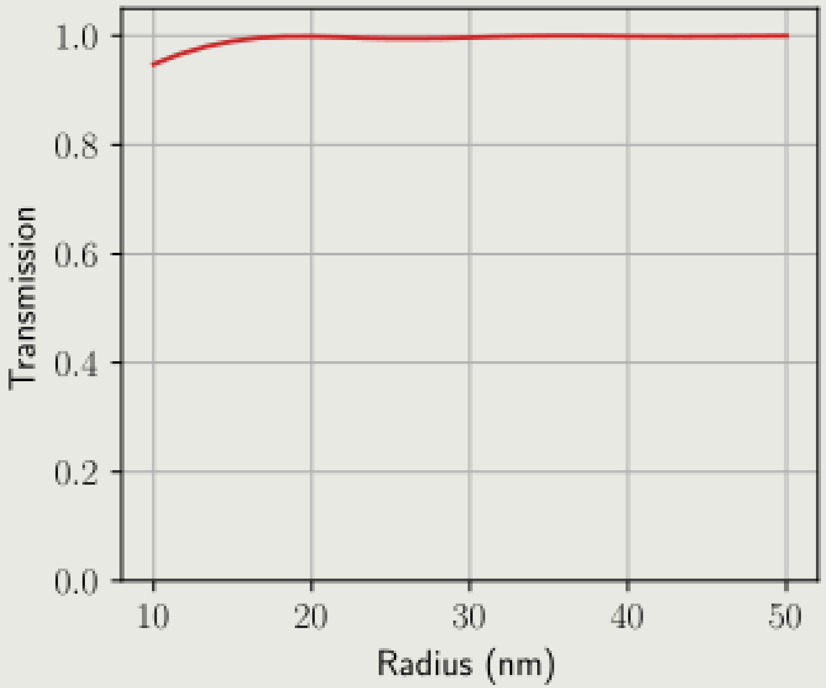
Transmission as a function of the radius

Parameters

- Potential width W: 8 nm
- Potential depth V_0: 0.25 eV
- Energy E: 0 eV

Transmission equals one for large radius

→ **No additional, spurious dissipation**



Application: interconnect coupler

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Hyperbolic secant potential $V(x,y) = -\frac{V_0}{\cosh(\beta x)}$ with $\beta = \frac{2\,\text{arccosh}(2)}{W}$ and W the full width at half maximum

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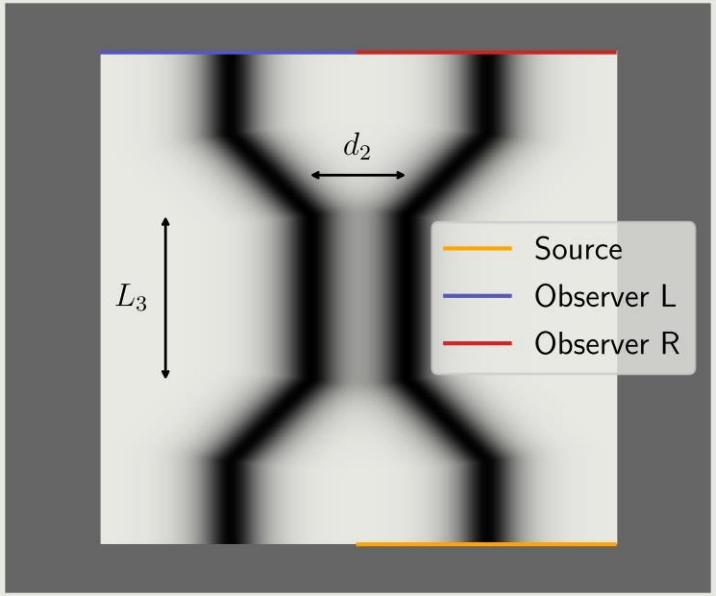


