Dirac operators in Graphene

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EMALCA, 12 de enero 2022

Outline

- Operators for Solid State Physics
- Bloch bands and Dirac points in graphene
- Bounded pieces of graphene

Based on joint work with Rafael Benguria, Søren Fournais and Edgardo Stockmeyer.

Quantum Mechanics

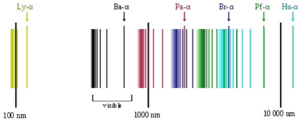
$\mathbb{C}^4$

$L^2(\mathbb{R}^3)\ \langle f, g\rangle = \int \bar{f} g$

- States : $\mathcal{H}$ Hilbert space
- An Hamiltonian H: self-adjoint
- Schrödinger's equation

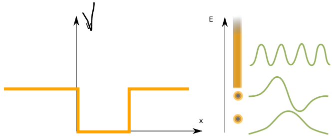
$$i\partial_t \Psi_t = H\Psi_t.$$

- Interpretation ?
- Spectral theorem



J. Bricmont, Making Sense of Quantum Mechanics, Springer

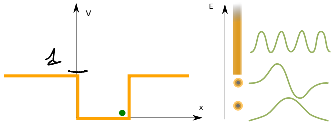
Spectral Theory



- Eigenvalues: $H\psi = \lambda\psi$

$\forall N \in \mathbb{N} \quad \psi_N \in \mathcal{H} \quad (\psi_N)_j = \begin{cases} \frac{e^{ipj}}{\sqrt{2N+1}} & \text{si } N^2 \le j \le N^2+2N \\ 0 & \text{si no} \end{cases}$

$(H\psi_N)_j = \begin{cases} \frac{e^{ip(j-1)} + e^{ip(j+1)}}{\sqrt{2N+1}} = (\psi_N)_j \, 2\cos(p) & \text{si } N^2+1 \le j \le N^2+2N-1 \\ \frac{e^{ip(j+1)}}{\sqrt{2N+1}} & \text{si } j = N^2,\ N^2-1 \\ \frac{e^{ip(j-1)}}{\sqrt{2N+1}} & N^2+2N,\ N^2+2N+1 \\ 0 & \text{si no} \end{cases}$



- Eigenvalues: $H\psi = \lambda\psi$ (Weyl)
- Essential spectrum: $\|(H-\lambda)\psi_n\| \to 0$, $\|\psi_n\| = 1$, $\psi_n \perp \psi_m$ $\quad n \neq m$

$\langle \psi_n, \psi_m \rangle = 0$

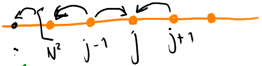
$\|(H - 2\cos(p))\psi_N\|^2 = \frac{4}{2N+1}$

$p \in [-\pi, \pi]$

Exampl

$(a_n)_{n\in\mathbb{Z}} \quad (b_n)_{n\in\mathbb{Z}}$

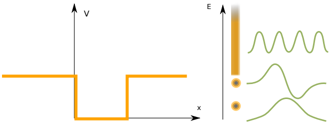
$\mathcal{H} := \ell^2(\mathbb{Z})$



$H_{ij} = \begin{cases} 1 & |i-j| = 1 \\ 0 & \text{else} \end{cases}$

$(Ha)_j = a_{j+1} + a_{j-1}$

Spectral Theory



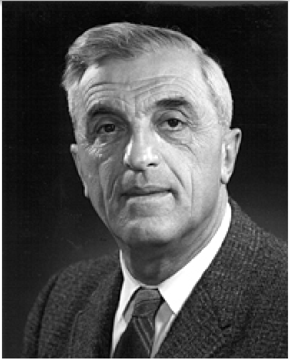
- Eigenvalues: $H\psi = \lambda\psi$
- Essential spectrum: $\|(H-\lambda)\psi_n\| \to 0$, $\|\psi_n\| = 1$, $\psi_n \perp \psi_m$
- Periodic potentials ?

Bloch–Floquet Theory

$\langle U\psi, U\varphi\rangle = \langle \psi, \varphi\rangle$

A unitary transformation to a family of operators on the states for a single cell, depening on a parameter in the dual lattice.

