Two aspects of Klein tunneling in graphene: supersymmetry and Dirac structure beyond the linear approximation

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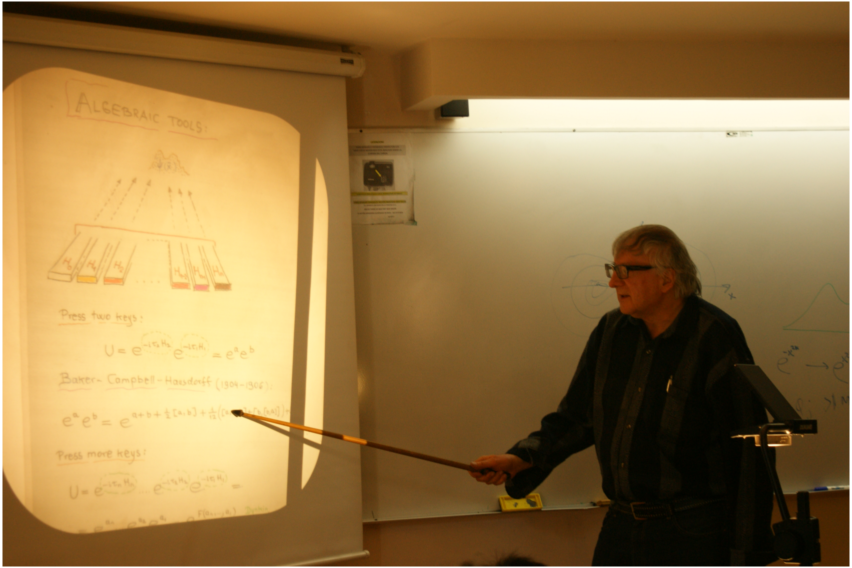
In honor of prof. Bogdan Mielnik



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- A. Contreras-Astorga, F. Correa, V. Jakubský, Phys. Rev. B. 102, 115429 (2020)

- N.A. Shah, A. Contreras-Astorga,F. Fillion-Gourdeau, M. A. H Ahsan, S. MacLean, M. Faizal, Phys. Rev. B 105, L161401 (2022).

Klein tunneling in graphene

Graphene is a 2D material made of a single-atom layer of carbon. In a tight binding model of graphene, the dispersion relation, expanded to the second order in $|k|a$, with the next to nearest neighbor hopping $t^{'}$ is given by

$$\epsilon_k^\lambda = -3t^{'} + \lambda\hbar v_F k + \frac{9a^2}{4} t^{'} k^2 - \lambda \frac{\hbar v_F k^2 a}{4} \cos(3\phi_k).$$

Then, at low energies and adding a potential term, the charge carriers are modeled by the 2D Dirac equation

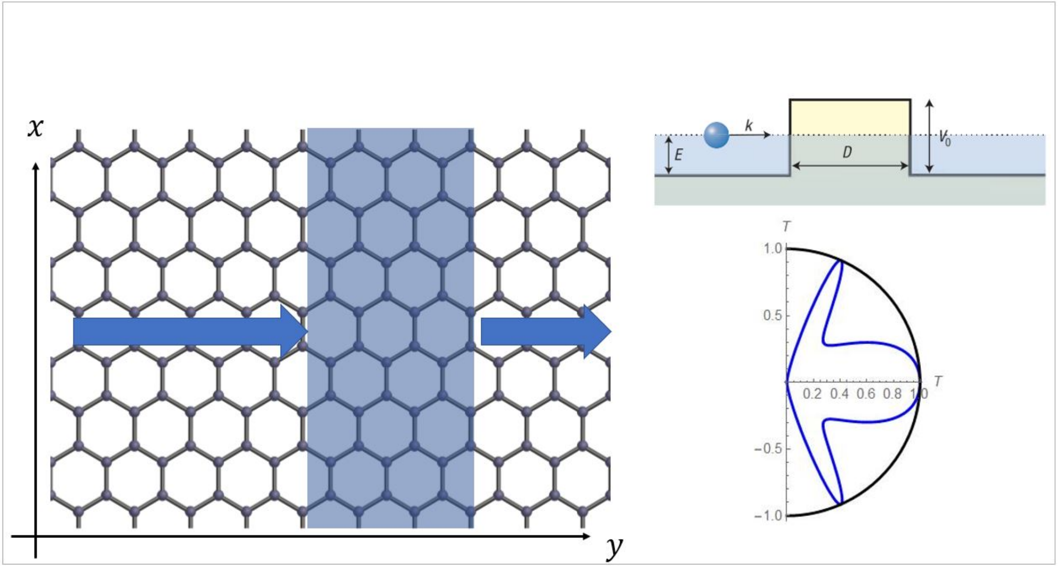
$$(\sigma \cdot \mathbf{p} + \mathbf{V})\,\psi(x,y) = (-i\sigma_1 \partial_x - i\sigma_2 \partial_y + \mathbf{V}(x,y))\,\psi(x,y) = E\psi(x,y)$$

