Pauli equation with complex boundary conditions

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Based on:

D. Kochan, D. Krejčiřík, RN, P. Siegl, to appear in *J. Phys. A: Math. Theor.*, arXiv:1203.5011

Outline of the talk

Motivation

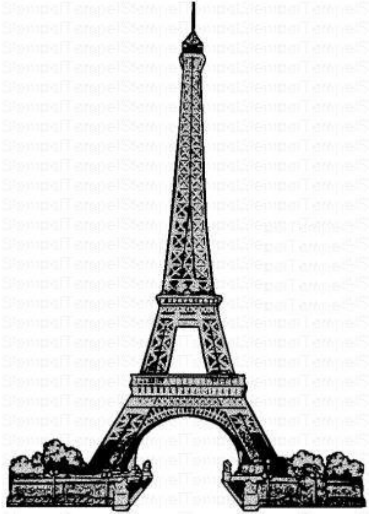
Mathematical model

Scattering motivation

Symmetries

Spectral analysis

Concluding remarks



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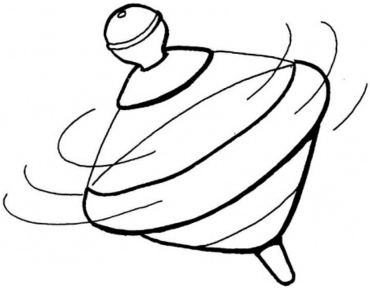
The motivation

- effort to extend Quantum mechanics with $\mathcal{PT}$-symmetric operators [BeBo98]

→ only similarity to self-adjoint operators [Mo02],[ScGeHa92]

- non-local self-adjoint operator → (non-self-adjoint) differential operator
- What about spin?



[BeBo98] 1998, Bender, Boettcher, *Physical Review Letters* 80

[Mo02] 2002, Mostafazadeh, *Journal of Mathematical Physics* 43

[ScGeHa92] 1992, Scholtz, Geyer, Hahne, *Annals of Physics* 213

Influence of the spin

- Pauli equation

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\Delta\Psi + \frac{\mu}{\hbar}\vec{B}\cdot\vec{L}\,\Psi + \frac{e^2}{8m}(\vec{B}\times\vec{x})^2\Psi + \mu\vec{B}\cdot\vec{\sigma}\,\Psi$$

  is $\mathcal{PT}$-symmetric on $\mathbb{R}^3$, not necessarily on $\Omega \subset \mathbb{R}^3$

- $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right)$

- complexification through boundary conditions

$$\frac{\partial\Psi}{\partial n} + A\Psi = 0 \qquad \text{on}\,\partial\Omega$$

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- complexification through boundary conditions

$$\frac{\partial\Psi}{\partial n} + A\Psi = 0 \qquad \text{on}\,\partial\Omega$$

- time-reversal operator $\mathcal{T}$ differs from complex conjugation

- for fermionic systems:

$$\mathcal{T}^2 = -1$$

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The model

- $H\Psi := -\frac{\hbar^2}{2m}\Delta\Psi + \frac{\mu}{\hbar}\vec{B}\cdot\vec{L}\,\Psi + \frac{e^2}{8m}(\vec{B}\times\vec{x})^2\Psi + \mu\vec{B}\cdot\vec{\sigma}\,\Psi$

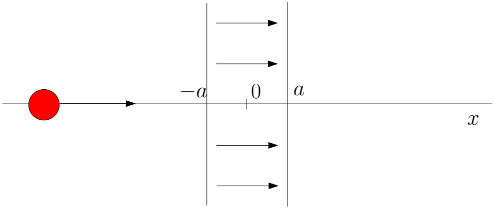
- homogeneous, time-independent field $\vec{B} := (0, 0, B)$

- $\vec{B}\cdot\vec{L}$ and $\vec{B}\times\vec{x}$ act in first two space variables
  $\vec{B}\cdot\vec{\sigma} = B\sigma_3$ acts in the third ($\sigma_3 = \mathrm{diag}(1, -1)$)

- $\Omega := \mathbb{R}^2 \times (-a, a)$

- matrix A constant on each connected component of $\partial\Omega$

→ separation of the problem → focus on the one dimensional problem in the third variable (denoted x)



