9.º Congresso do Comité Português da URSI
Lisboa 04/12/2015

INSTITUIÇÕES ASSOCIADAS

Diffractionless Propagation of Electron Waves in Graphene Superlattices

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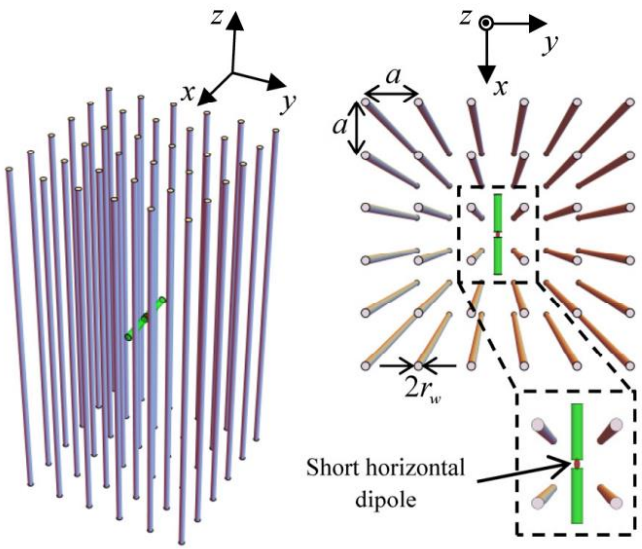
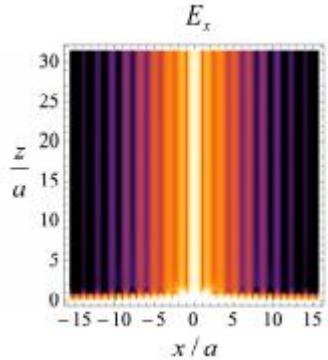
instituto de telecomunicações

Optical anisotropy

Super collimation of the radiation

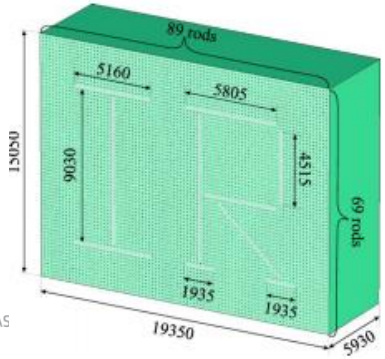




T. A. Morgado, M. G. Silveirinha, *http://arxiv.org/abs/1511.06714*

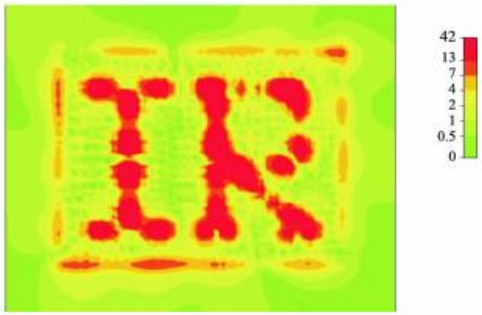
Increased Directionality!

Sub-wavelength imaging



Source Plane

Image Plane



Mário G. Silveirinha, Pavel A. Belov, and Constantin R. Simovski, *Phys. Rev. B* **75**, 035108, 2007

dfernandes@co.it.pt

Electronic anisotropy

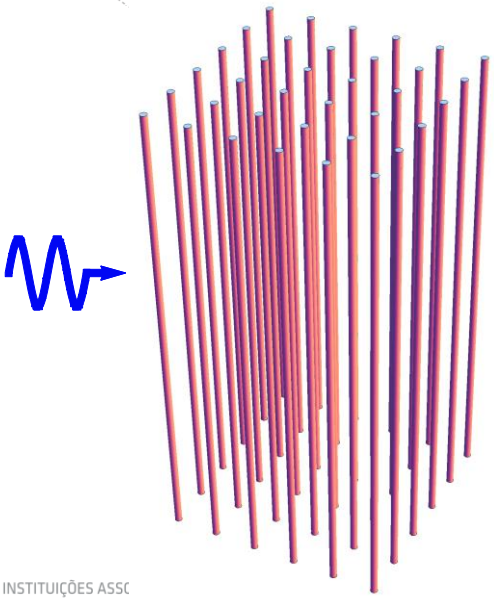
Maxwell Equations

$$\frac{\partial \mathbf{B}(\mathbf{r},t)}{\partial t} + \nabla \times \mathbf{E}(\mathbf{r},t) = 0$$

$$\varepsilon_0 \frac{\partial \mathbf{E}(\mathbf{r},t)}{\partial t} + \nabla \times \mathbf{H}(\mathbf{r},t) = \mathbf{J}_t(\mathbf{r},t)$$

Schrödinger Equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi(\mathbf{r},t) = i\hbar\frac{\partial \psi(\mathbf{r},t)}{\partial t}$$

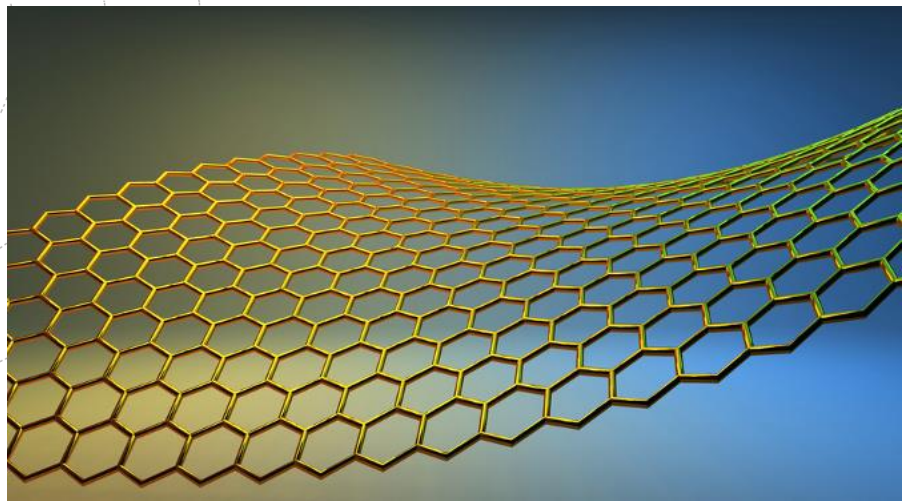


Can we obtain the same phenomena for electrons in graphene based-nanostructures?

