Spectra of graphene nanoribbons with armchair and zigzag boundary conditions

Petr Siegl

GFM University of Lisbon, Portugal

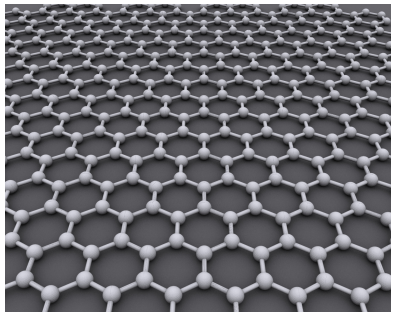
Joint work with P. Freitas (GFM-UL, Portugal)

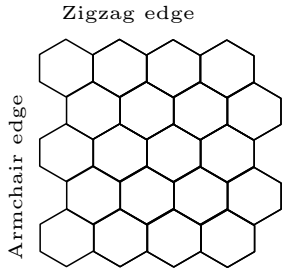
Outline

Introduction

Graphene

- 2D material, one layer sheet of carbon atoms





- many interesting physical properties
  - both metallic and semiconducting properties
  - anomalous quantum Hall effect, nonlinear Kerr effect, spintronics, Casimir effect, ...[a]
  - Nobel Prize in Physics for 2010 to A. Geim and K. Novoselov
- nanoribbons: strips of graphene[b]
- models: tight-binding (solid state physics), further approximations for low energies and long wavelenghts

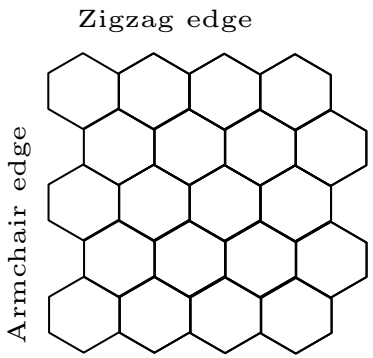
$\Rightarrow$ Dirac operator + boundary conditions[c d]

[a] A. H. Castro Neto et al. *Rev. Mod. Phys.* 81 (2009), pp. 109–162.
[b] M. Fujita et al. *J. Phys. Soc. Jpn.* 65 (1996), pp. 1920–1923.
[c] L. Brey and H. A. Fertig. *Phys. Rev. B* 73 (2006), p. 235411.
[d] A. R. Akhmerov and C. W. J. Beenakker. *Phys. Rev. B* 77 (2008), p. 085423.

Model

Domain $\Omega \subset \mathbb{R}^2$ and space

- finite rectangle (strip)
- arbitrary sufficiently regular
- infinite strip (waveguide)
- Hilbert space $L^2(\Omega, \mathbb{C}^k)$, $(k = 2, 4)$



Operator

$$H := \begin{pmatrix} 0 & \tau^* & 0 & 0 \\ \tau & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tau \\ 0 & 0 & -\tau^* & 0 \end{pmatrix}, \qquad \begin{aligned} \tau &:= -i\partial_1 + \partial_2, \\ \tau^* &:= -i\partial_1 - \partial_2 \end{aligned}$$

Boundary conditions

Zig-zag BC

$$\begin{aligned} \Psi_1(x_1, -b) &= 0, \\ \Psi_2(x_1, b) &= 0, \\ \Psi_3(x_1, -b) &= 0, \\ \Psi_4(x_1, b) &= 0. \end{aligned}$$

Armchair BC

$$\begin{aligned} \Psi_1(-a, x_2) &= \Psi_3(-a, x_2), \\ \Psi_2(-a, x_2) &= \Psi_4(-a, x_2) \\ \Psi_1(a, x_2) &= e^{\mathrm{i}\Theta}\Psi_3(a, x_2), \\ \Psi_2(a, x_2) &= e^{\mathrm{i}\Theta}\Psi_4(a, x_2), \quad \Theta \in \mathbb{R}. \end{aligned}$$

Model

Boundary conditions

Zig-zag BC

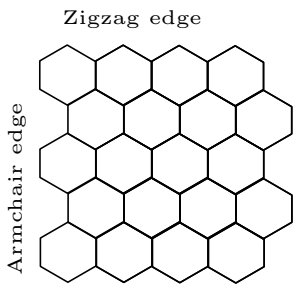
$$\begin{aligned}\Psi_1(x_1,-b)&=0,\\ \Psi_2(x_1,b)&=0,\\ \Psi_3(x_1,-b)&=0,\\ \Psi_4(x_1,b)&=0.\end{aligned}$$

Armchair BC

$$\begin{aligned}\Psi_1(-a,x_2)&=\Psi_3(-a,x_2),\\ \Psi_2(-a,x_2)&=\Psi_4(-a,x_2)\\ \Psi_1(a,x_2)&=e^{\mathrm{i}\Theta}\Psi_3(a,x_2),\\ \Psi_2(a,x_2)&=e^{\mathrm{i}\Theta}\Psi_4(a,x_2),\quad \Theta\in\mathbb{R}.\end{aligned}$$

Differences in boundary conditions

- armchair BC
  - only for specific directions
  - semi-conducting and metallic properties (depend on Θ)
- zig-zag BC
  - appropriate also for non-straight boundary
  - metallic behaviour, edge states
- substantial difference from the operator point of view
- realistic physical system: combination of zig-zag and armchair or manifolds (e.g. cylinder)



Armchair Example

Operator and BC

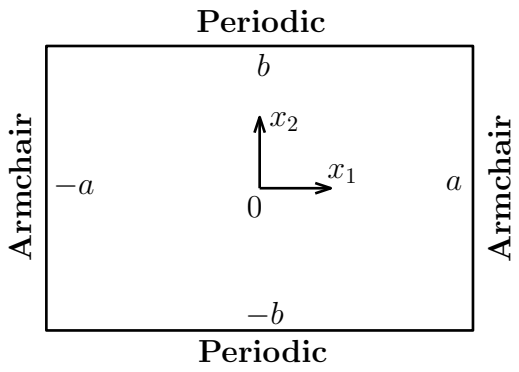
$$\dot{H}_{\mathrm{ap}} := \begin{pmatrix} 0 & \tau^* & 0 & 0 \\ \tau & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tau \\ 0 & 0 & -\tau^* & 0 \end{pmatrix}, \qquad \begin{aligned} \tau &:= -\mathrm{i}\partial_1 + \partial_2, \\ \tau^* &:= -\mathrm{i}\partial_1 - \partial_2 \end{aligned}$$

$$\mathrm{Dom}\,(\dot{H}_{\mathrm{ap}}) : \Psi \in C^1(\Omega, \mathbb{C}^4)$$

$$\begin{aligned} \text{Armchair}: \quad & \Psi_1(-a, x_2) = \Psi_3(-a, x_2), & \Psi_2(-a, x_2) = \Psi_4(-a, x_2) \\ & \Psi_1(a, x_2) = e^{\mathrm{i}\Theta}\Psi_3(a, x_2), & \Psi_2(a, x_2) = e^{\mathrm{i}\Theta}\Psi_4(a, x_2), \quad \Theta \in \mathbb{R}, \\ \text{Periodic}: \quad & \Psi_i(x_1, -b) = \Psi_i(x_1, b), (i = 1, \ldots, 4). \end{aligned}$$