$\mathbb{C}^2$

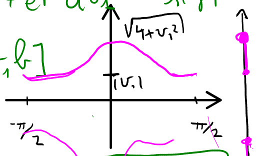


Example

$$H_{ij} = \begin{cases} v_1 & i=j=\text{even} \\ -v_1 & i=j=\text{odd} \\ 1 & |i-j|=1 \\ 0 & \text{else} \end{cases}$$

$$\psi_j = \begin{cases} e^{ipj}\, a & \text{si } j \text{ par} \\ e^{ipj}\, b & \text{si } j \text{ impar} \end{cases}$$

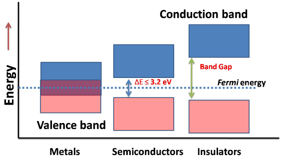
$$(H\psi)_j = \begin{cases} \left(e^{ip(j-1)} + e^{ip(j+1)}\right) b + e^{ipj} a v_1 & \text{si } j \text{ par} \\ e^{ipj}\left[(2\cos p)\, a - v_1 b\right] \end{cases}$$



$$h_p = \begin{pmatrix} v_1 & 2\cos p \\ 2\cos p & -v_1 \end{pmatrix}$$

$\sigma(H)$

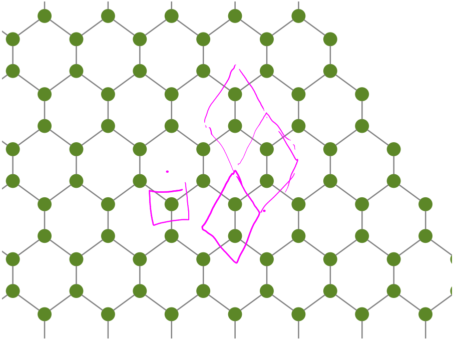
$\pm\sqrt{(2\cos p)^2 + v_1^2}$



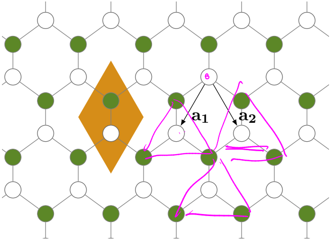
Graphene

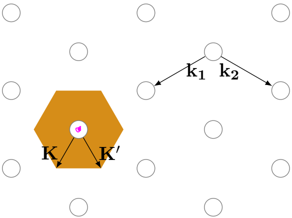
 

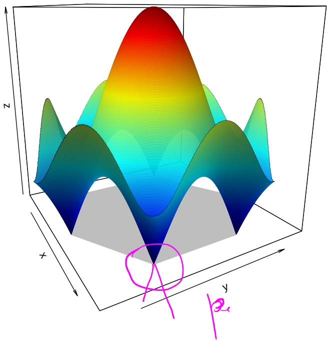
André Geim and Constantin Novoselov.



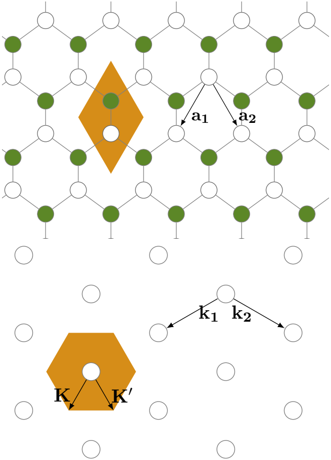
Band structure of Graphene

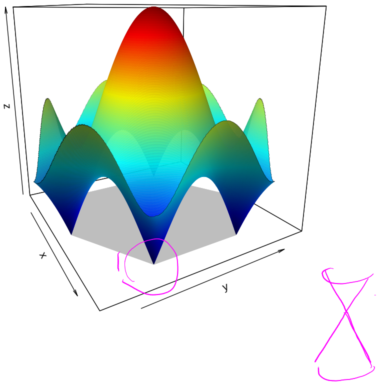






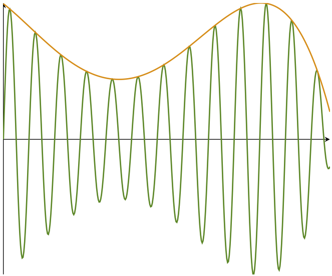
Band structure of Graphene - Tight-binding model

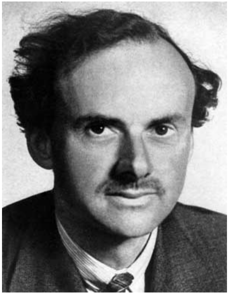




Wallace (1949), see also recent papers of Fefferman & Weinstein, Comech & Berkolaiko

Dirac - finally



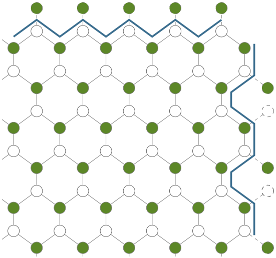


$\mathcal{H} = L^2(\mathbb{R}^2, \mathbb{C}^2)$

$$D = -i \begin{pmatrix} 0 & \partial_x - i\partial_y \\ -\partial_x + i\partial_y & 0 \end{pmatrix}$$

Dirac - in bounded domains ?

$$D = -i \begin{pmatrix} 0 & \partial_x - i\partial_y \\ -\partial_x + i\partial_y & 0 \end{pmatrix}$$



Muchas Gracias !