http://tinyurl.com/pbnhz92

Graphene

Graphene: a two dimensional carbon based material!



http://tinyurl.com/pbpcuku

KUNGL. VETENSKAPS-AKADEMIEN
THE ROYAL SWEDISH ACADEMY OF SCIENCES

THE NOBEL PRIZE IN PHYSICS 2010

INFORMATION FOR THE PUBLIC

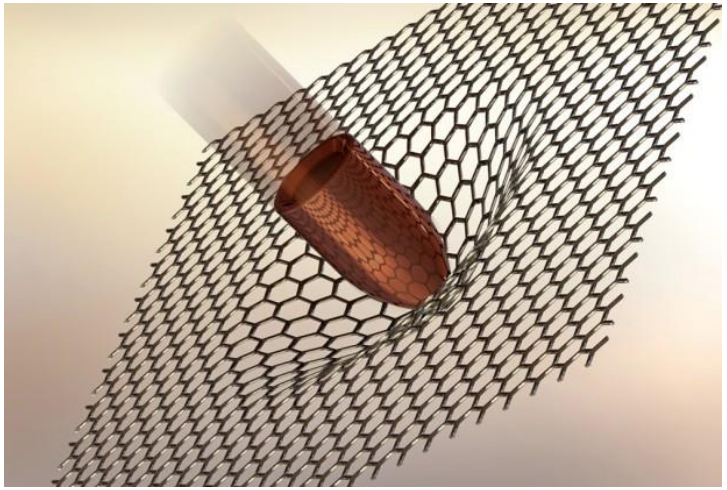
The Nobel Prize in Physics 2010 was awarded jointly to Andre Geim and Konstantin Novoselov *"for groundbreaking experiments regarding the two-dimensional material graphene"*

Special Properties of Graphene

- **Flexible and light, yet stronger than steel!!**

Dynamic mechanical behavior of multilayer graphene via supersonic projectile penetration

Jae-Hwang Lee[1,2,*], Phillip E. Loya[1], Jun Lou[1], Edwin L. Thomas[1,*]

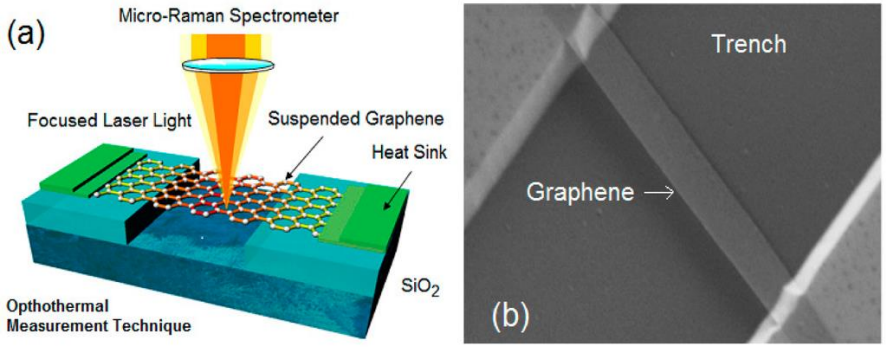


http://tinyurl.com/oy6zovh

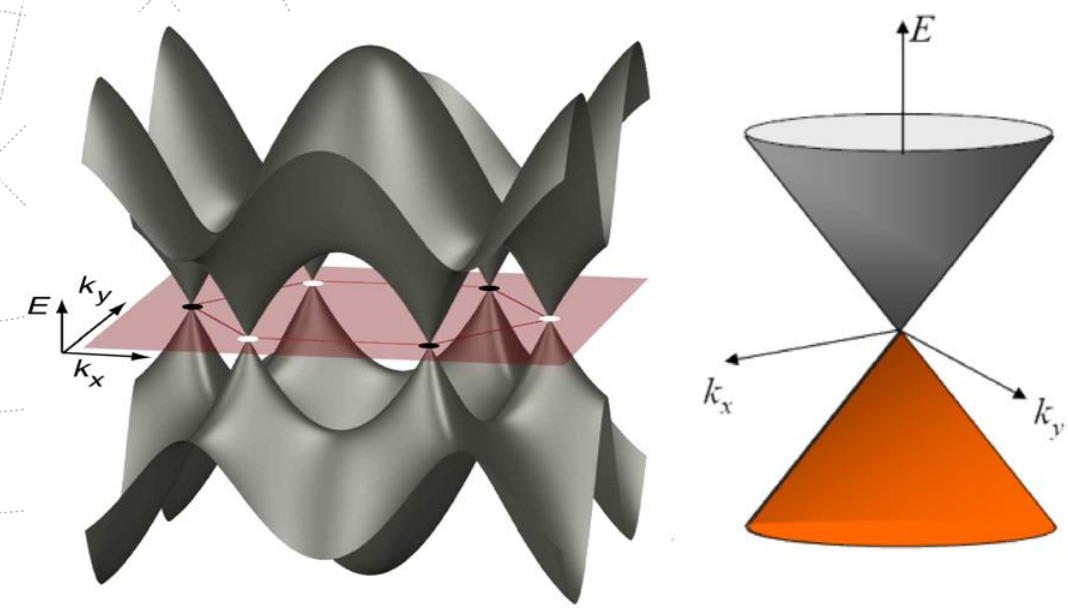
- **Excellent thermal conductor**

Graphene Thermal Properties: Applications in Thermal Management and Energy Storage

Jackie D. Renteria [1,2], Denis L. Nika [1,3] and Alexander A. Balandin [1,2,*]