Spectral problem for $\dot{H}^2_{\mathrm{ap}}$

$$\dot{H}^2_{\mathrm{ap}} = \begin{pmatrix} -\Delta & 0 & 0 & 0 \\ 0 & -\Delta & 0 & 0 \\ 0 & 0 & -\Delta & 0 \\ 0 & 0 & 0 & -\Delta \end{pmatrix}$$

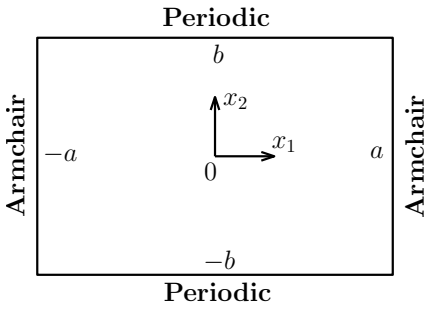


Armchair Example

Eigenvalues and eigenfunctions

- separation of variables: simple ODE problems
- eigenvalues:

$$\lambda_{m,n} = \sigma_m^2 + \zeta_n^2, \quad m, n \in \mathbb{Z},$$
$$\sigma_m = m\pi/b, \quad \zeta_n = n\pi/(2a) - \Theta/(4a).$$



- eigenfunctions:

$$\Psi_{m,n} = e^{\mathrm{i}\sigma_m x_2} \begin{pmatrix} Ae^{-\mathrm{i}\zeta_n x_1} \\ Be^{-\mathrm{i}\zeta_n x_1} \\ A(-1)^n e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_n x_1} \\ B(-1)^n e^{-\mathrm{i}\frac{\Theta}{2}} e^{\mathrm{i}\zeta_n x_1} \end{pmatrix}, \quad A, B \in \mathbb{C}.$$

- spectrum is discrete, $0 \in \sigma(\dot{H}_{\mathrm{ap}}^2)$ for some Θ
- eigenfunctions form orthonormal basis in $L^2(\Omega, \mathbb{C}^4)$, $\dot{H}_{\mathrm{ap}}^2$ is ess. self-adjoint
- spectrum of $\dot{H}_{\mathrm{ap}}$: $\pm\sqrt{\lambda_{m,n}}$ [a b]
- $\mathrm{Dom}\,(H_{\mathrm{ap}}) = W^{1,2}(\Omega, \mathbb{C}^4)$ + BC, graph norm $\|\dot{H}_{\mathrm{ap}}\Psi\|^2 + \|\Psi\|^2 = \|\Psi\|^2_{W^{1,2}}$

[a] L. Brey and H. A. Fertig. *Phys. Rev. B* 73 (2006), p. 235411.
[b] J Wurm et al. *New J. Phys.* 11 (2009), p. 095022.

Zigzag Example

Operator and BC

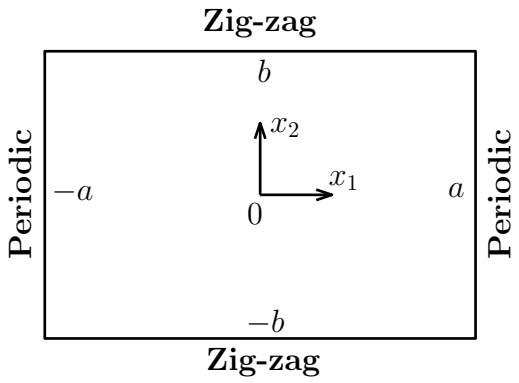
$$\dot{H}_{\mathrm{zp}} := \begin{pmatrix} 0 & \tau^* & 0 & 0 \\ \tau & 0 & 0 & 0 \\ 0 & 0 & 0 & -\tau \\ 0 & 0 & -\tau^* & 0 \end{pmatrix}, \qquad \begin{aligned} \tau &:= -\mathrm{i}\partial_1 + \partial_2, \\ \tau^* &:= -\mathrm{i}\partial_1 - \partial_2 \end{aligned}$$

$$\begin{aligned} \mathrm{Dom}\,(\dot{H}_{\mathrm{zp}}) &: \Psi \in C^1(\Omega, \mathbb{C}^4) \\ \mathrm{Zig-zag}: \quad & \Psi_1(x_1, -b) = 0, && \Psi_3(x_1, -b) = 0, \\ & \Psi_2(x_1, b) = 0, && \Psi_4(x_1, b) = 0, \\ \mathrm{Periodic}: \quad & \Psi_i(-a, x_2) = \Psi_i(a, x_2), (i = 1, \ldots, 4). \end{aligned}$$

Reduction

$$\dot{H}_{\mathrm{zp}} = \begin{pmatrix} 0 & \tau^* \\ \tau & 0 \end{pmatrix}$$

$$\begin{aligned} \mathrm{Zig-zag}: \quad & \Psi_1(x_1, -b) = 0, \ \Psi_2(x_1, b) = 0, \\ \mathrm{Periodic}: \quad & \Psi_i(-a, x_2) = \Psi_i(a, x_2) \end{aligned}$$



Zigzag Example

Spectrum of $\dot{H}^2_{\mathrm{zp}}$

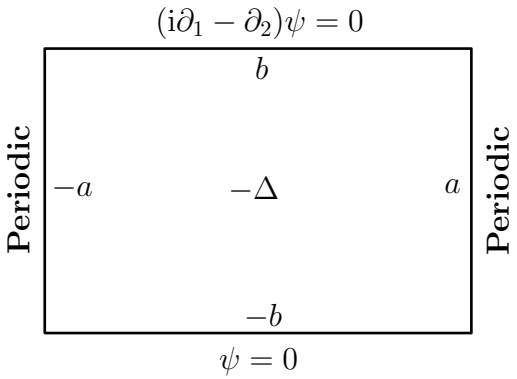
$$\dot{H}^2_{\mathrm{zp}} = \begin{pmatrix} -\Delta & 0 \\ 0 & -\Delta \end{pmatrix}$$

$$\begin{aligned} \mathrm{Zig-zag}: \quad & \Psi_1(x_1, -b) = 0, & \Psi_2(x_1, b) = 0, \\ & (\mathrm{i}\partial_1 - \partial_2)\Psi_1(x_1, b) = 0, & (\mathrm{i}\partial_1 + \partial_2)\Psi_2(x_1, -b) = 0, \\ \mathrm{Periodic}: \quad & \Psi_i(-a, x_2) = \Psi_i(a, x_2), & \\ & \partial_1\Psi_i(-a, x_2) = \partial_1\Psi_i(a, x_2). & \end{aligned}$$