where

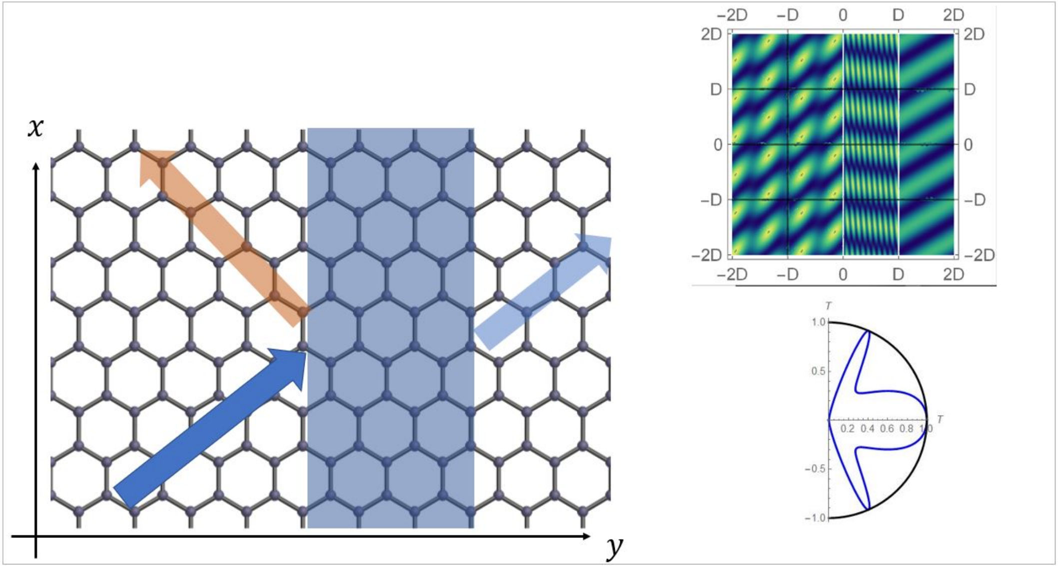
$$\mathbf{V}(x,y) = \sigma_0 \mathcal{V}_0(x,y) + \sigma_1 \mathcal{V}_1(x,y) + \sigma_2 \mathcal{V}_2(x,y) + \sigma_3 \mathcal{V}_3(x,y).$$

Our first goal is to construct an electric potential barrier $\mathcal{V}_0(x,y)$ with omnidirectional perfect transmission at specific energy (super - Klein tunneling).