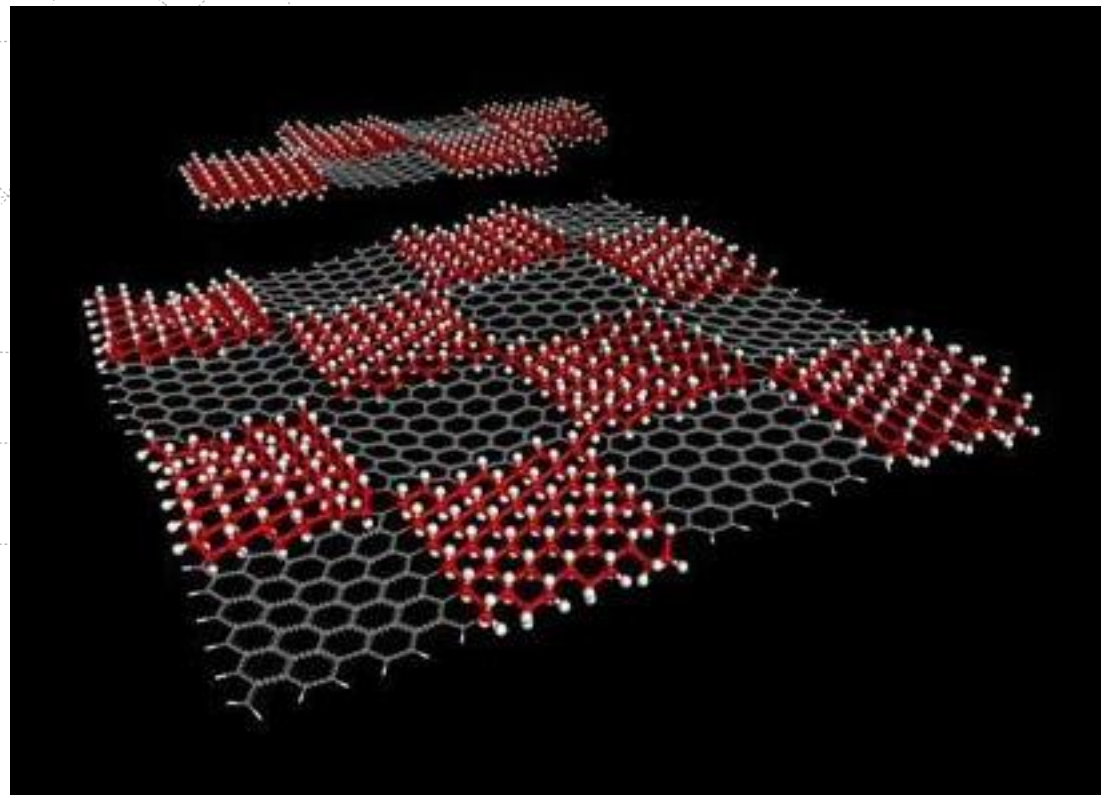
Electronic Properties of Graphene



Eva Y Andrei *et al*, *Rep. Prog. Phys.* **75** 056501, 2012

- **Linear energy dispersion.**
- **Zero effective mass.**
- **No bandgap.**

Graphene Superlattices

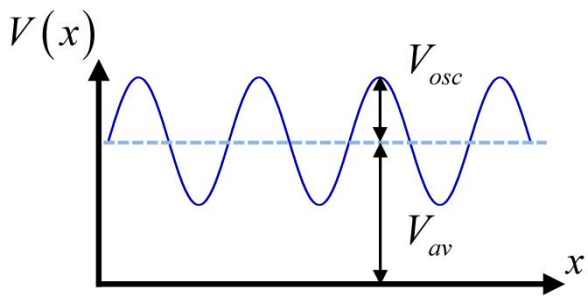


http://goo.gl/JGbgeC

- **Graphene based heterostructures**
- **Tailoring the potential ↔ gain control over the electron propagation.**

Graphene Superlattices – Effective Medium Model

Periodic 1-D potential $V(\mathbf{r}) = V(x) = V_{av} + V_{osc}(x)$

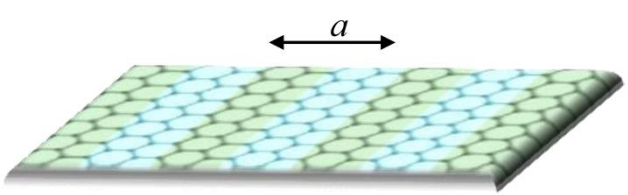


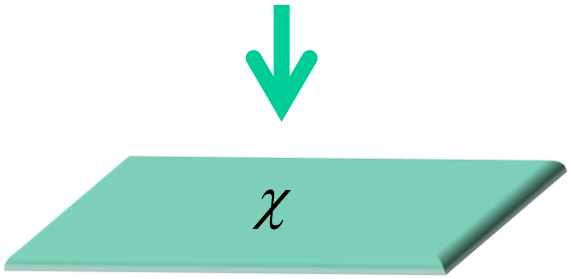
$$\left(\hat{H}\boldsymbol{\psi}\right)(\mathbf{r}) = \left[-i\hbar v_F \boldsymbol{\sigma}\cdot\nabla + V(\mathbf{r})\right]\cdot\boldsymbol{\psi}(\mathbf{r})$$

Effective medium theory

M. G. Silveirinha and N. Engheta 2012 *Phys. Rev. B* **85** 195413

D. E. Fernandes, M. G. Silveirinha and N. Engheta 2014 *Phys. Rev. B* **90**, 041406(R)





$$\left(\hat{H}_{ef}\boldsymbol{\psi}\right)(\mathbf{r}) = \left[-i\hbar v_F\left(\boldsymbol{\sigma}_x\hat{\mathbf{x}} + \chi\boldsymbol{\sigma}_y\hat{\mathbf{y}}\right)\cdot\nabla + V_{ef}\right]\cdot\boldsymbol{\psi}(\mathbf{r})$$

χ *anisotropy ratio* (depends on $V_{osc}(x)$)