Reduction II

$$\dot{H}^2_{\mathrm{zp}} = -\Delta$$

$$\begin{aligned} \mathrm{Zig-zag}: \quad & \psi(x_1, -b) = 0, & (\mathrm{i}\partial_1 - \partial_2)\psi(x_1, b) = 0, \\ \mathrm{Periodic}: \quad & \psi(-a, x_2) = \psi(a, x_2), & \partial_1\psi(-a, x_2) = \partial_1\psi(a, x_2). \end{aligned}$$

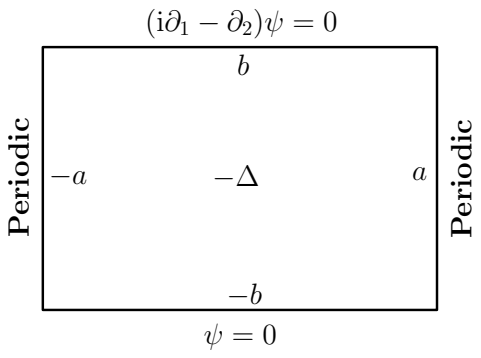


Zigzag Example

Spectrum of $\dot{H}^2_{\mathrm{zp}}$

- separation of variables:
  $\psi(x_1, x_2) = e^{-\mathrm{i}\sigma x_1}\xi(x_2)$
- periodic BC: $\sigma_m = m\pi/a, m \in \mathbb{Z}$
- "Cauchy-Riemann" BC:

$$\begin{cases} -\xi'' = \omega^2\xi & \text{in } (-b, b), \\ \xi = 0 & \text{at } -b, \\ \xi' - \sigma_m\xi = 0, & \text{at } b, \end{cases}$$



- $\lambda_{m,n} = \sigma_m^2 + \omega_{m,n}^2, \quad m \in \mathbb{Z}, n \in \mathbb{N}.$
- $\lambda_{m,1} \to 0$ as $m \to +\infty$, more precisely

$$\lambda_{m,1} = 4\sigma_m^2 e^{-4\sigma_m b} + \mathcal{O}(\sigma_m^4 e^{-8\sigma_m b}).$$

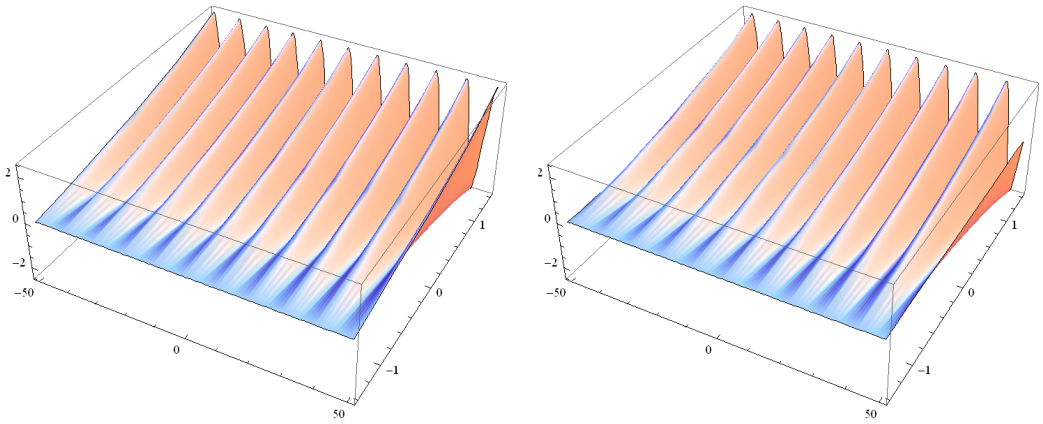
- $0 \in \sigma_{\mathrm{ess}}(\dot{H}^2_{\mathrm{zp}})$
- $\{\psi_{m,n}\}$ form orthonormal basis, $\sigma(\dot{H}_{\mathrm{zp}}) : \pm\sqrt{\lambda_{m,n}}$ [a] [b]

[a] L. Brey and H. A. Fertig. *Phys. Rev. B* 73 (2006), p. 235411.
[b] J Wurm et al. *New J. Phys.* 11 (2009), p. 095022.

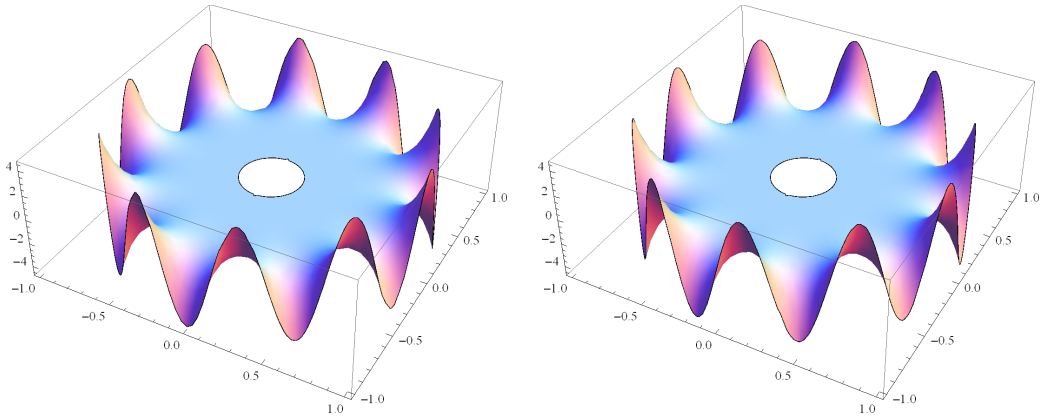
Zigzag Example

Eigenfunctions

- "usual" states: $\psi_{m,n} = e^{-\mathrm{i}\sigma_m x_1} \sin(\omega_{m,n}(x_2 + b))$
- "edge" states: $\psi_{m,n} = e^{-\mathrm{i}\sigma_m x_1} \sinh(\omega_{m,1}(x_2 + b))$, $m > m_0$



- analogous effect and calculations for annulus:



General situation

Aims

- understand spectra of Dirac operator with zigzag BC
- equivalently Laplacian with "Cauchy-Riemman" BC
- essential spectrum, explain and describe the edge states
- domains of definition
- perturbations by (diagonal) potential

Available mathematical literature

- 1995 K. M. Schmidt[a]
  - special case in 2D,
  - domains of definition, supersymmetry
- 1970 W. D. Evans[b c]
  - 3D problems (sphere and $\mathbb{R}^3$) with potentials
  - proofs based more on calculations (spherical symmetry, separation of variables)
  - perturbations, Glazman's decomposition method[d]

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[a] K. M. Schmidt. *The Quarterly Journal of Mathematics* 46 (1995), pp. 509–516.