The Hamiltonian

- $\mathscr{H} := L^2((-a, a); \mathbb{C}^2)$
- $\frac{\hbar^2}{2m} = 1$, $b = \mu B$

$$H_b := \begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b \end{pmatrix}$$

$$\mathrm{D}(H_b) := \left\{ \Psi \in H^2((-a, a); \mathbb{C}^2) \,\middle|\, \Psi'(\pm a) + A^{\pm}\Psi(\pm a) = 0, \quad A^{\pm} \in \mathbb{C}^{2,2} \right\}$$

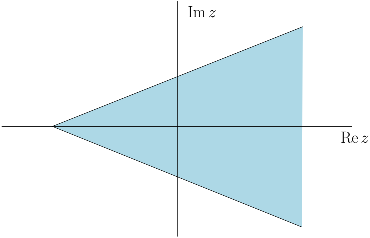
Sesquilinear form

- form associated with Hamiltonian: $h_b(\Phi, \Psi) := (\Phi, H_b\Psi)$

$$h_b(\Phi, \Psi) = (\Phi', \Psi') + b(\Phi, \sigma_3\Psi) + \overline{\Phi}^T(a)A^+\Psi(a) - \overline{\Phi}^T(-a)A^-\Psi(-a)$$
$$\mathrm{D}(h_b) := H^1((-a, a); \mathbb{C}^2),$$

- perturbation results $\rightarrow$ $h_b(\Phi, \Psi)$ is closed sectorial form

$\Rightarrow$ Representation theorem $\rightarrow$ a unique m-sectorial operator H_b on $\mathscr{H}$ such that $h_b(\Phi, \Psi) = (\Phi, H_b\Psi)$ for all $\Phi \in \mathrm{D}(h_b)$ and $\Psi \in \mathrm{D}(H_b) \subset \mathrm{D}(h_b)$



Adjoint operator

- in agreement with previous statements

$$H_b\Psi = \begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

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- H_b^* is easily found through $h_b^*(\Phi, \Psi) := \overline{h_b^*(\Psi, \Phi)}$

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$$H_b^*\Psi = \begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

$$\mathrm{D}(H_b^*) = \left\{ \Psi \in H^2((-a,a);\mathbb{C}^2) \,\middle|\, \Psi'(\pm a) + (A^{\pm})^*\Psi(\pm a) = 0 \right\}$$

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The scattering motivation

- generalized problem

$$\begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b + V(x) & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b + V(x) \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \lambda \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

where $V(x)$ is an electric potential supported in $(-a, a)$

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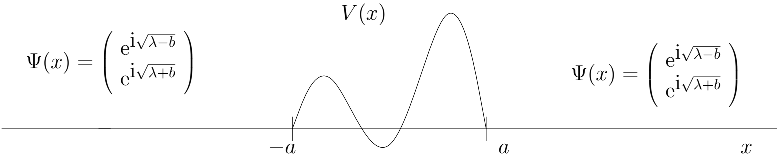
where $V(x)$ is an electric potential supported in $(-a, a)$

- Robin-type boundary conditions

$$\begin{pmatrix} \psi'_+(\pm a) \\ \psi'_-(\pm a) \end{pmatrix} + \begin{pmatrix} -\mathrm{i}\sqrt{\lambda - b} & 0 \\ 0 & -\mathrm{i}\sqrt{\lambda + b} \end{pmatrix} \begin{pmatrix} \psi_+(\pm a) \\ \psi_-(\pm a) \end{pmatrix} = 0$$



The scattering motivation

- solving the non-linear problem by one-parametric spectral problem [HCKrSi11]

$$\begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b + V(x) & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b + V(x) \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \lambda(\alpha) \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

$$\begin{pmatrix} \psi_+'(\pm a) \\ \psi_-'(\pm a) \end{pmatrix} + \begin{pmatrix} -\mathrm{i}\sqrt{\alpha - b} & 0 \\ 0 & -\mathrm{i}\sqrt{\alpha + b} \end{pmatrix} \begin{pmatrix} \psi_+(\pm a) \\ \psi_-(\pm a) \end{pmatrix} = 0$$

- solutions of the original problem are obtained using the dispersion relation

$$\lambda(\alpha_*) = \alpha_*$$

- solutions are perfect transmission energies
- complex points in the spectrum correspond to the loss of PTE's

[HCKrSi11] 2011, Hernandez-Coronado, Krejčiřík, Siegl, *Physics Letters A* 375

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Symmetries

How to choose $\mathcal{T}$ physically?

