### Spectral gap for graphene quantum dots

#### Vladimir Lotoreichik

#### in collaboration with T. Ourmières-Bonafos

Czech Academy of Sciences, Řež near Prague



#### Differential Operators on Graphs and Waveguides Graz, 26.02.2019

### 1 Dirac operator with $\infty$ -mass boundary conditions

### 2 Upper bounds on the size of the spectral gap



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3 Key ideas of the proof

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## Dirac differential expression in two dimensions

### Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

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#### First-order Dirac differential expression

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The off-diagonal entries resemble Cauchy-Riemann operators: interplay with complex analysis.

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$$\cdots \leq -\mu_2(\Omega) \leq -\mu_1(\Omega) < \mathsf{0} < \mu_1(\Omega) \leq \mu_2(\Omega) \leq \dots$$

 $\mu_1(\Omega) := \inf(\sigma(\mathsf{D}_\Omega) \cap \mathbb{R}_+)$  describes the size of the spectral gap.

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#### Massless Dirac operator in $\mathbb{R}^2$

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$$\mathsf{D}_{\mathbb{R}^2} + \underbrace{\mathcal{M}\sigma_3\chi_{\mathbb{R}^2\backslash\Omega}}_{\text{mass term}} \xrightarrow{\mathcal{M}\to\infty} \mathsf{D}_\Omega, \qquad \text{(in a proper sense)}.$$

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Eigenmodes of such GQD are effectively described by  $D_{\Omega}$ .

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Computing the quadratic form for  $\mathsf{D}^2_\Omega$  and applying the min-max principle:

$$\left(\mu_1(\Omega)\right)^2 = \inf_{u \in \operatorname{dom} \mathsf{D}_\Omega \setminus \{0\}} \mathsf{R}_\Omega[u] = \inf_{u \in \operatorname{dom} \mathsf{D}_\Omega \setminus \{0\}} \frac{\displaystyle \int_\Omega |\nabla u|^2 + \frac{1}{2} \displaystyle \int_{\partial \Omega} \kappa |u|^2}{\displaystyle \int_\Omega |u|^2}.$$

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Aim: to get a bound on  $\mu_1(\Omega)$  in the spirit of an isoperimetric inequality,

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### The analysis of the unit disk: unusual ground-state

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#### Proposition

 $\mu_1(\mathbb{D}) > 0$  is the smallest non-negative solution of  $J_0(\mu) = J_1(\mu)$ . An eigenfunction associated to  $\mu_1(\mathbb{D})$  is

$$u_{\circ}(r,\theta) := \begin{pmatrix} J_{0}(\mu_{1}(\mathbb{D})r) \\ ie^{i\theta}J_{1}(\mu_{1}(\mathbb{D})r) \end{pmatrix}$$

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- X Symmetric decreasing rearrangement.
- X Parallel coordinates.
- ✓ Conformal maps.
- Shrinking coordinates.

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 $\mathcal{H}(\mathbb{D})$  – the space of holomorphic functions on  $\mathbb{D}$ .

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### Hardy norm of $h \in \overline{\mathcal{H}(\mathbb{D})}$

$$\|h\|_{\mathcal{H}^{2}(\mathbb{D})} = \sup_{0 \le r < 1} \left(\frac{1}{2\pi} \int_{0}^{2\pi} |h(re^{i\theta})|^{2} \mathrm{d}\theta\right)^{1/2}$$

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## Intermezzo: Hardy spaces & conformal maps

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#### Theorem (VL-Ourmières-Bonafos-18)

$$\mu_1(\Omega) < \mu_1(\mathbb{D}) \left(\frac{2\pi}{|\Omega| + \pi r_{\mathrm{i}}^2}\right)^{1/2} \frac{1}{r_{\mathrm{c}}} \|f'\|_{\mathcal{H}^2(\mathbb{D})}.$$

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 Geometric estimates of  $||f'||_{\mathcal{H}^2(\mathbb{D})}$  

 Star-shaped (nearly circular): Warschawski-50, Specht-51, Gaier-62

 Convex: Kovalev-2017

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$$\begin{split} \Omega \text{ is convex in addition} \\ \textbf{r}_{i} &:= \min_{x \in \partial \Omega} |x| \\ \textbf{r}_{o} &:= \max_{x \in \partial \Omega} |x| \end{split}$$