Preferred direction of propagation for the electrons

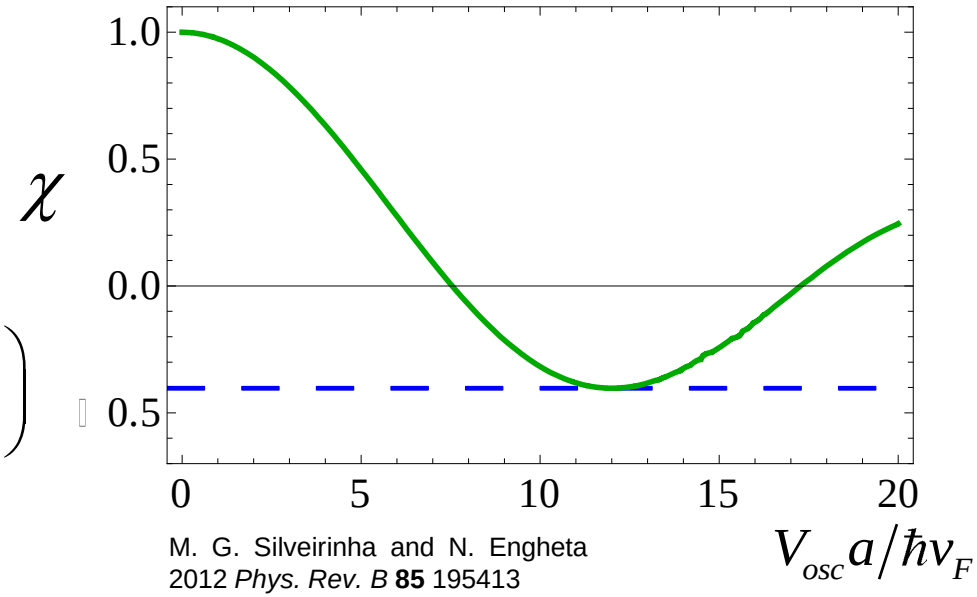
Tailoring Transport Properties of Electrons

- **Anisotropic velocity of propagation**

$$v_x = v_F$$

$$v_y = |\chi| v_F$$

$$V_{osc} \sin\left(\frac{2\pi x}{a}\right)$$

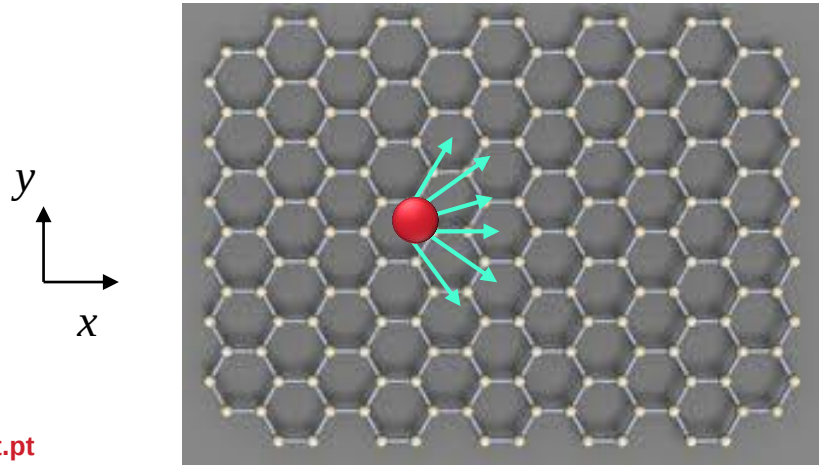


M. G. Silveirinha and N. Engheta 2012 *Phys. Rev. B* **85** 195413

Pristine Graphene: $\chi = 1$

No preferred direction of propagation!

$$v_y = v_x = v_F$$



Tailoring Transport Properties of Electrons

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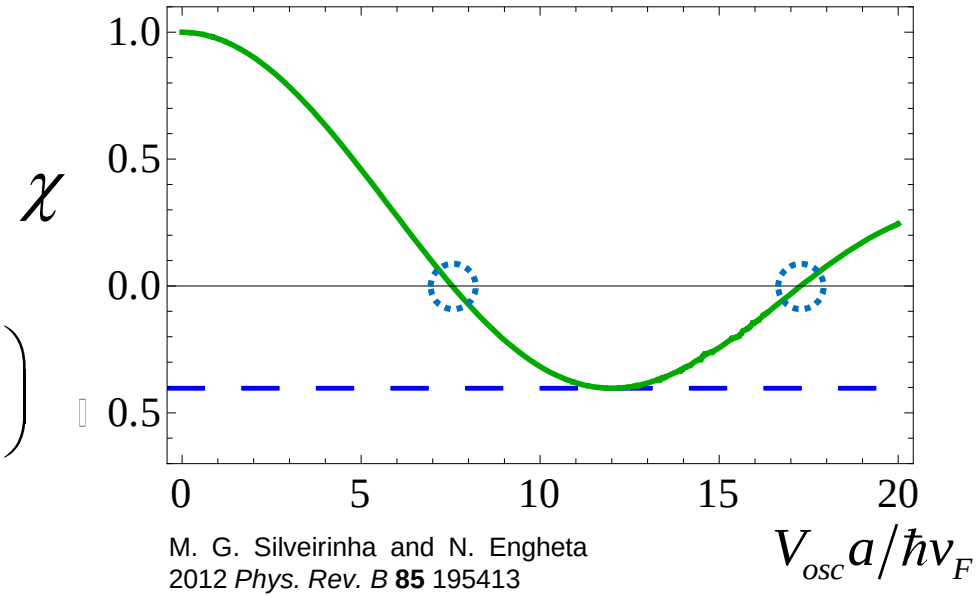


M. G. Silveirinha and N. Engheta 2012 *Phys. Rev. B* **85** 195413

Regimes of extreme anisotropy:

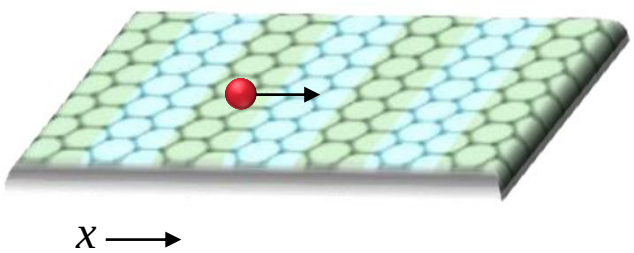
$$\frac{V_{osc} a}{\hbar v_F} = 7.55$$

$$\frac{V_{osc} a}{\hbar v_F} = 17.32$$

$$\chi = 0$$

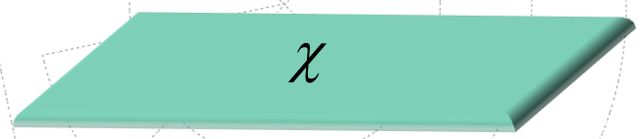
$$v_x = v_F$$
$$v_y = 0$$

Electrons tend to propagate only along the *x*-direction!!