Maxwell equations

$$\mathrm{rot}\vec{B} = \mu_0\vec{j} + \mu_0\varepsilon_0\frac{\partial\vec{E}}{\partial t} \qquad \mathrm{rot}\vec{E} = -\frac{\partial\vec{B}}{\partial t}$$

$$\mathrm{div}\vec{E} = \frac{\rho}{\varepsilon_0} \qquad \mathrm{div}\vec{B} = 0,$$

where $\vec{E}$ *is electric field intensity,* $\vec{B}$ *is magnetic field induction*

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- time-reversal $\mathcal{T}$:
  - charge density $\rho \to \rho$, current density $\vec{j} \to -\vec{j}$

  $\Rightarrow$ $\vec{E} \to \vec{E}$, $\vec{B} \to -\vec{B}$

Symmetries

How to choose $\mathcal{T}$ physically?

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Definition

We say that linear operator H_0 is $\mathcal{PT}$-symmetric if it satisfies the relation $[H_0, \mathcal{PT}] = 0$.

- $(\mathcal{P}\Psi)(x) := \Psi(-x)$, $\qquad (\mathcal{T}\Psi)(x) := (\mathrm{i}\sigma_2\mathcal{K}\Psi)(x) = \begin{pmatrix} \overline{\psi_-(x)} \\ -\overline{\psi_+(x)} \end{pmatrix}$,

  $(\mathcal{K}\Psi)(x) := \overline{\Psi(x)}$

Symmetry properties of H_b

Definition

We say that a densely defined operator H on a Hilbert space is S-self-adjoint if $H^* = S^{-1}HS$ for some bounded and boundedly invertible operator S.

Proposition

H_0 *is*

- $\mathcal{PT}$*-symmetric if, and only if,* $A^- = \mathcal{T}A^+\mathcal{T}$

H_b *is*

- $\mathcal{PK}$*-symmetric if, and only if,* $A^- = -\mathcal{K}A^+\mathcal{K}$
- *self-adjoint if, and only if,* $(A^\pm)^* = A^\pm$
- $\mathcal{P}$*-self-adjoint if, and only if,* $A^- = -(A^+)^*$
- $\mathcal{T}$*-self-adjoint if, and only if,* $(A^\pm)^* = -\mathcal{T}A^\pm\mathcal{T}$
- $\mathcal{K}$*-self-adjoint if, and only if,* $(A^\pm)^* = -\mathcal{K}A^\pm\mathcal{K}$

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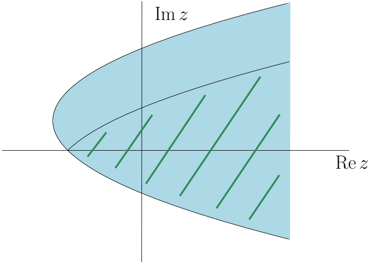
Basic notions about the spectrum of H_b

- S-self-adjointness with an antilinear $S \Rightarrow$ empty residual spectrum [BoKr08]
  - $\lambda \in \sigma_{\mathrm{p}}(H_b) \quad \Leftrightarrow \quad \overline{\lambda} \in \sigma_{\mathrm{p}}(H_b^*)$
  - $\sigma_{\mathrm{r}}(H_b) = \left\{ \lambda \in \mathbb{C} | \ \bar{\lambda} \in \sigma_{\mathrm{p}}(H_b^*) \quad \& \quad \lambda \notin \sigma_{\mathrm{p}}(H_b) \right\}$

- spectrum is enclosed in a parabola

- $\mathcal{PK}$-symmetry $\Rightarrow$ spectrum is symmetric with respect to the real axis



[KrSi10] 2008, Borisov, Krejčiřík, *Integral Equations Operator Theory* 62

Basic notions about the spectrum of H_b

- H_b is an operator with compact resolvent $\Rightarrow$ spectrum is purely discrete
- implicit equation for the eigenvalues

$$\begin{aligned}
&\Big(\det(A^+) + \det(A^-) - a_{11}^+ a_{22}^- - a_{22}^+ a_{11}^-\Big)\, k_- k_+ \cos(ak_-) \cos(ak_+) \\
&+ \Big(\det(A^+) \det(A^-) + a_{11}^+ a_{11}^- k_-^2 + a_{22}^+ a_{22}^- k_+^2 + k_-^2 k_+^2\Big) \sin(ak_-) \sin(ak_+) \\
&+ \Big(-\det(A^+) a_{22}^- + a_{22}^+ \det(A^-) + (-a_{11}^+ + a_{11}^-) k_-^2\Big)\, k_+ \sin(ak_-) \cos(ak_+) \\
&+ \Big(-\det(A^+) a_{11}^- + a_{11}^+ \det(A^-) + (-a_{22}^+ + a_{22}^-) k_+^2\Big)\, k_- \cos(ak_-) \sin(ak_+) \\
&+ \Big(a_{21}^+ a_{12}^- + a_{12}^+ a_{21}^-\Big)\, k_- k_+ = 0,
\end{aligned}$$

