Spectrum of graphene quantum dots

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Eigenvalues and Inequalities
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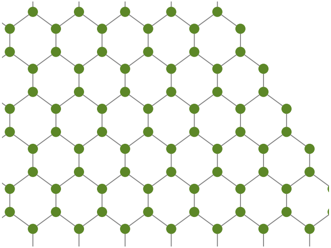
Outline

joint work with Rafael Benguria, Søren Fournais and Edgardo Stockmeyer

- Graphene quantum dots
- Boundary conditions and self-adjointness
- An inequality for eigenvalues
- Semi-classical expansion for eigenvalue sums

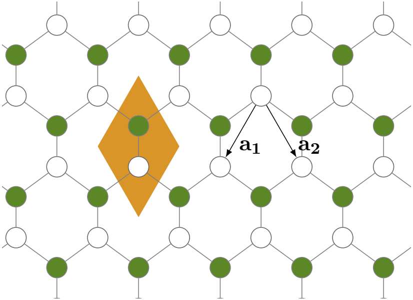
Graphene

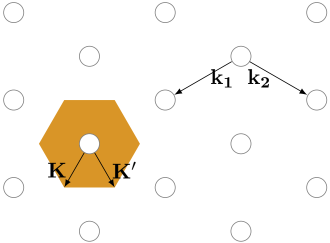


Andre Geim and Constantin Novoselov*

*pictures ©The Nobel Foundation

Band structure of graphene





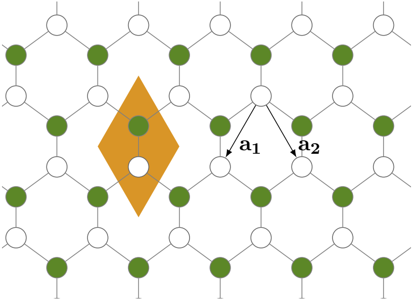
Dirac points : tight-binding* or general case*

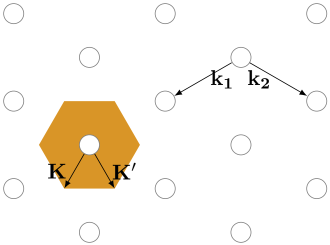
$$H_{\text{t.b.}} = -t \sum_{n,i} |A, n\rangle \langle B, n + a_i| + \text{h.c.}$$

*Wallace, 1949

*Fefferman, Weinstein, 2012

Band structure of graphene

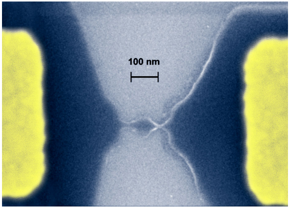




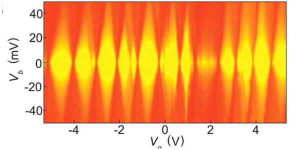
- plane wave $\mathbf{K}$, $\mathbf{K}'$ + envelope
- components for each sublattice
- full description : two Dirac points

$$T = v_f \hbar(-i\boldsymbol{\sigma} \cdot \nabla) = -i \begin{pmatrix} 0 & \partial_x - i\partial_y \\ \partial_x + i\partial_y & 0 \end{pmatrix}$$