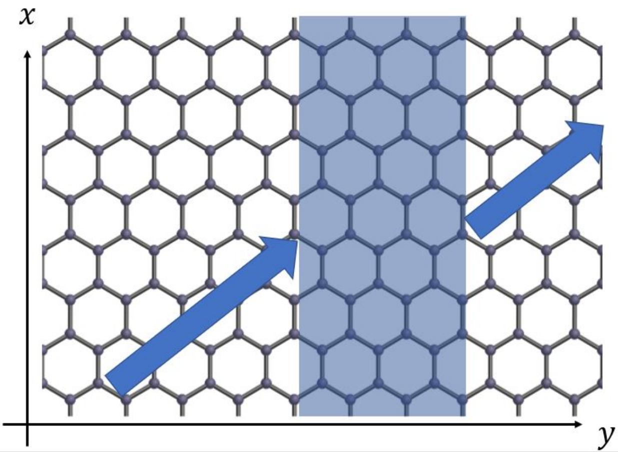
Klein tunneling in graphene

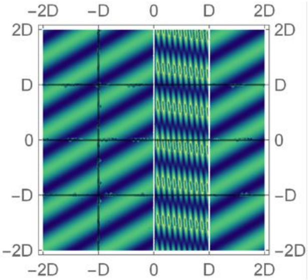


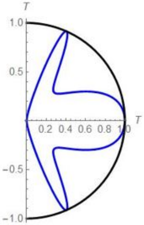
Klein tunneling in graphene



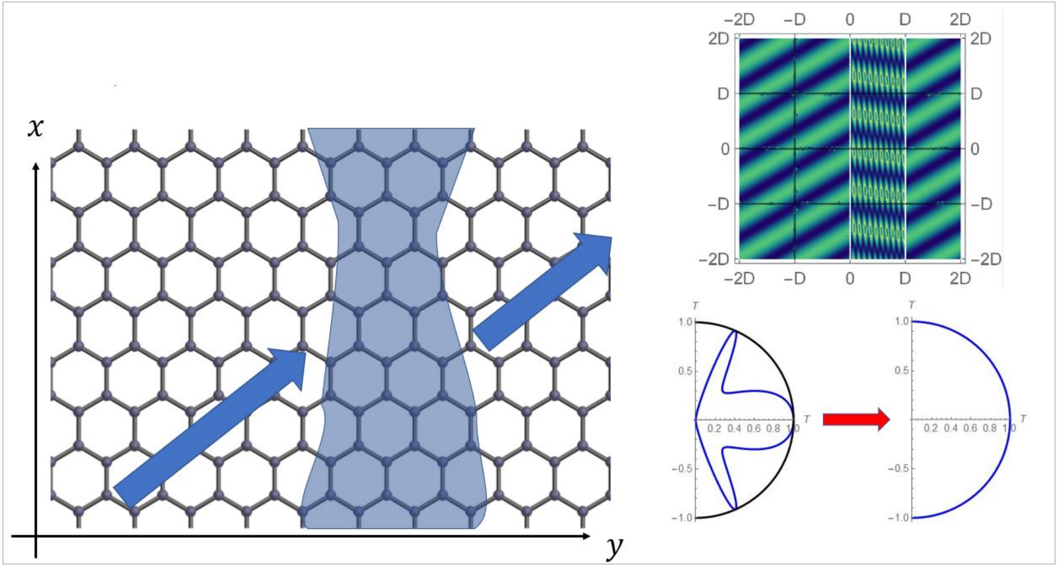
Klein tunneling in graphene



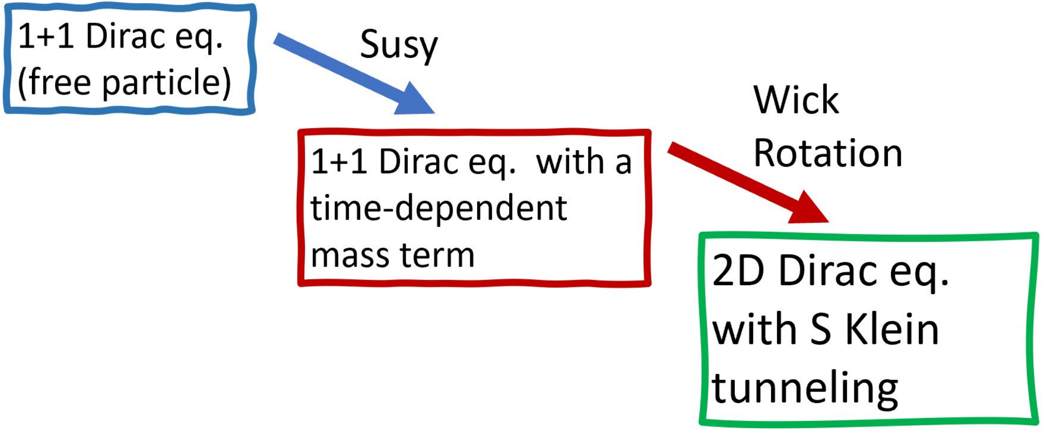




Super-Klein tunneling in graphene



Super-Klein tunneling in graphene



Time-dependent susy transformations

It relies on the operator L that intertwines the operator H_0, with an operator H_1 that represents the new quantum system,

$$LH_0 = H_1 L.$$

Let us use it with a $1+1$ Dirac operator $H_0\psi = (i\partial_t - i\sigma_2\partial_z - \mathbf{V}_0(z,t))\psi = 0$. Susy is based on the choice of two vectors u_1, u_2 that are solutions of $H_0 u_j = 0$. We can use them to compose a matrix $\mathbf{u} = (u_1, u_2)$ that also satisfies

$$H_0\mathbf{u} = 0.$$

Once the matrix $\mathbf{u}$ is fixed, the operators L and H_1 are

$$L = \partial_z - \mathbf{u}_z\mathbf{u}^{-1}, \quad H_1 \quad = \quad H_0 - i[\sigma_2, \mathbf{u}_z\mathbf{u}^{-1}].$$

Given a solution ψ of $H_0\psi = 0$, the spinor $\phi = L\psi$, will be a solution of $H_1\phi = 0$.