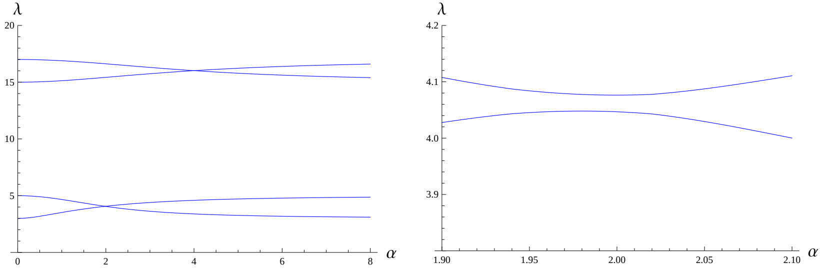
where $k_\pm = \sqrt{\lambda \mp b}$

$A^{\pm} = \begin{pmatrix} 0 & i\alpha \\ -i\alpha & 0 \end{pmatrix}$ - Self-adjoint example

Spectrum of H

$$\tan(ak_+)\cot(ak_-) + \tan(ak_-)\cot(ak_+) = -\frac{k_+^2 k_-^2 + \alpha^4}{\alpha^2}$$

$A = A^* \Rightarrow$ spectrum is real.



$A^{\pm} = \begin{pmatrix} i\alpha \pm \beta & 0 \\ 0 & i\alpha \pm \beta \end{pmatrix}$ - Decoupled non-Hermitian example

Spectrum of H

$$\Big(-2\beta k_- \cos(2ak_-) + (k_-^2 - \alpha^2 - \beta^2)\sin(2ak_-)\Big)$$
$$\times \Big(-2\beta k_+ \cos(2ak_+) + (k_+^2 - \alpha^2 - \beta^2)\sin(2ak_+)\Big) = 0$$

Studied for fixed β [KrSi10]

- $\beta = 0$
- $\beta > 0$
- $\beta < 0$

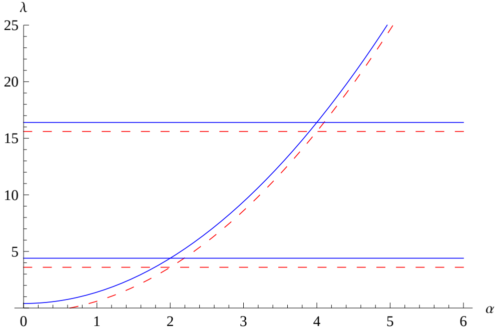
[KrSi10] 2010, Krejčiřík, Siegl, *Journal of Physics A: Mathematical and Theoretical* 43

$A^{\pm} = \begin{pmatrix} \mathrm{i}\alpha \pm \beta & 0 \\ 0 & \mathrm{i}\alpha \pm \beta \end{pmatrix}$ - Decoupled non-Hermitian example

Spectrum of H for $\beta = 0$
[KrBiZn06]

$$(k_-^2 - \alpha^2)(k_+^2 - \alpha^2)\sin(2ak_-)\sin(2ak_+) = 0$$

$$\lambda_{j,\pm} = \begin{cases} \alpha^2 \pm b, \\ \left(\frac{j\pi}{2a}\right)^2 \pm b \end{cases}$$



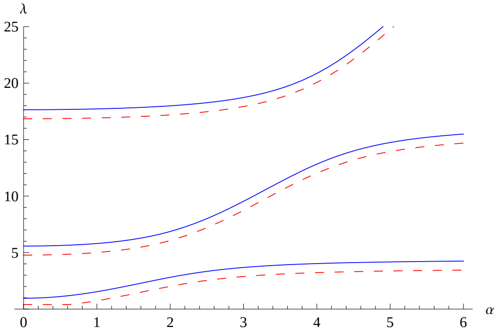
[KrBiZn06] 2006, Krejčiřík, Bíla, Znojil, *Journal of Physics A: Mathematical and General* 39

$A^{\pm} = \begin{pmatrix} i\alpha\pm\beta & 0 \\ 0 & i\alpha\pm\beta \end{pmatrix}$ - Decoupled non-Hermitian example

Spectrum of H for $\beta > 0$

$$\Big(-2\beta k_- \cos(2ak_-) + (k_-^2 - \alpha^2 - \beta^2)\sin(2ak_-)\Big)$$
$$\times \Big(-2\beta k_+ \cos(2ak_+) + (k_+^2 - \alpha^2 - \beta^2)\sin(2ak_+)\Big) = 0$$

Spectrum is real.