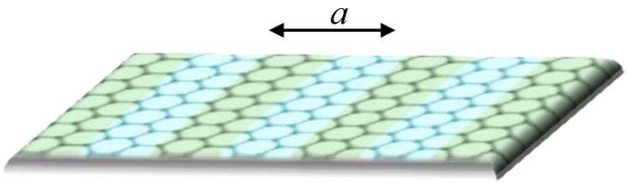


Bare GSL

GSL– Effective medium model $\chi = 0$

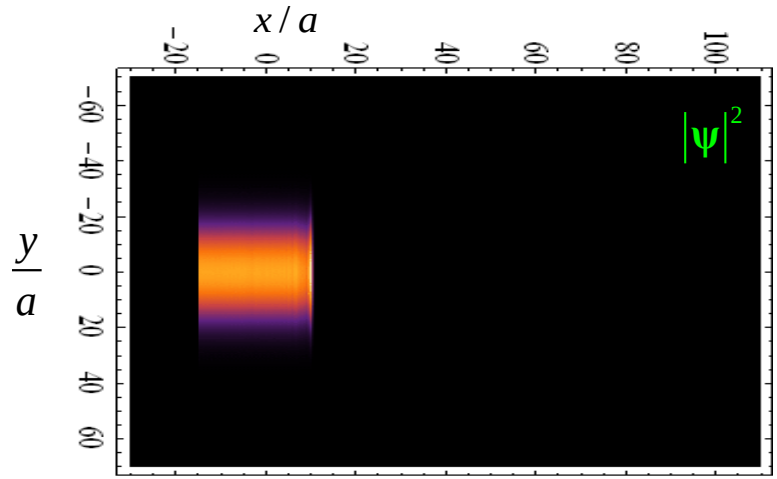


GSL– Microscopic model $\frac{V_{osc} a}{\hbar v_F} = 7.55$

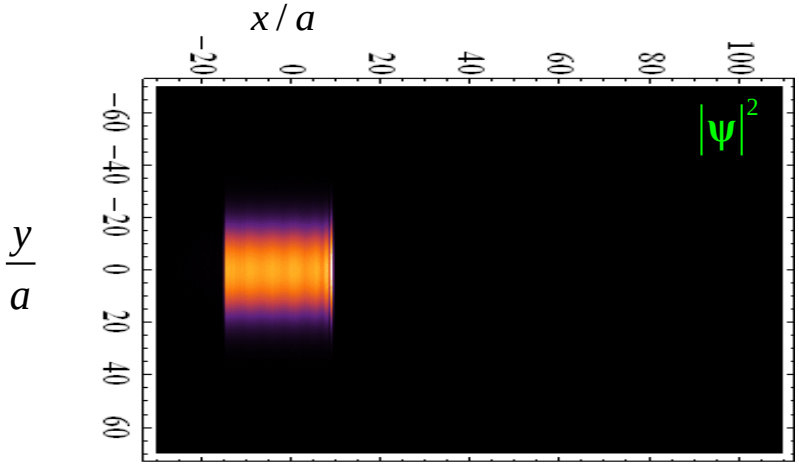


$R = 10a \quad a = 10\text{nm} \quad (V_{\text{av}} - E_0)\, a / \hbar v_F = 0.1 \quad E_0 a / \hbar v_F = 0.2$