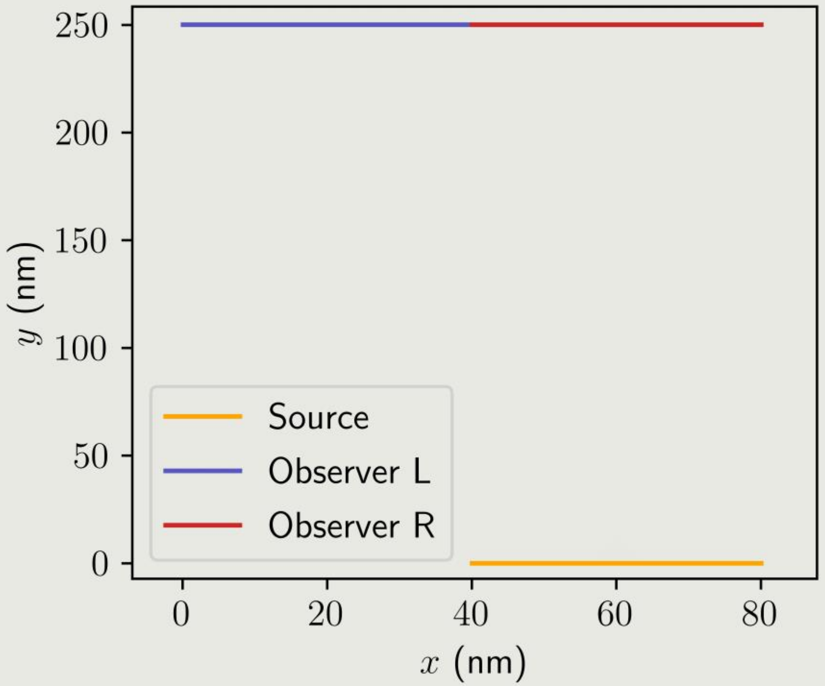
Application: interconnect coupler

Snapshots

Parameters

- Potential width W: 8 nm
- Potential depth V_0: 0.25 eV
- Energy E: 0 eV
- Length coupling region L_3: 150 nm
- Distance interconnects coupling region d_2: 15 nm

Transfer of mass from right to left waveguide



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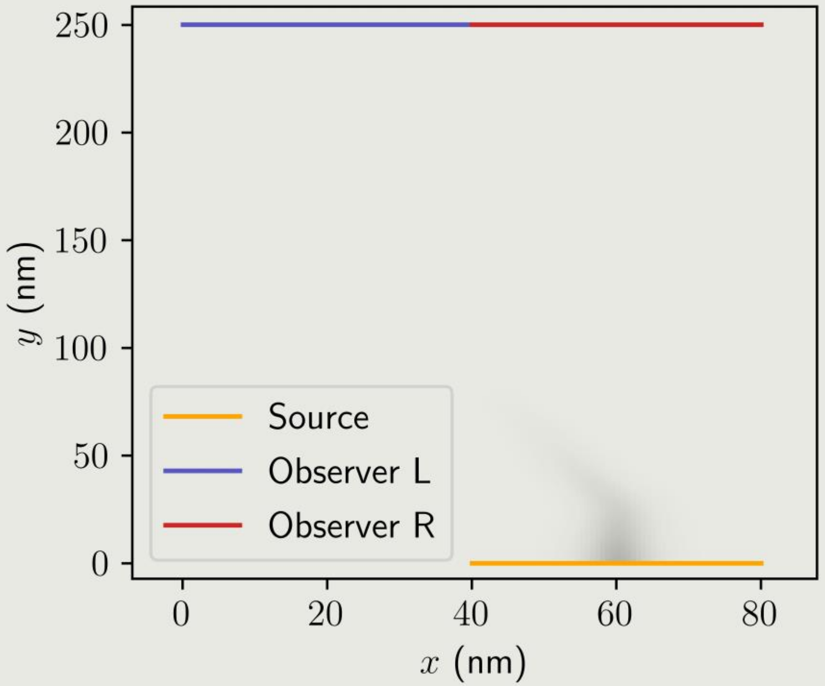