[b] W. D. Evans. *The Quarterly Journal of Mathematics* 21 (1970), pp. 89–99.

[c] W. D. Evans. *Proceedings of the London Mathematical Society* s3-21 (1970), pp. 651–673.

[d] I. M. Glazman. *Direct methods of qualitative spectral analysis of singular differential operators*, 1965.

Definition of operator

Lemma (Self-adjointness):

Let T be closed, densely defined operator. Then

$$H = \begin{pmatrix} 0 & T^* \\ T & 0 \end{pmatrix}$$

is self-adjoint.

- we search for closed realization of $\tau = -\mathrm{i}\partial_1 + \partial_2$ and its adjoint τ^*

Proposition (SUSY):

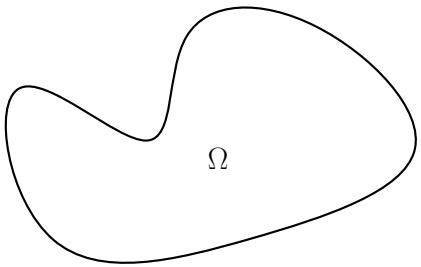
Let T be densely defined and closed. T^*T, TT^* are associated with the closed symmetric quadratic forms $t_{T^*T}[\psi] := \|T\psi\|^2$, $t_{TT^*}[\psi] := \|T^*\psi\|^2$ defined on $\mathrm{Dom}\,(T)$, $\mathrm{Dom}\,(T^*)$, respectively. Moreover, $\sigma(TT^*) \cup \{0\} = \sigma(T^*T) \cup \{0\}$.

- T^*T corresponds to Laplacian with "Cauchy-Riemann" BC
- $\mathrm{Dom}\,(T)$ is its form-domain
- proofs in 1993 Thaller[a]

[a] B. Thaller. Springer, 1993.

Schmidt's case

- arbitrary (sufficiently regular) domain Ω
- $H = \begin{pmatrix} 0 & \tau^* \\ \tau & 0 \end{pmatrix}$
- different BC (not precisely zig-zag): $\psi_1 \restriction \partial\Omega = 0$



Theorem [Schmidt'95]

[a] Let $\tau_0 := -\mathrm{i}\partial_1 + \partial_2$ be defined on $\mathrm{Dom}\,(\tau_0) := C_0^\infty(\Omega)$. Then

$$\tau := -\mathrm{i}\partial_1 + \partial_2,$$
$$\mathrm{Dom}\,(\tau) := W_0^{1,2}(\Omega),$$

is the closure of τ_0 and the adjoint reads

$$\tau^* := -\mathrm{i}\partial_1 - \partial_2,$$
$$\mathrm{Dom}\,(\tau^*) := \{\psi \in L^2(\Omega) \cap W_{\mathrm{loc}}^{1,2}(\Omega) : \tau^*\psi \in L^2(\Omega)\}.$$

[a] K. M. Schmidt. *The Quarterly Journal of Mathematics* 46 (1995), pp. 509–516.

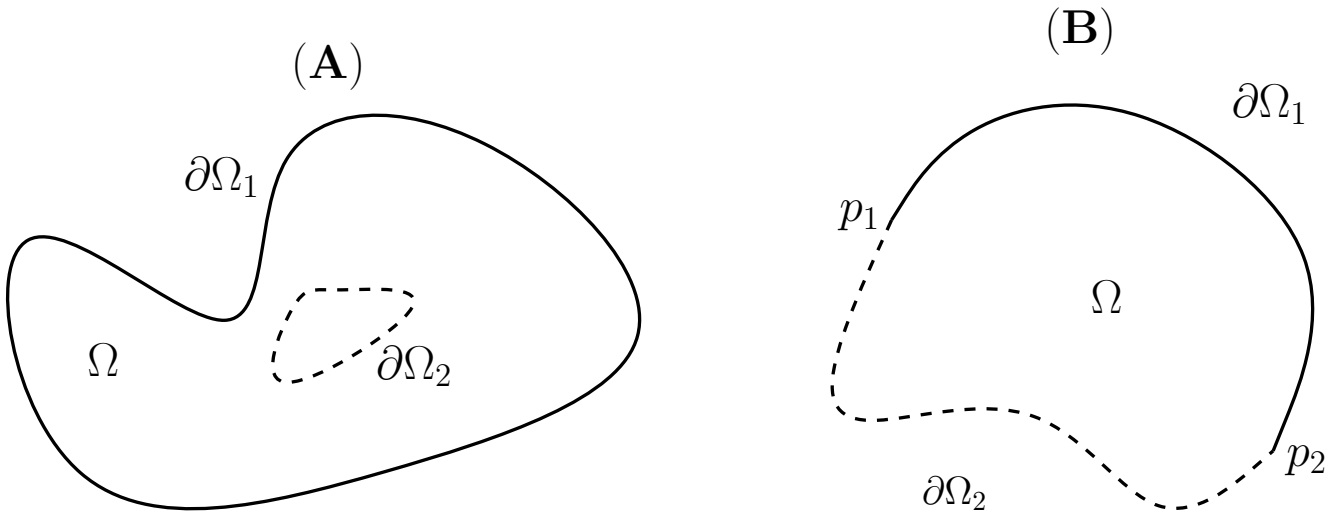
Schmidt's case

Corollaries [Schmidt'95]