Time animations



Effective medium model

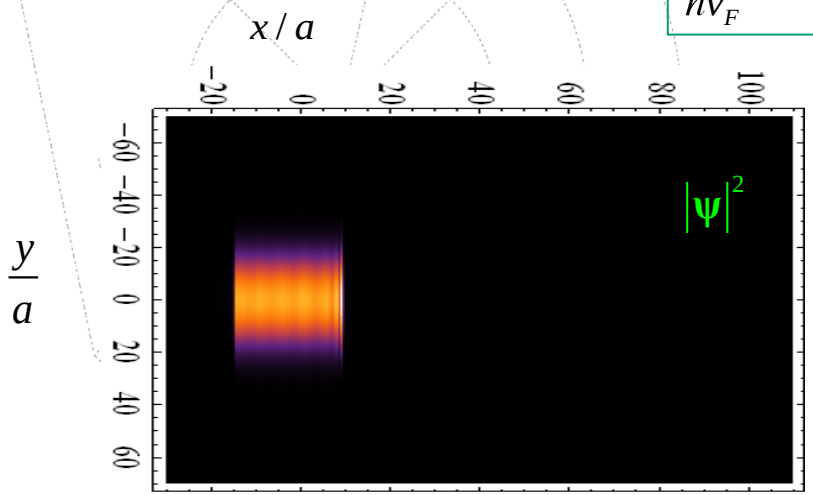


Microscopic model

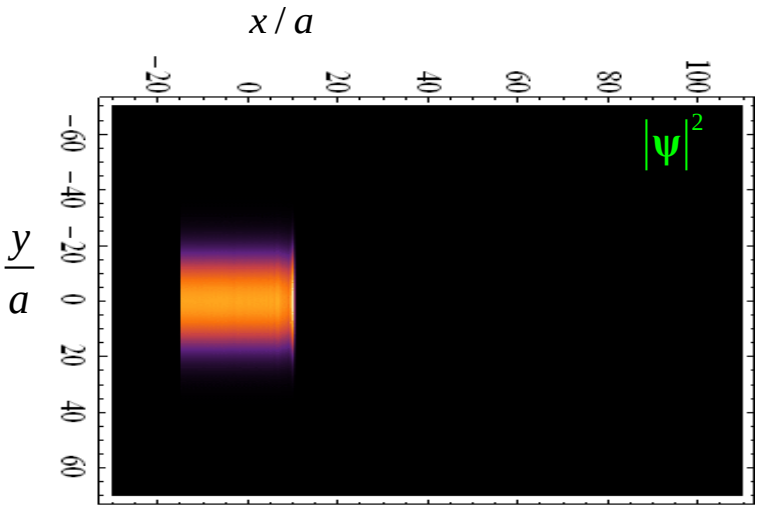
GSLs vs. Pristine Graphene

Time animations

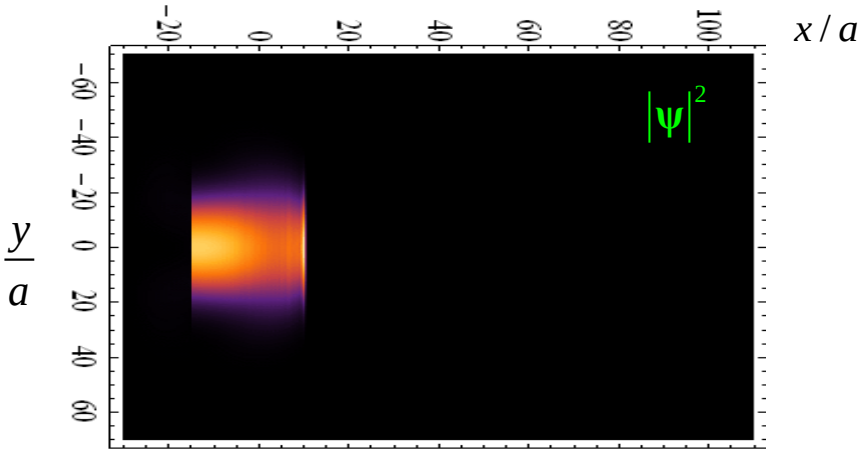
Graphene superlattice – Microscopic model $\frac{V_{osc}a}{\hbar v_F} = 7.546$



Graphene superlattice – Effective medium model $\chi = 0$



Pristine Graphene $\chi = 1$

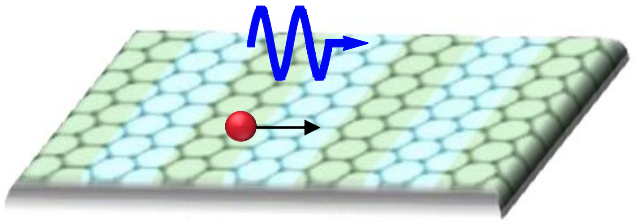


Conclusions

•Tailoring the electric potential in GSLs allows to obtain nondiffractive propagation.

•GSLs may be used for miniaturization of electronic devices.

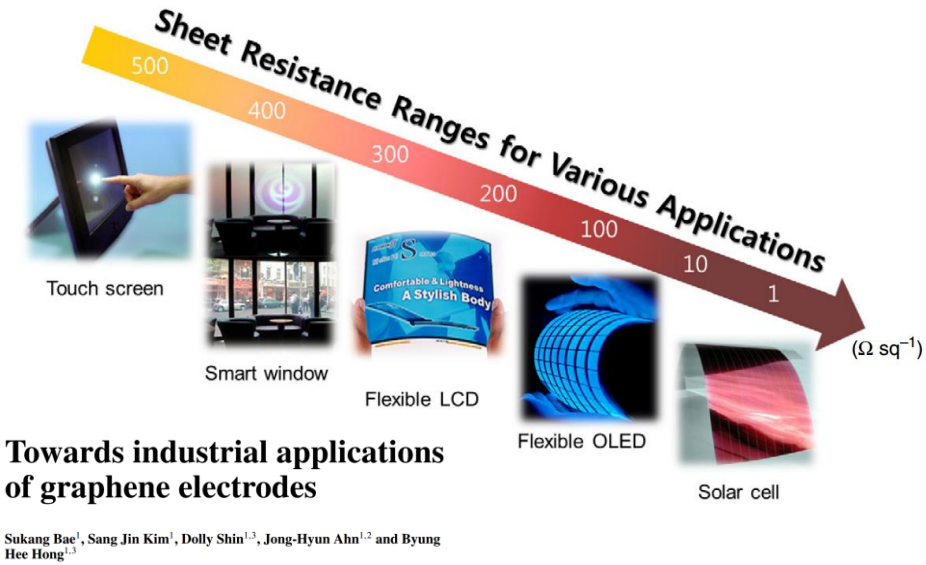
•Electronic anisotropy creating optical anisotropy!! (Work in progress).



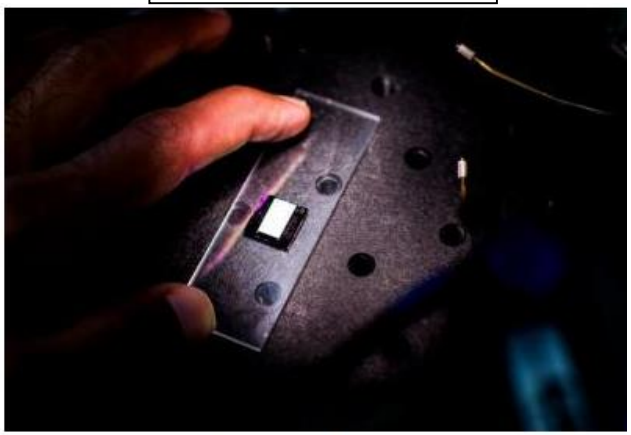
•Enhanced nonlinearities in graphene superlattices (solitons, bistability, high-order harmonics generation ,…).

Potential Applications of Graphene Structures

Transparent and flexible electrodes



Sensors



http://tinyurl.com/odb7ksz

Solar cells

http://tinyurl.com/pwf6fvt

Graphene batteries and supercapacitors

Optoelectronics

And much more…

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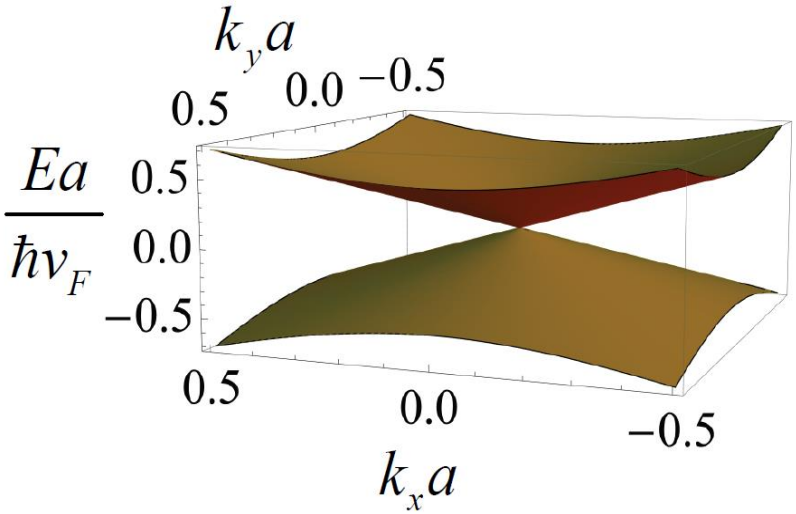
Energy Dispersion of Graphene Superlattices