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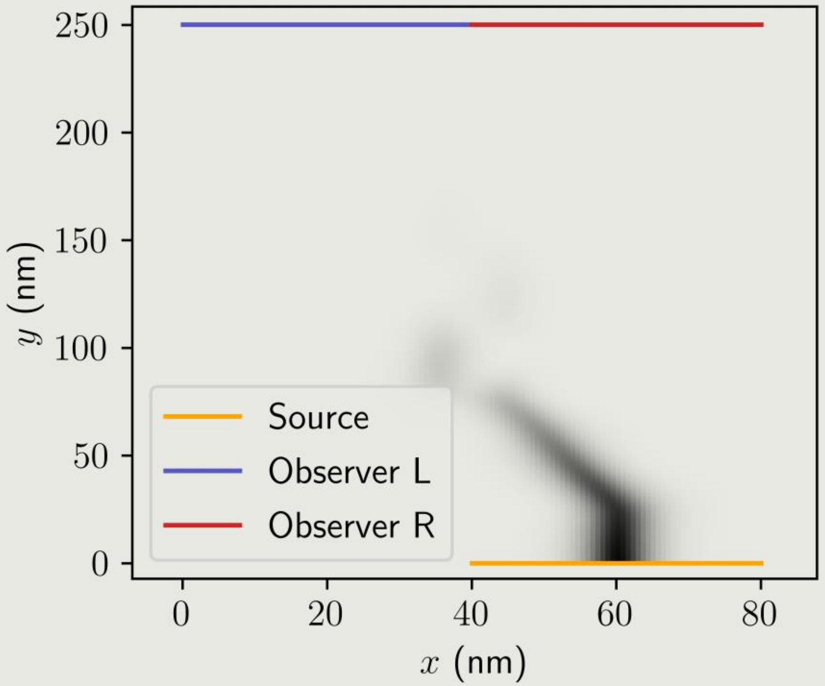

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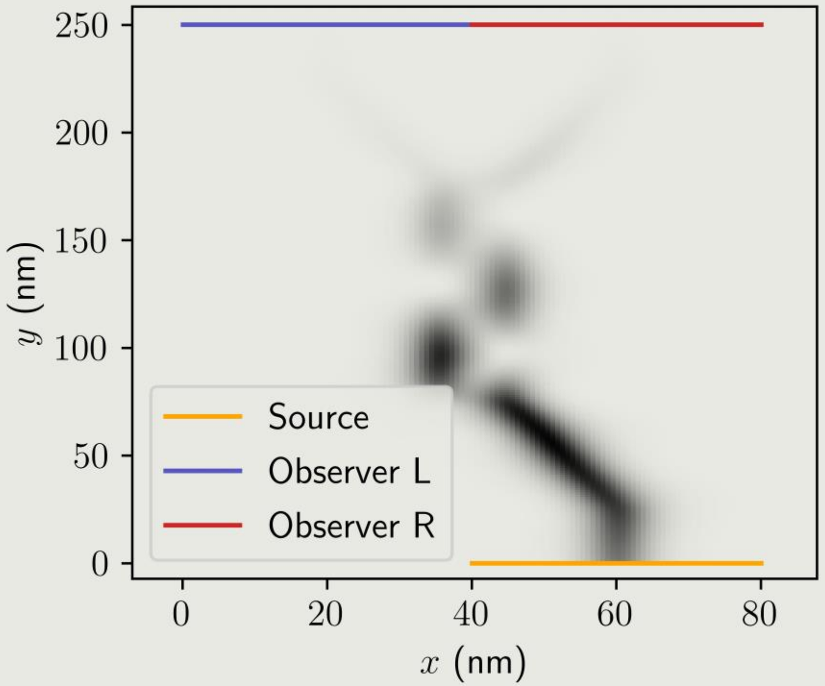