- $H = \begin{pmatrix} 0 & \tau^* \\ \tau & 0 \end{pmatrix}$ is self-adjoint.
- $H^2 = \begin{pmatrix} \tau^*\tau & 0 \\ 0 & \tau\tau^* \end{pmatrix}$
- $\tau^*\tau = -\Delta_D$, *i.e.* $\mathrm{Dom}\,(\tau^*\tau) = W_0^{1,2}(\Omega) \cap W^{2,2}(\Omega)$.
- $\sigma(\tau^*\tau) = \sigma(-\Delta_D)$, *i.e.* discrete spectrum
- $\mathrm{Dom}\,(\tau^*)$ is larger than $W^{1,2}(\Omega)$
- $0 \in \sigma_{\mathrm{ess}}(\tau\tau^*)$, 0 is eigenvalue of infinite multiplicity
- $\{(x_1 + ix_2)^n\} \subset \mathrm{Ker}(\tau\tau^*)$
- $\sigma(\tau\tau^*) = \sigma(\tau^*\tau) \cup \{0\}$

More general situation

Complementary (**A**) and interchanging (**B**) BC



- in both cases:
$$\psi_1 \restriction \partial\Omega_1 = 0, \qquad \psi_2 \restriction \partial\Omega_2 = 0.$$
- we search for closed realization of τ and its adjoint
- description of domains of definition
- analysis of spectra

More general situation

Proposition [Freitas,PS] (**A**)

Let Ω be a bounded connected domain with a locally Lipschitz boundary $\partial\Omega$ that is made up of two nonempty connected components $\partial\Omega_i$ $(i = 1, 2)$ with $\operatorname{dist}(\partial\Omega_1, \partial\Omega_2) > 0$.
Let A be the operator acting as $A\psi := \tau\psi$ on the domain

$$\operatorname{Dom}(A) := \{\psi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1) : \psi \restriction \partial\Omega_1 = 0,\ \tau\psi \in L^2(\Omega)\},$$

where $W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1)$ means the functions from $W^{1,2}(\Omega')$ for any $\Omega' \subset \Omega$, $\overline{\Omega'} \subset \Omega \cup \partial\Omega_1$.
Then A is closed and A^* acts as $A^*\phi := \tau^*\phi$ on the domain

$$\operatorname{Dom}(A^*) := \{\phi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_2) : \phi \restriction \partial\Omega_2 = 0,\ \tau^*\phi \in L^2(\Omega)\}.$$

Remarks

- proof is a modification of Schmidt's case[a]
- A is a closure of τ defined on smooth functions satisfying BC

[a] K. M. Schmidt. *The Quarterly Journal of Mathematics* 46 (1995), pp. 509–516.

More general situation

Proposition [Freitas,PS] (B)

Let Ω be a bounded connected domain with locally Lipschitz and connected boundary $\partial\Omega$. Let further $p_i \in \partial\Omega$ be two distinct points such that $\partial\Omega = \partial\Omega_1 \cup \partial\Omega_2 \cup \{p_1, p_2\}$. If B_0 is an operator acting as τ on the domain

$$\mathrm{Dom}\,(B_0) := \{\psi \in C^\infty(\Omega) : \exists \psi_0 \in C_0^\infty(\mathbb{R}^2), \psi = \psi_0 \restriction \Omega, \mathrm{supp}\,\psi \cap \overline{\partial\Omega_1} = \emptyset\},$$

then B_0 is closable and

$$\mathscr{D}_0 + \mathscr{D}_{\mathrm{loc}} \subset \mathrm{Dom}\,(B) \subset \mathscr{D},$$

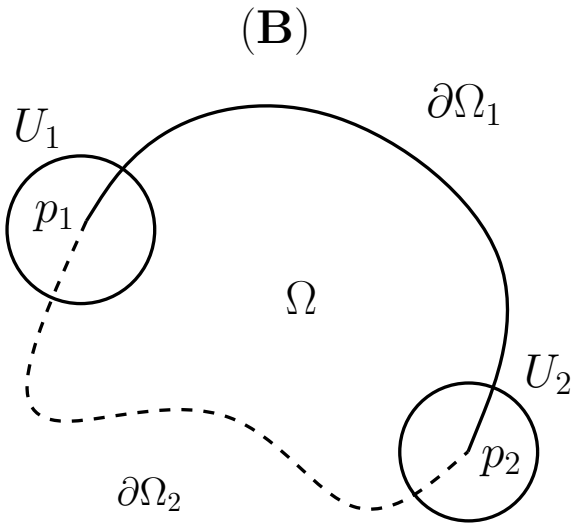
where

$$\begin{aligned}
\mathscr{D}_0 :=& \{\psi_1 \in W^{1,2}(\Omega) : \psi_1 \restriction \partial\Omega_1 = 0\},\\
\mathscr{D}_{\mathrm{loc}} :=& \{\psi_2 \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1) : \exists U_i \subset \mathbb{R}^2 \text{ open neighborhoods of } p_i,\ (i = 1, 2),\\
& \psi_2 \restriction U_{1,2} = 0, \tau\psi_2 \in L^2(\Omega)\},\\
\mathscr{D} :=& \{\psi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_1) : \psi \restriction \partial\Omega_1 = 0, \tau\psi \in L^2(\Omega)\}.
\end{aligned}$$

The adjoint operator $B_0^* = B^*$ reads

$$\begin{aligned}
& B_0^*\phi = \tau^*\phi,\\
& \mathrm{Dom}\,(B_0^*) = \{\phi \in L^2(\Omega) \cap W^{1,2}_{\mathrm{loc}}(\Omega \cup \partial\Omega_2) : \phi \restriction \partial\Omega_2 = 0, \tau^*\phi \in L^2(\Omega)\} =: \mathscr{D}^*.
\end{aligned}$$

More general situation



Remarks

- proof again a modification of the Schmidt's case
- part with $\mathscr{D}_0$ due to 2003 Kříž[a] and 2002 Dittrich & Kříž[b]
  - quantum waveguides with interchanging Dirichlet and Neumann boundary conditions
  - precise description of form and operator $(-\Delta)$ domains (larger than $W^{2,2}$)
- it is open if $\mathscr{D} \subset \mathrm{Dom}\,(B)$

[a] Jan Kříž. PhD thesis. Charles University Prague, 2003.

[b] J. Dittrich and J. Kříž. *Journal of Mathematical Physics* 43 (2002), pp. 3892–3915.