Stationary states energy dispersion:

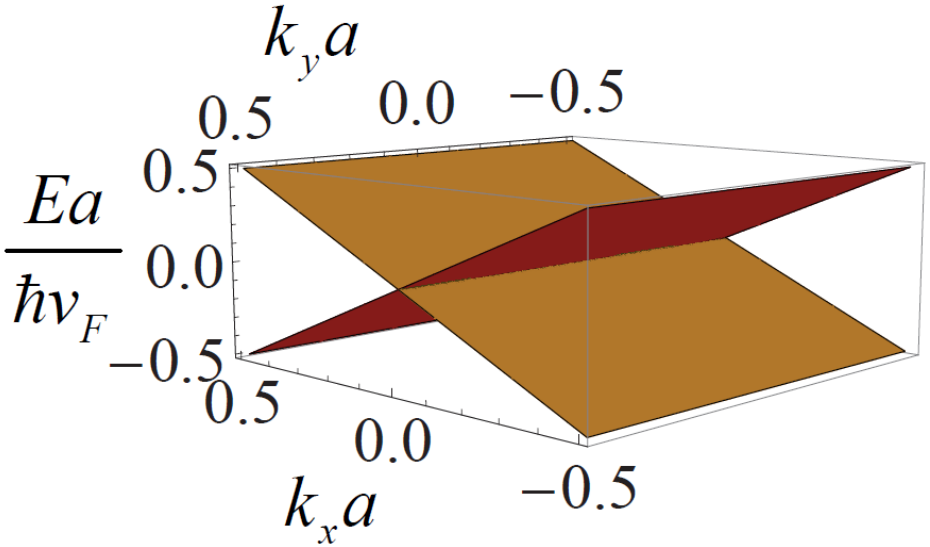
$$|E| = \hbar v_F \sqrt{k_x^2 + \chi^2 k_y^2}$$

$$\mathbf{v} = \nabla_k E/\hbar = v_F \frac{\left(k_x, \chi^2 k_y\right)}{|\mathbf{k}|}$$

Pristine Graphene $\chi = 1$

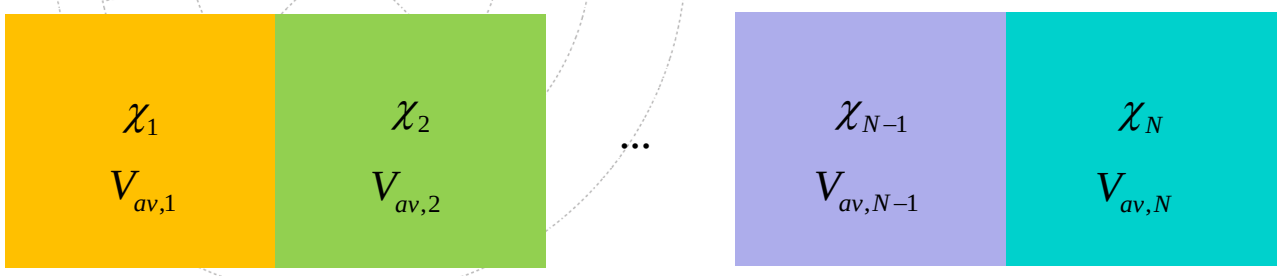


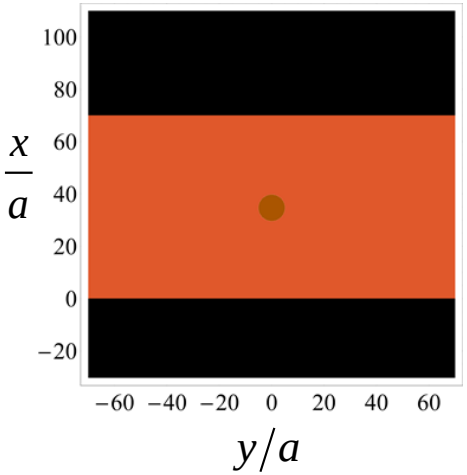
Superlattice in extreme anisotropy regime $\chi = 0$



FDTD algorithm

- Characterization of electron wave propagation in complex GSL structures





- Determining the scattering properties of GSL slabs.

- Characterization of the optical properties of graphene structures (conductivity).
  Work in progress…

FDTD Algorithm

- Effective medium model

$$\left(\hat{H}_{ef}\boldsymbol{\psi}\right)(\mathbf{r}) = i\hbar\frac{\partial}{\partial t}\boldsymbol{\psi} - i\hbar v_F \mathbf{j}$$

$$\hat{H}_{ef} = \left[-i\hbar v_F\left(\boldsymbol{\sigma}_x\hat{\mathbf{x}} + \chi\boldsymbol{\sigma}_y\hat{\mathbf{y}}\right)\cdot\nabla + V_{ef}\right] \qquad \boldsymbol{\psi} = \begin{Bmatrix}\psi_1\\ \psi_2\end{Bmatrix} \qquad \mathbf{j} = \begin{Bmatrix} j_1\\ j_2\end{Bmatrix}$$

Ficticious electron source

- Time update equations:

$$\frac{\partial\psi_1}{\partial t} = -v_F\left(\frac{d}{dx} - i\chi\frac{d}{dy}\right)\psi_2 + \frac{V_{ef}}{i\hbar}\psi_1 + j_1$$

$$\frac{\partial\psi_2}{\partial t} = -v_F\left(\frac{d}{dx} + i\chi\frac{d}{dy}\right)\psi_1 + \frac{V_{ef}}{i\hbar}\psi_2 + j_2$$