Wick rotation

Let us have the initial equation in the following form,

$$H\psi = (i\partial_t - i\sigma_2\partial_z - \mathbf{V}(z,t))\psi = 0,$$

where the matrix potential $\mathbf{V}(z,t)$ is supposed to be Hermitian.
By using the following change of the coordinates

$$z = ix, \quad \partial_z = -i\partial_x, \quad t = y, \quad \partial_t = \partial_y.$$

then multiplying by σ_3 from the left and making the rotation $\mathbf{U} = e^{i\frac{\pi}{4}\sigma_1}$, we get the following 2D stationary equation for zero energy in terms of x and y,

$$\widetilde{H}(x,y) = (-i\sigma_1\partial_x - i\sigma_2\partial_y + \widetilde{\mathbf{V}}(x,y))\widetilde{\psi}(x,y) = 0$$

with the potential term $\widetilde{\mathbf{V}}(x,y) = \mathbf{U}\sigma_3\mathbf{V}(ix,y)\mathbf{U}^{-1}$.

Wick rotation

A few comments are in order.

- This transformation can render the Dirac operator $\widetilde{H}$ non-Hermitian in general.
- The transformation also makes profound changes into the character of the potential term. With

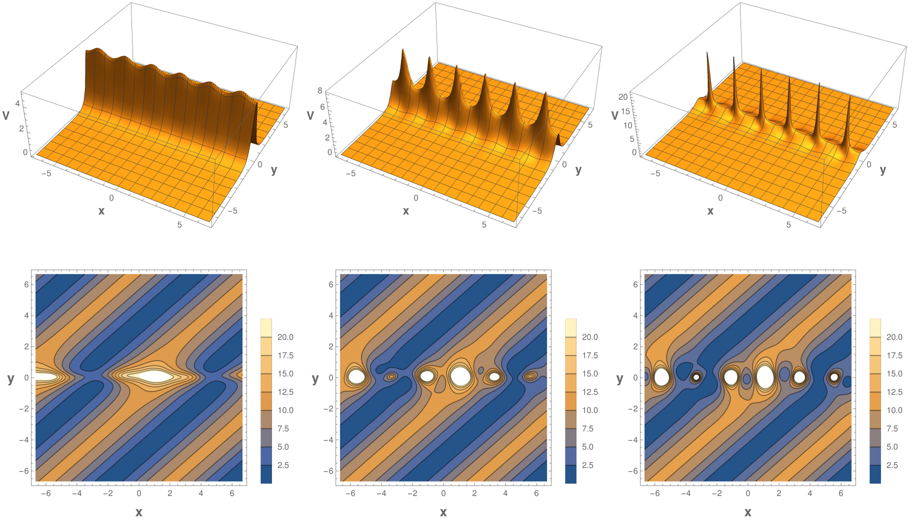
$$\mathbf{V}(z,t) = \sigma_0 \mathcal{V}_0(z,t) + \sigma_1 \mathcal{V}_1(z,t) + \sigma_2 \mathcal{V}_2(z,t) + \sigma_3 \mathcal{V}_3(z,t).$$

  we get

$$\widetilde{\mathbf{V}}(x,y) = \sigma_0 \mathcal{V}_3(ix,y) - i\sigma_1 \mathcal{V}_2(ix,y) + \sigma_2 \mathcal{V}_0(ix,y) - i\sigma_3 \mathcal{V}_1(ix,y).$$

  In particular, the mass term turns into the electrostatic potential.
- The Wick rotation describes the system at a single energy.