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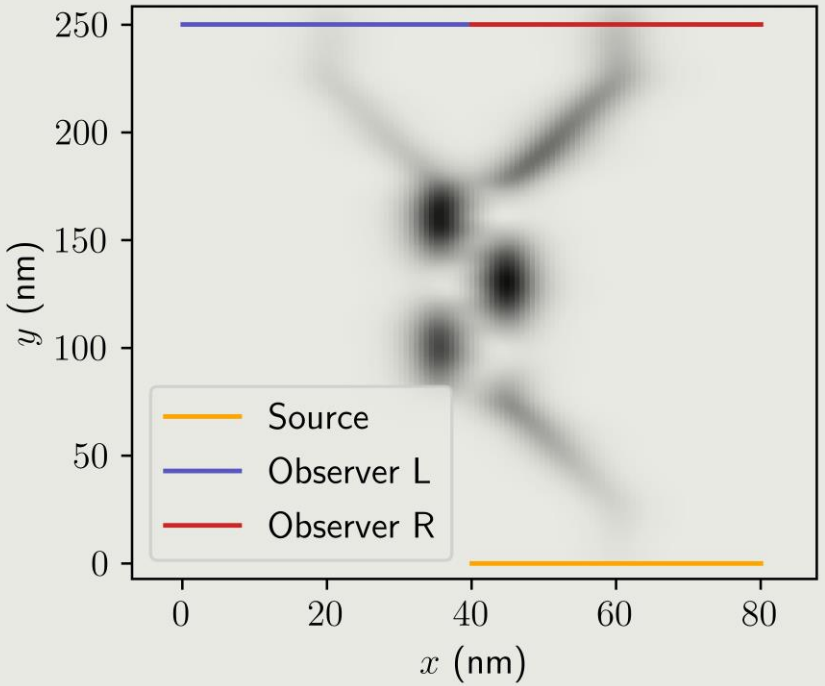

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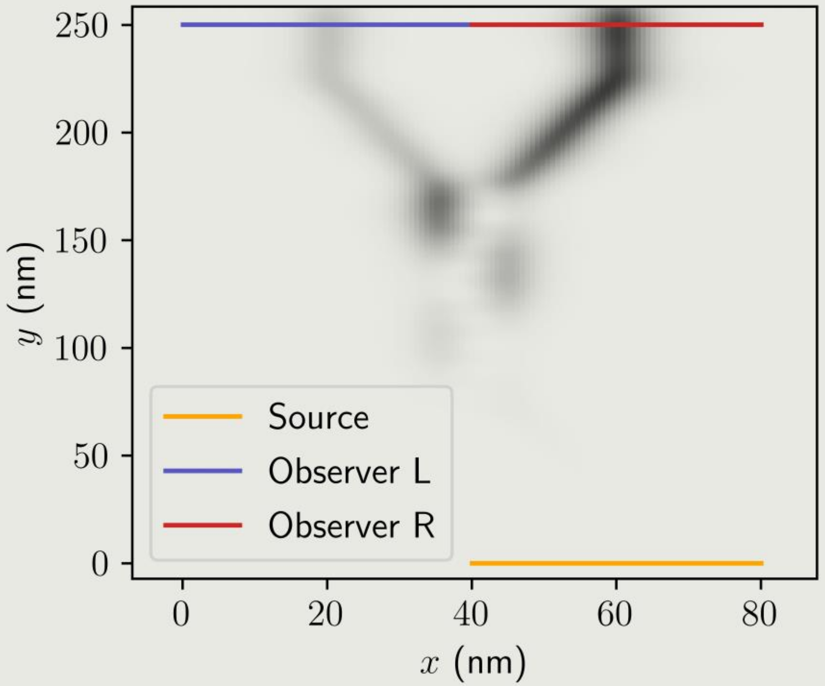

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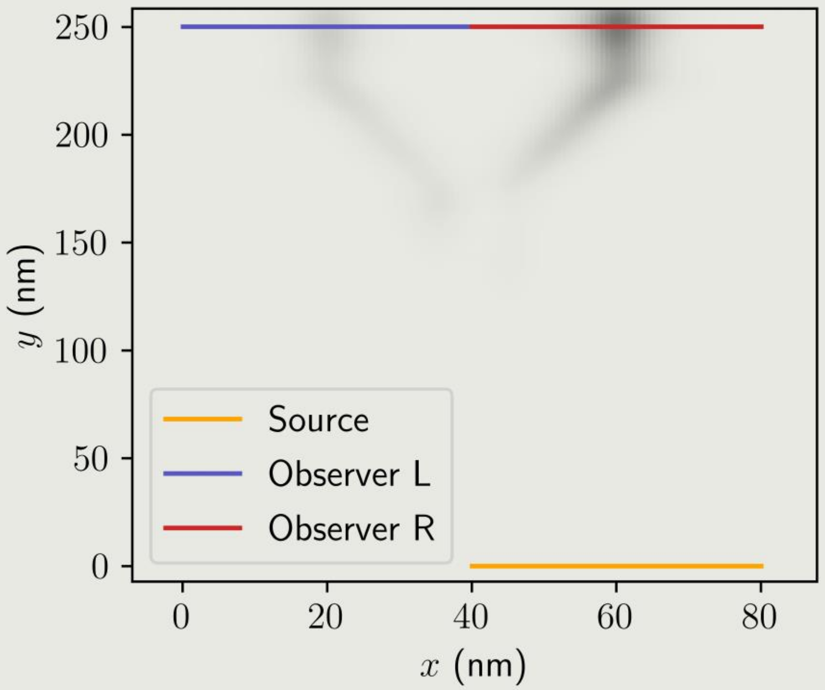