Coupling between ψ_1 and ψ_2

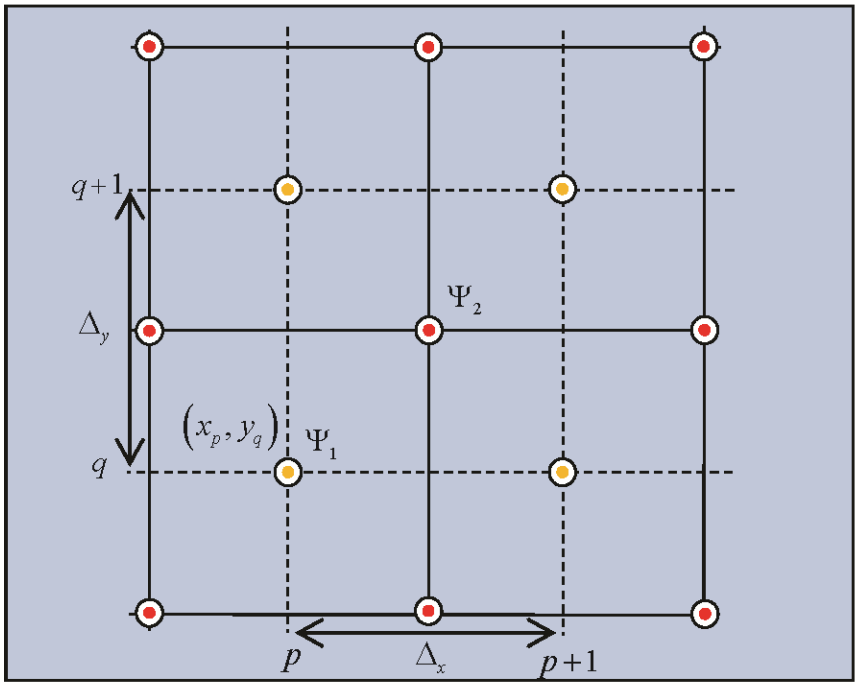
Discretization

- Rectangular Yee-*like* mesh:

$$F(x,y,t) = F(p\Delta x, q\Delta y, n\Delta t) \equiv F(p,q,n)$$

$$\psi_1(p,q,n) \equiv \psi_{1,p,q}^{n}$$

$$\psi_2\left(p+\frac{1}{2}, q+\frac{1}{2}, n+\frac{1}{2}\right) \equiv \psi_{2,p+\frac{1}{2},q+\frac{1}{2}}^{n+\frac{1}{2}}$$



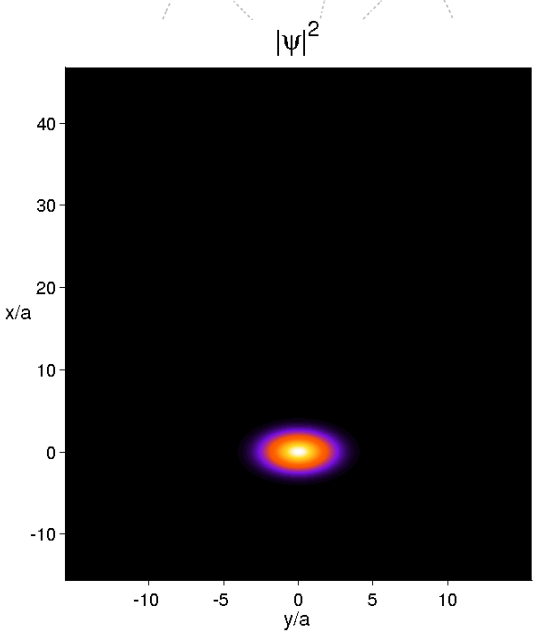
Derivatives → Finite Difference (FD) method

$$\frac{\partial}{\partial i} F(i) = \frac{F(i+\Delta i) - F(i)}{\Delta i}$$

$$i = x, y, t$$

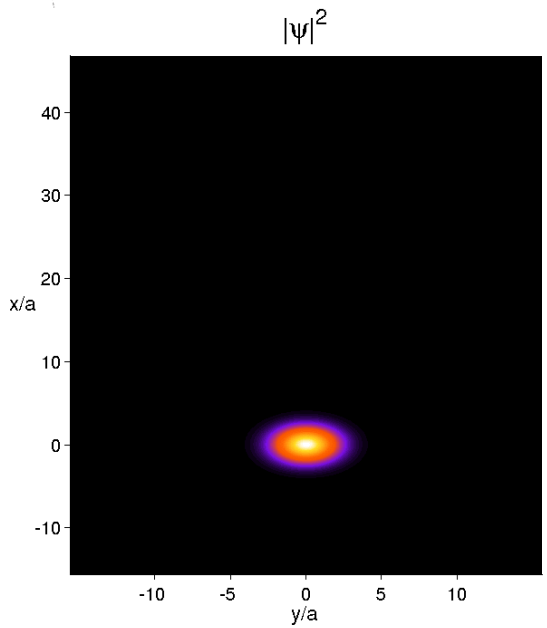
Time Evolution of Initial Electronic States

Time animations



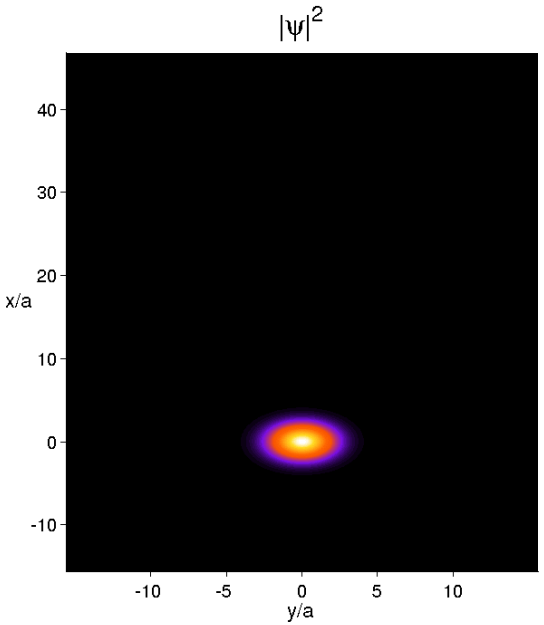
$\chi = 1.0$

$$\frac{V_{osc} a}{\hbar v_F} = 0$$



$\chi = 0.7$

$$\frac{V_{osc} a}{\hbar v_F} = 3.58$$



$\chi = 0$

$$\frac{V_{osc} a}{\hbar v_F} = 7.55$$