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$$\mathcal{F}_{\mathrm{K}}(\Omega) := \left(\frac{2\pi}{|\Omega| + \pi r_{\mathrm{i}}^2}\right)^{1/2} \left(\frac{r_{\mathrm{i}}}{r_{\mathrm{c}}}\right)^{2\frac{\omega}{r_{\mathrm{i}} - r_{\mathrm{c}}}}$$



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Inspired by  $\lambda_1^{\mathrm{Dir}}(\Omega) \leq \frac{|\partial \Omega|}{2r|\Omega|} \lambda_1^{\mathrm{Dir}}(\mathbb{D})$  for convex  $\Omega$ 's (Pólya-Szegő-51)

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### Proposition (Reverse Faber-Krahn)

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Ellipse  $\Omega_x$  with axes a = 1 + x and  $b = \frac{1}{1+x}$ 

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### Private communication with L. Kovalev

It might be impossible to bound  $||f'||_{\mathcal{H}^2(\mathbb{D})}$  asymptotically better.

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### Definition (Nearly circular domains)

Bounded  $C^3$ -domain  $\Omega \subset \mathbb{R}^2$ , star-shaped with respect to the origin and parametrized by  $\rho = \rho(\theta)$ , is called *nearly circular* if

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Theorem (VL-Ourmières-Bonafos-18)

$$\mu_1(\Omega) < \mu_1(\mathbb{D}) \left(\frac{2\pi}{|\Omega| + \pi r_i^2}\right)^{\frac{1}{2}} \frac{r_o}{r_c} \left(\frac{1+\rho_\star}{1-\rho_\star}\right)^{1/2}.$$

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### Dirac operator with $\infty$ -mass boundary conditions

### 2 Upper bounds on the size of the spectral gap

3 Key ideas of the proof

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Szegő proved in 1954 a reverse Faber-Krahn for the  $1^{st}$  non-trivial Neumann EV via conformal maps.

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#### Updated test function

$$u_{\star} := \begin{pmatrix} J_0(r\mu_1(\mathbb{D})) \\ \mathsf{in}(\theta) J_1(r\mu_1(\mathbb{D})) \end{pmatrix} \circ f^{-1}, \quad \text{where} \quad \mathsf{n}(\theta) := \nu_1(f(e^{\mathsf{i}\theta})) + \mathsf{i}\nu_2(f(e^{\mathsf{i}\theta})).$$

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#### Lemma

 $u_{\star} \in \operatorname{dom} \mathsf{D}_{\Omega}.$ 

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### Eigenvalues

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Estimates of 
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 through  $\mathcal{D}_{\mathbb{D}}, \mathcal{N}_{\mathbb{D}}$   
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## An upper bound involving the conformal map

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# Estimates of $\mathcal{D}_{\Omega}, \mathcal{N}_{\Omega}$ through $\mathcal{D}_{\mathbb{D}}, \mathcal{N}_{\mathbb{D}}$ $\mathcal{D}_{\Omega} > \left(\frac{|\Omega| + \pi r_{i}^{2}}{2\pi}\right) \mathcal{D}_{\mathbb{D}}$ and $\mathcal{N}_{\Omega} \leq \frac{1}{r_{c}^{2}} \|f'\|_{\mathcal{H}^{2}(\mathbb{D})}^{2} \mathcal{N}_{\mathbb{D}}.$

#### An upper bound on $\mu_1(\Omega)$

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V. Lotoreichik (NPI CAS)

Spectral gap for graphene quantum dots

V. Lotoreichik (NPI CAS)

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The disk or not the disk?  

$$\begin{cases}
|\Omega| = \pi & \stackrel{??}{\Longrightarrow} & \mu_1(\Omega) > \mu_1(\mathbb{D}).
\end{cases}$$

## Thank you

V. Lotoreichik (NPI CAS)

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V.L. and T. Oumières-Bonafos, A sharp upper bound on the spectral gap for convex graphene quantum dots, arXiv:1812.03029.



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Thank you for your attention!