Example: Super-Klein tunneling



$c_1 = 2, \; c_2 = 1$ $\qquad$ $c_1 = 0.2, \; c_2 = 0.1$ $\qquad$ $c_1 = 0.04, \; c_2 = 0.02$

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Dirac structure beyond the linear approximation

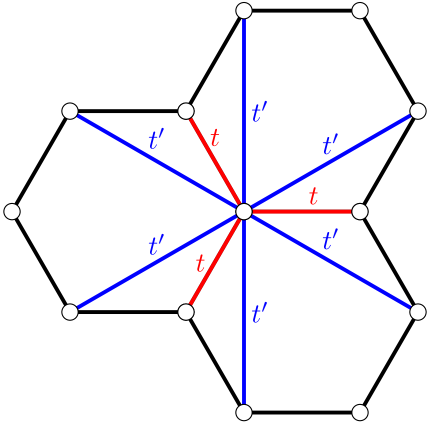


Figure: Graphene hexagonal lattice with nearest (t) and next-to-nearest (t') hopping energies.

Graphene's dispersion relation, expanded to the second order in $|k|a$, with the next to nearest neighbor hopping t' is given by

$$\epsilon_k^{\lambda} = -3t' + \lambda\hbar v_F k + \frac{9a^2}{4} t' k^2 - \lambda\frac{\hbar v_F k^2 a}{4}\cos(3\phi_k).$$

Our second goal is to investigate the effect of next-to-the-nearest atom hopping on Klein tunneling in graphene.

Dirac structure beyond the linear approximation

The Hamiltonian operator becomes:

$$\hat{H} = v_F \left[\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}} - \alpha(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}})(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}})\right] = v_F \left[\boldsymbol{\sigma} \cdot \hat{\boldsymbol{p}} - \alpha \hat{p}^2 \sigma_0\right].$$

To study Klein tunnelling, we consider free waves scattering on a $n - p - n$ junction. Thus, an electric static barrier potential $V(x) = V_0 \Theta(x) \Theta(D - x)$, where D is the potential length, is introduced in the GDS resulting in

$$\begin{aligned}\hat{H}\, \Psi(\boldsymbol{r}) &= \left\{ v_F \left[-i\hbar \boldsymbol{\sigma} \cdot \nabla + \alpha \hbar^2\, \sigma_0\, \nabla^2 \right] + V(x) \right\} \Psi(\boldsymbol{r}) \\ &= E_G\, \Psi(\boldsymbol{r}).\end{aligned}$$

Dirac structure beyond the linear approximation

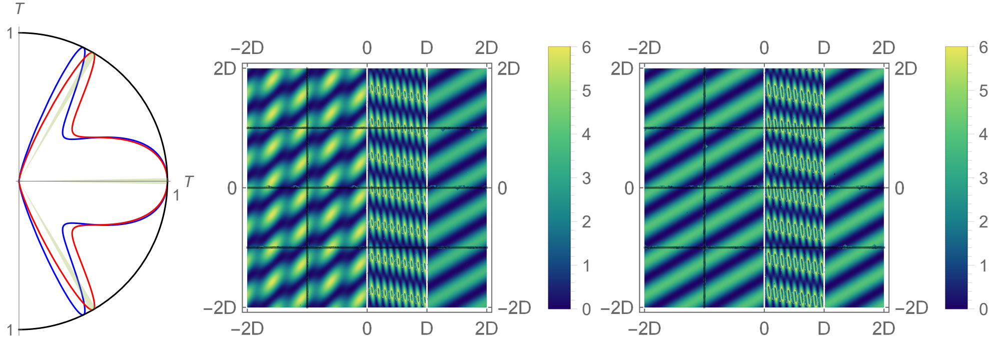


Figure: **Left**: Transmission probability T vs T_G. **Center**: Probability density in the $x-y$ plane of the superposition of two plane waves, $\Phi = \Psi(k_0, 0) + \Psi(k_0, \pi/3)$, considering only the linear regime. **Right**: $||\Phi||^2$ using the Generalized Dirac structure.

Dirac structure beyond the linear approximation

The dispersion relation for massless particles in many quantum gravity models is of the form $\epsilon_{\mathrm{grav},\boldsymbol{p}} = F(p)$, where F is usually a polynomial. One particular model has been extensively studied in which the dispersion relation is given by

$$\epsilon_{\mathrm{grav},\boldsymbol{p}} = c_1 p + c_2 p^2,$$

where $c_{1,2}$ are some coefficients.
We make a connection between graphene and quantum gravity models by neglecting the trigonal warping term. The energy becomes

$$\epsilon_{\boldsymbol{p}}^{\lambda} = v_F \left(\lambda p - \alpha p^2\right),$$

where $\alpha = \frac{3}{2}\frac{|t'|}{t}\frac{a}{\hbar} > 0$. Obviously, this has the same form as $\epsilon_{\mathrm{grav},\boldsymbol{p}}$ with the connection provided by the mapping $c_1 \to v_F \lambda$ and $c_2 \to -v_F \alpha$.