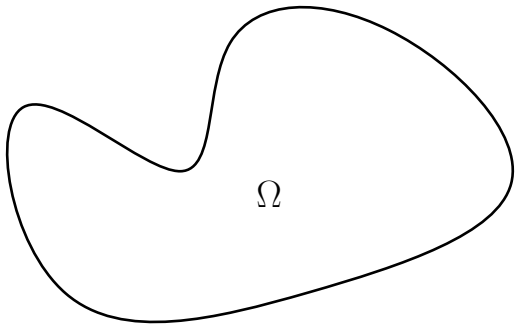
Zero is not an eigenvalue

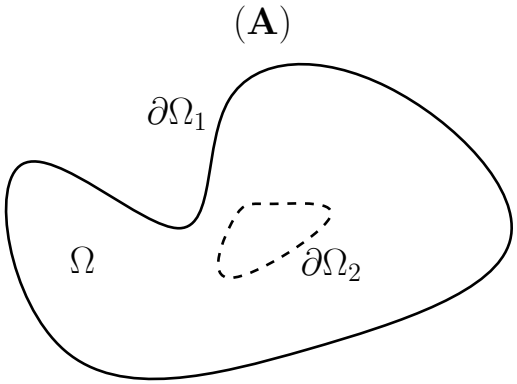
Proposition [Freitas,PS]

Zero is not an eigenvalue of either T^*T or TT^*, for $T = A, B$.

Proof and remarks

- eigenfunction ψ_0 satisfies $-\Delta\psi_0 = 0$ and $(-\mathrm{i}\partial_1 + \partial_2)\psi_0 = 0$ in any $\Omega' \subset \Omega$, $\overline{\Omega'} \subset \Omega \cup \partial\Omega_1$
- domains of definition (A, B) + embedding theorems $\Rightarrow \psi_0 \in C^\infty(\Omega')$ and $\psi_0 \in C(\overline{\Omega'})$
- ψ_0 is a holomorphic function in Ω' + zero on part of the boundary (with positive measure) $\Rightarrow \psi_0 = 0$





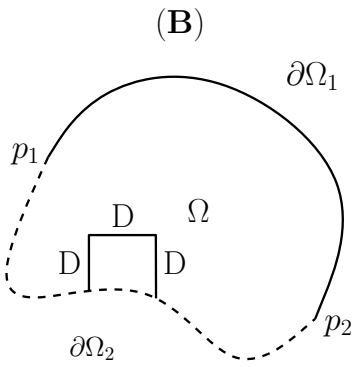
Zero is in the essential spectrum

Proposition [Freitas,PS]

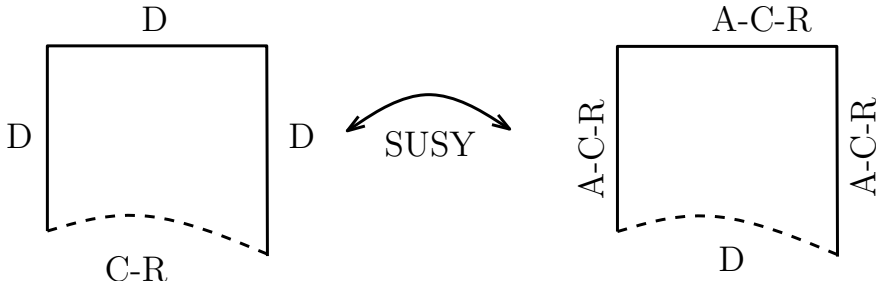
Zero is in the essential spectrum of both $T^* T$ and TT^*, $T = A, B$.

Proof and remarks

- Dirichlet bracketing argument



- SUSY and description of domains of definition



- particular singular sequence from "zig-zag – periodic" example
- 0 is not an eigenvalue

Local compactness

Local compactness of resolvent

- 0 is in the essential spectrum $\Rightarrow$ the resolvent of H^2 and H is not compact
- $\chi_K(H-z)^{-1}$ might be compact for compact $K \subset \Omega$
- local compactness of resolvent: typical for Schrödinger operators in $L^2(\mathbb{R}^n)$[a]
  - essential spectrum $\Leftrightarrow$ "behaviour at infinity"
  - singular sequences corresponding to $\lambda \in \sigma_{\text{ess}}$ must vanish in limit in every compact subset of $\mathbb{R}^n$
- for Dirac operators in $L^2(\mathbb{R}^n)$ valid as well[b]

[a] P. D. Hislop and I. M. Sigal. Springer Verlag, 1996.
[b] B. Thaller. Springer, 1993.

Proposition [Freitas,PS]

Let $\varphi_{1,2} \in C_0^\infty(\mathbb{R}^2)$ be such that $\operatorname{supp}\varphi_1 \cap \partial\Omega_2 = \emptyset$ and $\operatorname{supp}\varphi_2 \cap \partial\Omega_1 = \emptyset$. Then

$$\begin{pmatrix} \varphi_1 & 0 \\ 0 & \varphi_2 \end{pmatrix} \begin{pmatrix} -z & A^* \\ A & -z \end{pmatrix}^{-1}$$

is a compact operator in $L^2(\Omega, \mathbb{C}^2)$ for any $z \in \mathbb{C} \setminus \mathbb{R}$.

Edge states

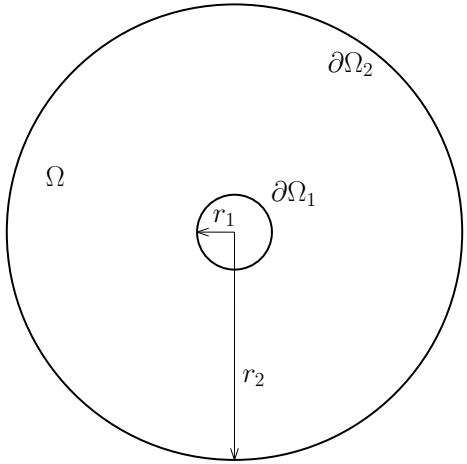
Proof

- description of domains of definition
- $\|\tau\psi\|^2 + \|\psi\|^2 = \|\psi\|^2_{W^{1,2}}$ for $\psi \in W_0^{1,2}$