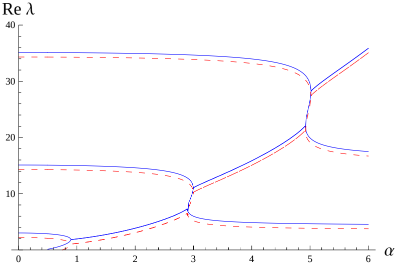


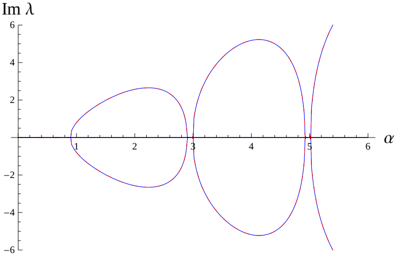
$A^{\pm} = \begin{pmatrix} i\alpha\pm\beta & 0 \\ 0 & i\alpha\pm\beta \end{pmatrix}$ - Decoupled non-Hermitian example

Spectrum of H for $\beta < 0$

$$\left(-2\beta k_- \cos(2ak_-) + (k_-^2 - \alpha^2 - \beta^2)\sin(2ak_-)\right)$$
$$\times \left(-2\beta k_+ \cos(2ak_+) + (k_+^2 - \alpha^2 - \beta^2)\sin(2ak_+)\right) = 0$$

- complex-conjugated pairs of eigenvalues appear in the spectrum.
- simultaneously at most only two pairs





$A^{\pm} = \begin{pmatrix} i\alpha \pm \beta & 0 \\ 0 & i\alpha \pm \beta \end{pmatrix}$ - Decoupled non-Hermitian example

Existence of the (bounded) metric operator

$$\Theta := \begin{pmatrix} I + K & 0 \\ 0 & I + K \end{pmatrix}$$

- K is an integral operator with kernel [KrSiZe11]

  $$K(x, y) := e^{i\alpha(x-y)-\beta|x-y|} \left(c + i\alpha \operatorname{sgn}(x-y) \right),$$

  where c is an arbitrary constant

- metric is positive if β is positive and large; or α is small; or $|\alpha|$ and $|c|$ are small

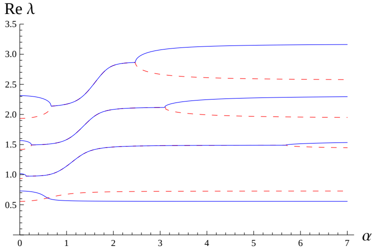
[KrBiZn06] 2006, Krejčiřík, Siegl, Železný, *Preprint* arXiv:1108.4946

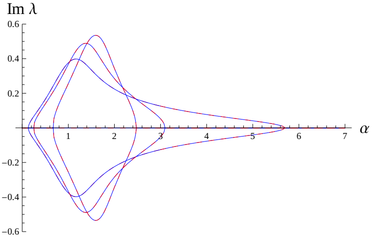
$A^{\pm} = \begin{pmatrix} 0 & \pm i\alpha \\ \pm i\alpha & 0 \end{pmatrix}$ - Coupled non-Hermitian example

Spectrum of H

$$4\alpha^2 k_+ k_- \cos(ak_+)^2 \cos(ak_-)^2 + 4\alpha^2 k_+ k_- \sin(ak_+)^2 \sin(ak_-)^2 = -(k_+ k_- + \alpha^4) \sin(2ak_+) \sin(2ak_-).$$

- complex-conjugated pairs of eigenvalues appear in the spectrum.
- simultaneously multiple pairs





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Concluding remarks

- investigation of the role of spin in $\mathcal{PT}$-symmetric quantum mechanics
- special attention to the physical choice of operator $\mathcal{T}$ ($\mathcal{T}^2 = -1$)
- physical realisation (scattering, metric)

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- special attention to the physical choice of operator $\mathcal{T}$ ($\mathcal{T}^2 = -1$)
- physical realisation (scattering, metric)

? connected boundary conditions

? similarity transformations

? self-adjoint counterparts of H_b

Thank you for your attention!