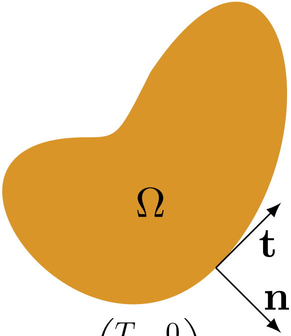
Graphene Quantum Dots



A graphene quantum dot between two leads*



Coulomb blockade diamonds in a 15 nm graphene SET*

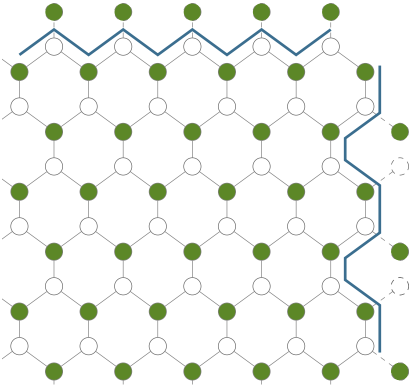


$$V \equiv \begin{pmatrix} T & 0 \\ 0 & T \end{pmatrix}$$

*Picture from *www.graphene.org*

*Picture from Science 2008 Vol. 320, Issue 5874, pp. 356-358

Boundary conditions



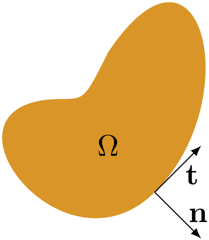
Zigzag BC:
$\phi_2 = 0$ at boundary

Armchair BC:
superposition from both valleys $= 0$

Infinite mass BC:*
$T + \sigma_3 M \mathbf{1}_{\Omega^c}$ with $M \to \infty$

*(Berry-Mondragon, 1987) and (Stockmeyer-Vugalter 2015)

Boundary conditions : matrix form



$$A\gamma\phi = \gamma\phi$$

$$A_{\text{z.z.}} = \begin{pmatrix} \sigma_3 & 0 \\ 0 & -\sigma_3 \end{pmatrix}$$

$$A_{\text{a.c.}} = \begin{pmatrix} 0 & \boldsymbol{t}\cdot\boldsymbol{\sigma} \\ \boldsymbol{t}\cdot\boldsymbol{\sigma} & 0 \end{pmatrix}$$

$$A_{\infty-\text{m.}} = \begin{pmatrix} \boldsymbol{t}\cdot\boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{t}\cdot\boldsymbol{\sigma} \end{pmatrix}$$

Boundary conditions: general form

$$\langle u, Tv \rangle = \langle Tu, v \rangle - i \int_{\partial\Omega} (u, \boldsymbol{n} \cdot \boldsymbol{\sigma}\, v)_{\mathbb{C}^2}$$

$$A_\eta = \cos(\eta) \boldsymbol{\sigma} \cdot \boldsymbol{t} + \sin(\eta) \sigma_3,$$

Definition

D_η acts as $-i\boldsymbol{\sigma} \cdot \nabla$ on

$$\mathcal{D}(D_\eta) \equiv \{u \in H^1(\Omega, \mathbb{C}^2) | A_\eta \gamma u = \gamma u\}.$$

- Symmetric
- Self-adjoint ?

Domain of self-adjoint extension

Theorem

$\Omega \subset \mathbb{R}^2$ a bounded C^2-domain, η a C_1-function such that $\cos\eta \neq 0$. Then D_η is self-adjoint on

$$\mathcal{D}(D_\eta) \subset H^1.$$

- Hypothesis: $u_2 = B(t_1 + it_2)u_1$,
- Result: $\|Du\|^2 + \|u\|^2 \sim \|\nabla u\|^2 + \|u\|^2$ on the domain
- Elliptic boundary value problems (Hörmander, Booß- Bavnek and Wojchiechowski)
- Or : proof "by hand"
- Corners: Le Treust, Ourmières-Bonafos, 2017

Zigzag BC or $\cos\eta = 0$

$$u = \begin{pmatrix} f \\ g \end{pmatrix} \text{ and } g = 0 \text{ at } \partial\Omega$$

$$D = -2i \begin{pmatrix} 0 & \partial_z \\ \partial_{z^*} & 0 \end{pmatrix}$$

$$Du = -2i \begin{pmatrix} \partial_z g \\ \partial_{z^*} f \end{pmatrix}$$

Solution: $g \equiv 0$ and f holomorphic.