Corollaries

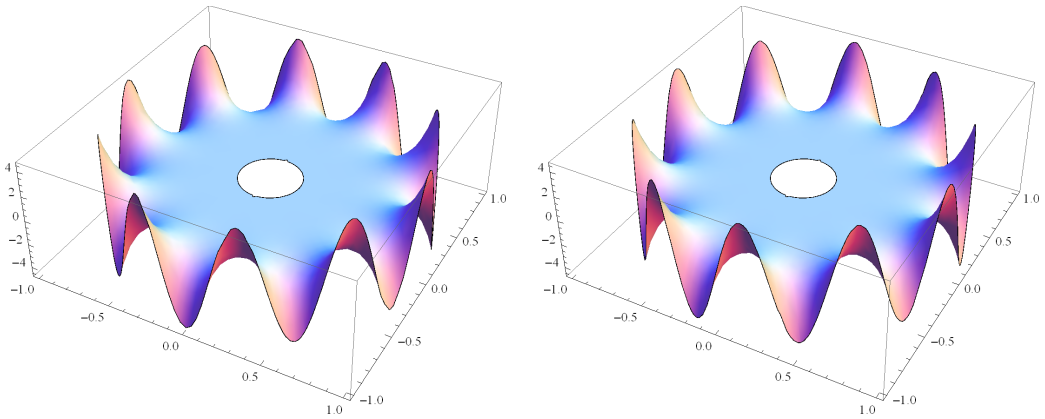
- 0 is the only point of essential spectrum of H in case (A)
  - singular sequences must squeeze to $\partial\Omega_1$ for $(\Psi_n)_2$ and $\partial\Omega_2$ for $(\Psi_n)_1$
  - we can construct a singular sequence $\{\Phi_n\}$ for which $(\Phi_n)_1$ and $(\Phi_n)_2$ are orthogonal
  - $\|(H-\lambda)\Phi_n\|^2 = \|\tau(\Phi_n)_1\|^2 + \|\tau^*(\Phi_n)_2\|^2 + |\lambda|^2\|\Phi_n\|^2 \to 0$
  - then $\Phi_n \to 0$, but $\|\Phi_n\| = 1$
- sequence of eigenfunctions associated with eigenvalues tending to zero must vanish in limit in every compact subset of Ω
  - explanation of features of edge states

Example annulus



Edge states

- $\lambda_{m,1} = \frac{-4m(1-m)}{r_2^2}\left(\frac{r_1}{r_2}\right)^{-2m} + \mathcal{O}\left(m^4(r_1/r_2)^{-4m}\right)$, as $m \to -\infty$



Potential perturbations

Proposition [Freitas,PS] (**A**)

Let $V \in L^\infty(\Omega)$ be a real potential. Let $U_\delta := \{x \in \Omega : \mathrm{dist}(x, \partial\Omega) < \delta\}$ and let denote $m_\delta := \operatorname{ess\,inf}_{U_\delta} V$, $M_\delta := \operatorname{ess\,sup}_{U_\delta} V$. Then $\sigma_{\mathrm{ess}}(H^A_{zz} + V) \subset \cap_{\delta>0}[m_\delta, M_\delta]$.

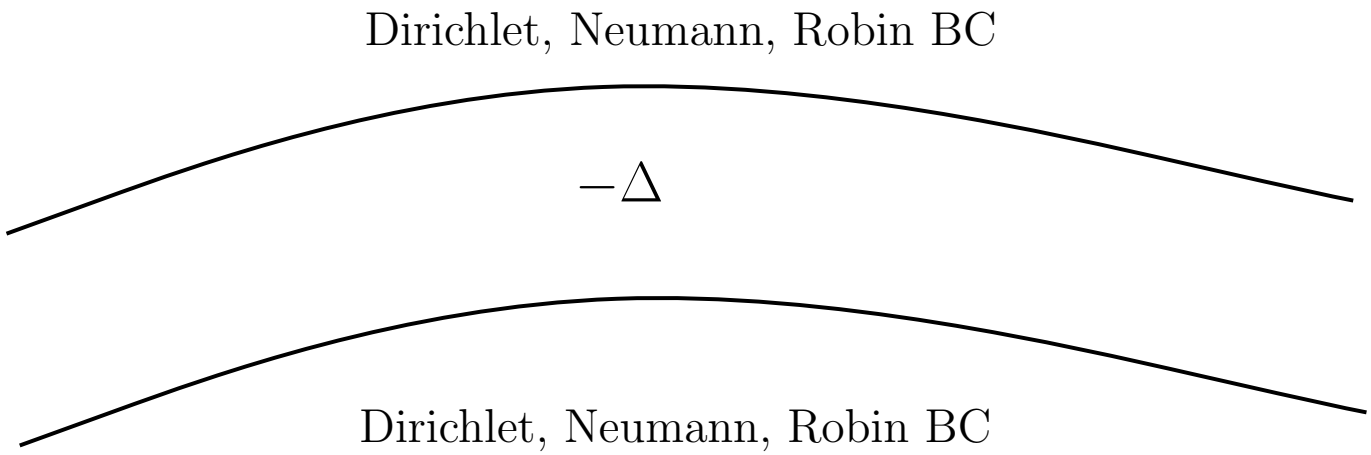
Proof and remarks

- proof: properties of singular sequences (local compactness) + simple estimates + criterion from Glazman[a]
- inspired by an analogous result of Evans[b] for Dirac operator in 3D ball
- if V is continuous: $\sigma_{\mathrm{ess}}(H + V) \subset [\min_{\partial\Omega} V, \max_{\partial\Omega} V]$
- further amendments possible
- weaker variant in (**B**) case

[a] I. M. Glazman. *Direct methods of qualitative spectral analysis of singular differential operators*, 1965.

[b] W. D. Evans. *Proceedings of the London Mathematical Society* s3-21 (1970), pp. 651–673.

Quantum waveguides



Motivation and literature

- straight planar strips: $\sigma_{\mathrm{ess}}(H) = [E_0, +\infty)$
  - E_0 depends on BC: $E_0^{(D)} = 2\pi/d$, $E_0^{(N)} = 0$
- what happens if the waveguide is bended?
  - bound states below essential spectrum[a b]
  - similar effects for strips on manifolds[c]
  - in 3D also twisting: oposite effect (Hardy inequality)[d]
- graphene waveguides?

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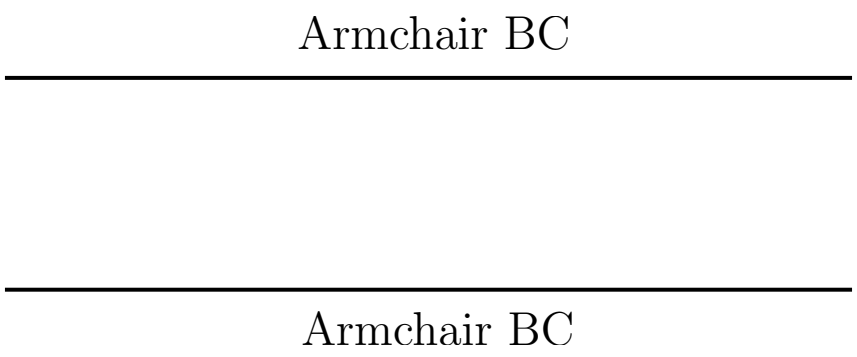
[a] P. Exner and P. Šeba. *J. Math. Phys.* 30 (1989), pp. 2574–2580.