Dirac structure beyond the linear approximation

The mathematical structure of graphene is consistent with the framework of the generalized uncertainty principle (GUP). In this framework, one postulates the existence of generalized position and momentum operators $\hat{\boldsymbol{X}}$, $\hat{\boldsymbol{P}}$ that obey a modified commutation relation:

$$[\hat{X}_i, \hat{P}_j] = i\hbar \left[\delta_{ij} - \alpha \left(\delta_{ij}\hat{P} + \frac{\hat{P}_i\hat{P}_j}{\hat{P}}\right)\right].$$

These relations imply a minimal measurable length $(\Delta x)_{\min} \sim \hbar\alpha$ and a maximal measurable momentum $(\Delta p)_{\min} \sim \alpha^{-1}$.
In graphene, the generalized commutation relations is fullfilled by

$$\hat{\boldsymbol{X}} = \hat{\boldsymbol{x}} \quad \text{and} \quad \hat{\boldsymbol{P}} = \hat{\boldsymbol{p}}(1 - \alpha\hat{p}),$$

with $[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij}$. The operators $\hat{\boldsymbol{X}}$, $\hat{\boldsymbol{P}}$ can be interpreted as the high-energy position and momentum, respectively, while $\hat{\boldsymbol{x}}$, $\hat{\boldsymbol{p}}$ are their low-energy counterparts.

Summary

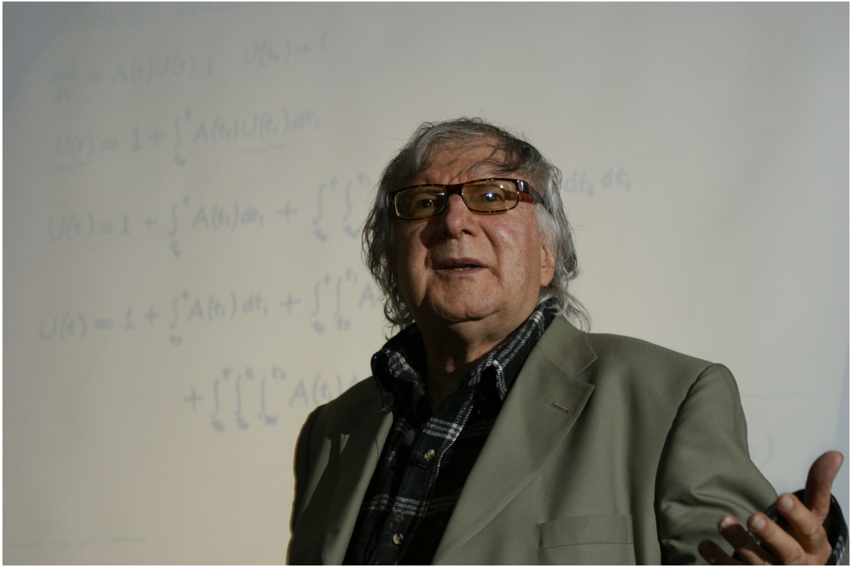
- We presented a technique to obtain a truly 2D electrostatic barrier that presents the Super-Klein tunneling phenomenon. The incident wave bounces on the barrier. However, for an specific energy, the interference is such that the reflected wave gets completely annihilated and the waves incoming from any direction get perfectly transmitted up to a phase shift.

- We studied the effect of next-to-the-nearest atom hopping on quantum transport in graphene. The effective quantum dynamics obtained was used to obtain an emergent generalized Dirac structure, which captured the effects of discrete topology and which is reminiscent of Lorentz-breaking quantum gravity models.

- It was proposed that such effects can be tested by measuring transmittance through $n-p-n$ graphene junctions using a pump-probe experiment.

- Graphene can be used as an analogue for Lorentz violating phenomena, which remain very elusive in high-energy particle physics experiments.

Thank you professor Bogdan Mielnik



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