Proof for $\cos\eta \neq 0$

$$i \int_{\partial\Omega} (\boldsymbol{n}\cdot\boldsymbol{\sigma}\,\gamma v, \gamma u)_{\mathbb{C}^2} = \langle Tu, v\rangle - \langle u, Tv\rangle$$

$$i \int_{\partial\Omega} (\boldsymbol{n}\cdot\boldsymbol{\sigma}\,\gamma v, \phi)_{\mathbb{C}^2} = \langle v, TE\phi\rangle - \langle Tv, E\phi\rangle$$

$$\mathcal{D}(D_\eta^*) = \{u \in L^2 | Tu \in L^2, A_\eta \gamma u = \gamma u \in H^{-1/2}\}$$

Proof for $\cos\eta \neq 0$

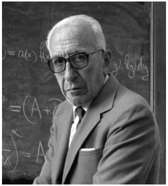
$$\mathcal{D}(D_\eta^*) = \{u \in L^2 | Tu \in L^2, A_\eta \gamma u = \gamma u \in H^{-1/2}\}$$

Check if

$$\mathcal{D}(D_\eta^*) \subset H^1$$

$$i \int_{\partial\Omega} (\boldsymbol{n}\cdot\boldsymbol{\sigma}\, \gamma v, \phi)_{\mathbb{C}^2} = \langle v, TE\phi\rangle - \langle Tv, E\phi\rangle$$

- Calderón projector γS
- $\gamma S \boldsymbol{n}\cdot\boldsymbol{\sigma}\, \gamma v$ is in $H^{1/2}$
- Boundary condition: $(A_\eta - 1)\gamma v = 0$



Alberto Calderón*

Spectrum

Boundary conditions

$$u_2 = B(t_1 + it_2)u_1, \quad B \neq 0$$

- Discrete spectrum (compact resolvent)
- No zero eigenvalue if sign B constant

Spectral gap

Theorem

Ω simply connected, B constant. If λ is an eigenvalue of D_η, then

$$\lambda^2 \geq \frac{2\pi}{|\Omega|} \min(B^2, B^{-2}).$$

- Case $B = 1$: Raulot (2006)
- Not sharp : when $B = 1$, $\Omega =$ unit disc, $\lambda_1 \sim 1.435 > \sqrt{2}$

Spectral gap

Theorem

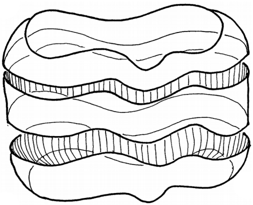
Ω simply connected, $B = 1$,

$$\lambda^2 \geq \frac{2\pi}{|\Omega|}.$$

Theorem (Bär, 1992)

Ω a compact surface of genus 0,

$$\lambda^2 \geq \frac{4\pi}{\mathrm{vol}\Omega}.$$



Spectral gap : idea of proof

- $B = 1$ is sufficient.
- Use the energy functional (Lichnerowicz formula) : for $u, v \in \mathcal{D}(D)$

$$(Du, Dv) = (\nabla u, \nabla v) + \frac{1}{2}\int_{\partial\Omega} (u, v)_{\mathbb{C}^2}(s)\kappa(s)\,\mathrm{d}s$$

- Define a modified connection

$$\widetilde{\partial}_j = \partial_j - i\frac{1}{2}\sigma_j - \sigma_f\sigma_j,$$

and compute

$$\int_\Omega e^{-2f}\sum_j \left(\widetilde{\partial}_j u, \widetilde{\partial}_j u\right)_{\mathbb{C}^2}$$

Spectral gap : idea of proof

- Apply to an eigenfunction and after a few integrations by parts and commutators...

$$\frac{\lambda^2}{2}\|e^{-f}u\|^2 \geq \left\langle e^{-2f}u, (-\Delta f)u \right\rangle + \int_{\partial\Omega} e^{-2f}\,(u,u)_{\mathbb{C}^2}\,(\frac{\kappa}{2} + \boldsymbol{n}\cdot\nabla f).$$

$$\begin{cases} -\Delta f = C & \text{in } \Omega, \\ \boldsymbol{n}\cdot\nabla f = -\kappa/2 & \text{in } \partial\Omega. \end{cases}$$

Finally...

$$\lambda^2 \geq \frac{2\pi}{|\Omega|}$$

Semi-classics for eigenvalues

Theorem

$$\mathrm{Tr}[h^2 D^2 - 1]_- = h^{-2}\frac{|\Omega|}{4\pi} + h^{-1}\int_{\partial\Omega}\Theta(B(s))\,\mathrm{d}s + o(h^{-1})$$

where $\Theta(B) = \frac{1}{6\pi}\frac{(1-|B|)^2}{|B|}$.