[b] David Krejčiřík and Jan Kříž. *Publ. RIMS, Kyoto University* 41 (2005), pp. 757–791.

[c] David Krejčiřík. *J. Geom. Phys.* 45 (2003), pp. 203–217.

[d] T. Ekholm, H. Kovařík, and D. Krejčiřík. *Arch. Ration. Mech. Anal.* 188 (2008), pp. 245–264.

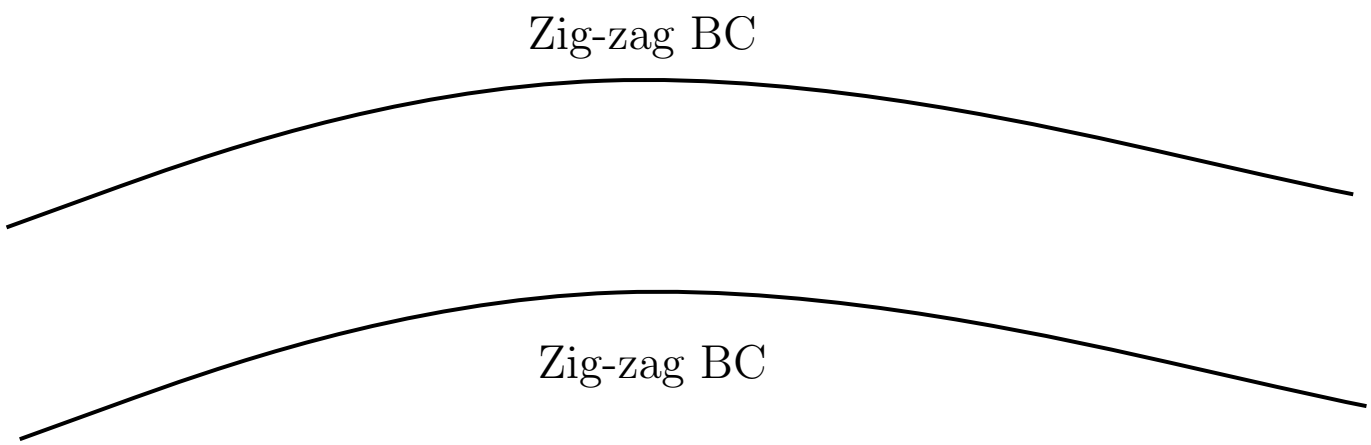
Armchair waveguide



Proposition [Freitas,PS]

$\sigma(H_{\mathrm{ac}}) = \sigma_{\mathrm{ess}}(H_{\mathrm{ac}}) = (-\infty, -E_0] \cup [E_0, +\infty)$, where $E_0 := \min_{n\in\mathbb{Z}} |\zeta_n|$ with $\zeta_n = n\pi/(2a) - \Theta/(4a)$.

Zig-zag waveguide



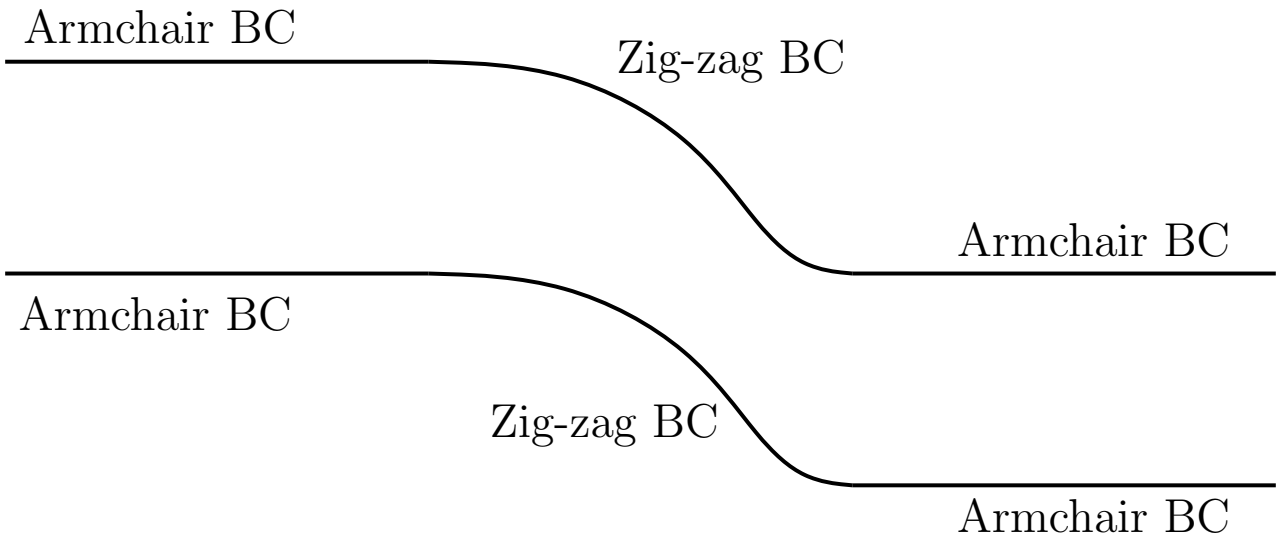
Proposition [Freitas,PS]

Let Ω be asymptotically straight, *i.e.* $\gamma(s) \to 0$ as $s \to \pm\infty$, then $\sigma_{\mathrm{ess}}(H_{\mathrm{zz}}) = \mathbb{R}$.

Proof

- construction of singular sequences for straight waveguide
- $\sigma_{\mathrm{ess}}(H) = \mathbb{R}$ due to edge states
- singular sequences can be modified for bent waveguide

Armchair–Zig-zag waveguide



Remarks

- difficulties with definition of operator H: essentially self-adjoint or more extensions?
- for H^2 definition via quadratic forms (Friedrichs extension)
- for H^2: $\sigma_{\mathrm{ess}}(H^2) \supset \{0\} \cup [E_0^2, +\infty)$
- variational techniques in the gap (if any) of essential spectrum (much harder)

Summary and further directions

Summary

- spectra of graphene nanoribbons
- armchair and zigzag boundary conditions
- 0 in essential spectrum
- edge states and their properties
- potential perturbations
- waveguides

Further directions

- physical restrictions for appearance of edge states (necessary high-frequencies)
- optimization problems (number, highest/lowest energies) for edge states
- non-trivial geometry (manifolds), lattice defects, magnetic fields (off-diagonal perturbations)
- combined wavequides
- non-self-adjoint perturbations (gains/losses)