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Snapshots

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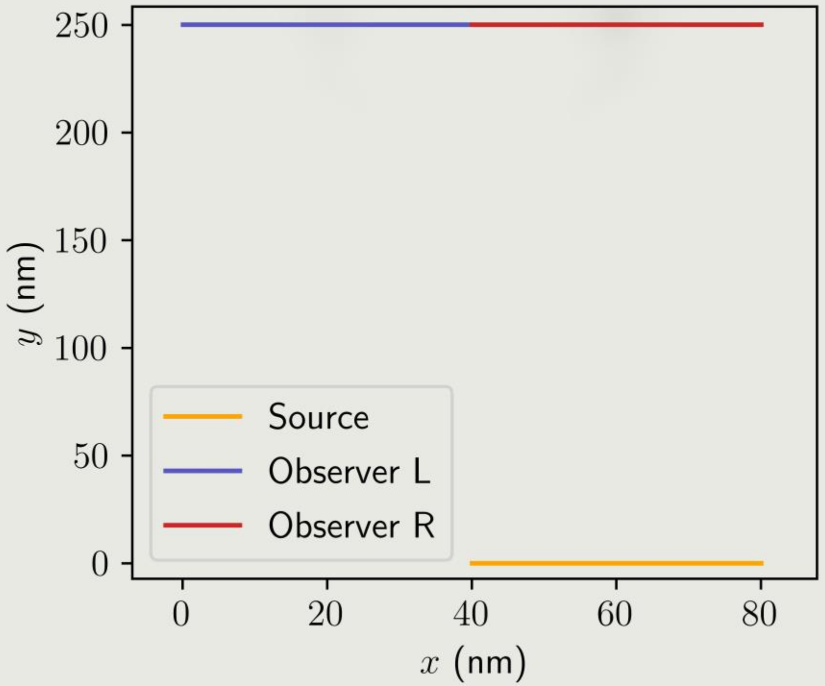


Application: interconnect coupler

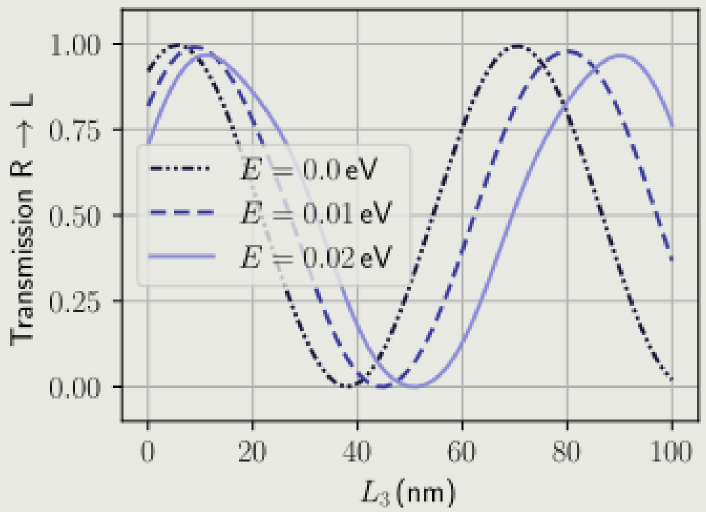
Transmission as a function of the length of the coupling region