Hermann Weyl*

*Picture © MFO

Semi-classics for eigenvalues

Theorem

$$\mathrm{Tr}[h^2 D^2 - 1]_- = h^{-2}\frac{|\Omega|}{4\pi} + h^{-1}\int_{\partial\Omega}\Theta(B(s))\,\mathrm{d}s + o(h^{-1})$$

where

$$\Theta(B) = \frac{1}{6\pi}\frac{(1-|B|)^2}{|B|}.$$

- Proof cf. Frank, Geisinger, 2012
- Absence of boundary term for $B = 1$ in Berry, Mondragon, 1987.
- Heat Trace for $B = 1$ in Bramson, Gilkey, 1992.

Semi-classics for eigenvalues

Variational problem

$$-\operatorname{Tr}[H]_- = \inf_{0 \le \gamma \le 1} \operatorname{Tr}[H\gamma].$$

Localization $\sim l^{-2}$
Coordinate transform error $\sim lh^{-2}$

Semi-classics for eigenvalues

Example : Bulk term

$$\mathrm{Tr}[\phi H \phi]_-$$

Upper bound

$$\begin{aligned} &\leq \mathrm{Tr}(\phi [H]_- \phi) \\ &\leq \mathrm{Tr}(\phi [H_{\mathbb{R}^2}]_- \phi) = 2 \int_\Omega \phi^2(x)\,\mathrm{d}x \int_{\mathbb{R}^2} [h^2 p^2 - 1]_- \frac{\mathrm{d}p}{(2\pi)^2} \end{aligned}$$

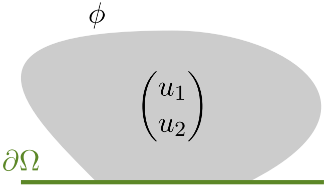
Lower bound

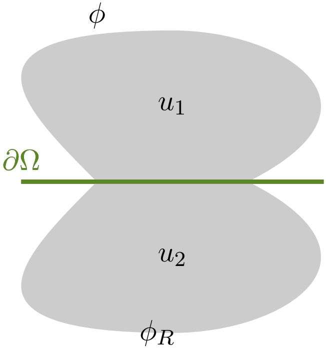
$$\begin{aligned} &\geq \mathrm{Tr}(\phi H \phi [H_{\mathbb{R}^2}]_-^0) \\ &= \int_\Omega \int_{|hp|\leq 1} \sum_{i=1,2} |D\phi(x) e^{ikx} e_i|^2 - |\phi(x) e^{ikx} e_i|^2 \frac{\mathrm{d}p}{(2\pi)^2}\,\mathrm{d}x \end{aligned}$$

Semi-classics for eigenvalues

Boundary term with $B = 1$

$$(Du, Dv) = (\nabla u, \nabla v) + \frac{1}{2}\int_{\partial\Omega} (u, v)_{\mathbb{C}^2}(s)\kappa(s)\,\mathrm{d}s$$





Semi-classics for eigenvalues

Boundary term with $B \neq 1$

$$\beta = \frac{|1-b^2|}{1+b^2}, \quad \nu = \mathrm{sign}(1-b^2), \quad \text{and } \eta = \frac{k+il}{|k+il|}.$$

Then the solutions are

$$e_{\pm,k,l}(x,y) = e^{ikx} \frac{1}{|\eta \mp b|} \begin{pmatrix} -(\eta^* \mp b)e^{ily} + (\eta \mp b)e^{-ily} \\ \mp(1 \mp b\eta)e^{ily} \pm (1 \mp b\eta^*)e^{-ily} \end{pmatrix},$$

$$\widetilde{e}_k(x,y) = e^{ikx} \sqrt{\frac{2|k|\beta}{b^2+1}} e^{-\nu k \beta y} \begin{pmatrix} 1 \\ b \end{pmatrix}$$

Thank you !