Spectral gap for graphene quantum dots

Vladimir Lotoreichik

in collaboration with T. Ourmières-Bonafos

Czech Academy of Sciences, Řež near Prague

Analysis and Applications
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Outline

1. Dirac operator with ∞-mass boundary conditions
2. Upper bounds on the size of the spectral gap
3. Key ideas of the proof

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First-order Dirac differential expression

$$\mathcal{D} = -\mathrm{i}(\sigma_1\partial_1 + \sigma_2\partial_2) = -\mathrm{i}\begin{pmatrix} 0 & \partial_1 - \mathrm{i}\partial_2 \\ \partial_1 + \mathrm{i}\partial_2 & 0 \end{pmatrix}.$$

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

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

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$$\dots \le -\mu_2(\Omega) \le -\mu_1(\Omega) < 0 < \mu_1(\Omega) \le \mu_2(\Omega) \le \dots$$

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

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Large mass in the exterior of Ω

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

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Eigenmodes of such GQD are effectively described by D_Ω.

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Computing the quadratic form for D_Ω^2 and applying the min-max principle:

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

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

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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

$$u_\circ(r,\theta) := \begin{pmatrix} J_0(\mu_1(\mathbb{D})r) \\ \mathrm{i}e^{\mathrm{i}\theta} J_1(\mu_1(\mathbb{D})r) \end{pmatrix}.$$

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

Intermezzo: Hardy spaces & conformal maps

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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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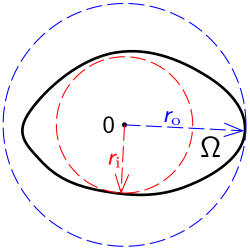

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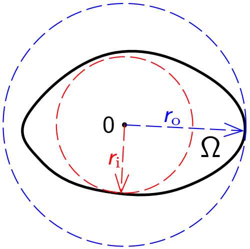

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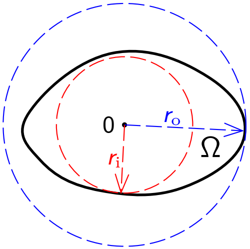

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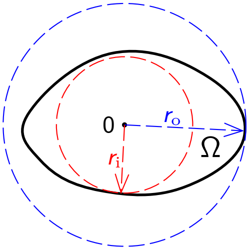

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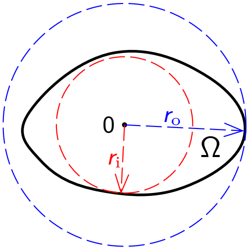

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$$\|f'\|_{\mathcal{H}^2(\mathbb{D})} \leq r_c \left(\frac{r_i}{r_c}\right)^{2\frac{r_o - r_c}{r_i - r_c}} \qquad \text{(Kovalev-17)}$$

$$\mathcal{F}_K(\Omega) := \left(\frac{2\pi}{|\Omega| + \pi r_i^2}\right)^{1/2} \left(\frac{r_i}{r_c}\right)^{2\frac{r_o - r_c}{r_i - r_c}}.$$

Theorem (VL-Ourmières-Bonafos-18)

$\mu_1(\Omega) \leq \mu_1(\mathbb{D})\mathcal{F}_K(\Omega)$.

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

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$$\mathcal{F}_{\rm K}(\Omega) = \mathcal{F}_{\rm K}(\mathbb{D}_r) = \frac{1}{r} \qquad \Longrightarrow \qquad \mu_1(\Omega) \le \mu_1(\mathbb{D}_r).$$

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

$$\mathcal{F}_{\mathrm{K}}(\Omega_x) = \left(\frac{1 + 2x + x^2}{1 + x + \frac{x^2}{2}}\right)^{\frac{1}{2}} (1+x)^{8+8x+4x^2} = 1 + \frac{17x}{2} + \mathcal{O}(x^2), \quad x \to 0^+$$

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Private communication with L. Kovalev

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

Back to the 60s: Gaier's estimate of $\|f'\|_{\mathcal{H}^2(\mathbb{D})}$

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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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Outline

1. Dirac operator with ∞-mass boundary conditions

2. Upper bounds on the size of the spectral gap

3. Key ideas of the proof

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Lemma

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The disk or not the disk?

$$\begin{cases} |\Omega| = \pi \\ \Omega \not\cong \mathbb{D} \end{cases} \quad \overset{??}{\Longrightarrow} \quad \mu_1(\Omega) > \mu_1(\mathbb{D}).$$

Thank you

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V. L. and T. Oumières-Bonafos, A sharp upper bound on the spectral gap for graphene quantum dots, *to appear in Math. Phys. Anal. Geom.*, arXiv:1812.03029.

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Thank you for your attention!