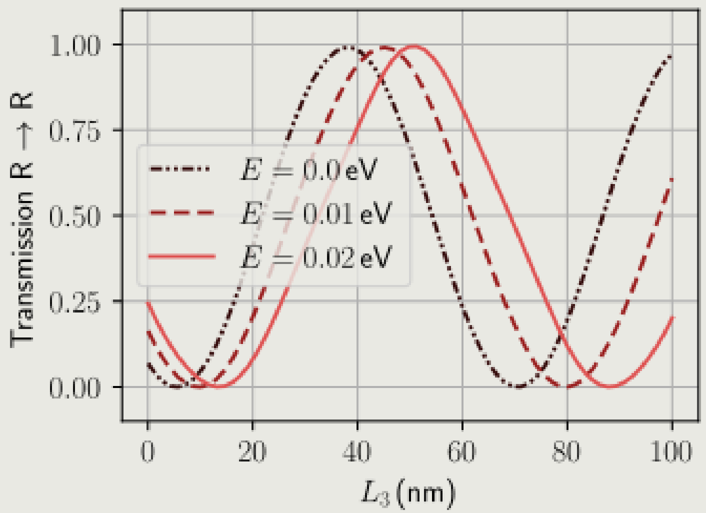
Parameters

- Potential width W: 8 nm
- Potential depth V_0: 0.25 eV
- Distance interconnects coupling region d_2: 15 nm

Transmission oscillates as a function of the length of the coupling region

Larger energy E results in larger oscillation period





Application: interconnect coupler

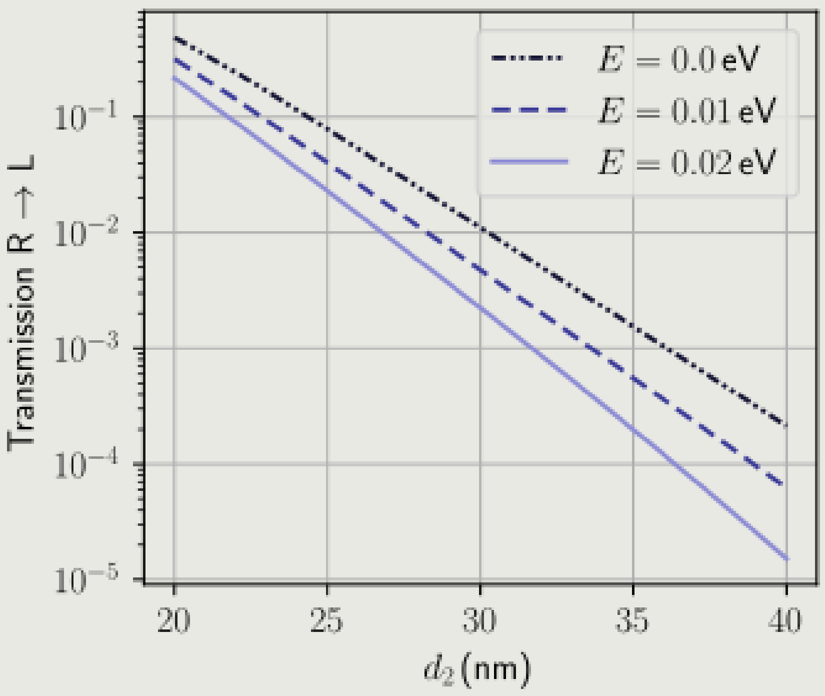
Transmission as a function distance between interconnects

Parameters

- Potential width W: 8 nm
- Potential depth V_0: 0.25 eV
- Length coupling region L_3: 100 nm

Transmission decreases exponentially with d_2, the distance between the interconnects in the coupling region

Larger energy E results in weaker coupling



Conclusion

Besides CNTs and GNRs, **electrostatically induced interconnects in graphene** are a possible alternative for Cu in future interconnects

Novel simulation technique for (2+1)D Dirac equation based on partitioned Runge-Kutta timestepping

Comparison with analytical solution showed that method is **fourth-order accurate and conservative**

Numerical method was employed to **analyze interconnect structures such as bends and couplers**

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