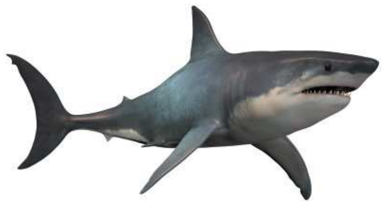
Do similar potential shapes lead to similar physical results?

A case study with two $\mathcal{PT}$-symmetric potentials

Géza Lévai

Institute for Nuclear Research (ATOMKI)
Debrecen, Hungary



PHHQP seminar, February 3, 2022

What is a quantum mechanical potential?

It represents the interaction of quantum mechanical particles

It is not the only way to account for this – see, e.g. PDM

Its concept is deeply rooted in physics

It has a classical correspondent

It is easy to visualize

Weak–strong, attractive–repulsive, long-range–short-range, etc.
In most cases it is an approximation, but sometimes it is reality

The solutions, i.e. the wave functions carry all physical information

It can be extended to the complex domain

Mainly to account phenomenologically for the loss of flux

With an opposite sign it can also account for increasing flux

$\mathcal{PT}$ *symmetry appears as a fine balance of these effects*

Problem: *the intuitive insight fades away with increasing non-hermiticity*

Symmetries generally have characteristic effect on the energy spectrum $[H, O] = 0$

$\mathcal{PT}$ symmetry is no exception $O = \mathcal{PT}$

$\mathcal{P}$: $x \to -x$ space reflection

$\mathcal{T}$: $t \to -t$ time reflection, essentially complex conjugation

For potentials in one dimension: $V^*(-x) = V(x)$

Real component: even function of x

Imaginary component: odd function of x

Delicate balance of emissive (gain) and absorptive (loss) regions

Mathematical interpretation

Relaxing the Hermiticity requirement

A special case of pseudo-Hemiticity

Unusual consequences:

Real energy eigenvalues... that can turn into complex conjugate pairs

Breakdown of $\mathcal{PT}$ symmetry

History: from a mathematical curiosity to optical experiments

Exact methods helped a lot in the understanding of $\mathcal{PT}$QM

Exact spectrum, wave functions, transmission and reflection coefficients

Even in the vicinity of critical parameter domains: at the **breakdown of $\mathcal{PT}$ symmetry**

We learned about interesting features

Potentials with the **same real** but **different imaginary** components may behave in essentially different way

The complexification of discrete energy eigenvalues occurs in a limited domain:

For **moderate** *imaginary potential component the E_n stay real*

A **too strong** *imaginary potential component may "freeze in" the E_n at real values* (See e.g. $\mathrm{i}x^3$)

Examples are the $\mathcal{PT}$-symmetric Scarf II and Rosen–Morse II potentials

For the Rosen–Morse II the E_n are always real

It has **finite, non-vanishing** imaginary potential component

Is this going to be the same in **other similar potentials** too?

The Scarf II potential

$$V(x) = -v_r \frac{1}{\cosh^2 x} + \mathrm{i} v_i \frac{\sinh x}{\cosh^2 x}\,, \qquad v_r = \left(\frac{\alpha+\beta}{2}\right)^2 + \left(\frac{\alpha-\beta}{2}\right)^2 - \frac{1}{4}\,, \quad v_i = 2\left(\frac{\beta+\alpha}{2}\right)\left(\frac{\beta-\alpha}{2}\right)$$

Relations for the parameters:

$\mathcal{PT}$ symmetry: $\Longrightarrow$ α, β are real **or** imaginary

$\alpha \leftrightarrow \beta$: $\Longrightarrow$ $V(x) \leftrightarrow V(-x)$

$V(x)$ invariant under $\alpha \leftrightarrow -\alpha$ $\Longrightarrow$ $q\alpha \equiv \pm\alpha$ quasi-parity

$$\psi_n^{(q)}(x) = C_n^{(q)} (1 - \mathrm{i}\sinh(x))^{\frac{q\alpha}{2}+\frac{1}{4}} (1 + \mathrm{i}\sinh(x))^{\frac{\beta}{2}+\frac{1}{4}} P_n^{(q\alpha,\beta)}(\mathrm{i}\sinh(x))$$

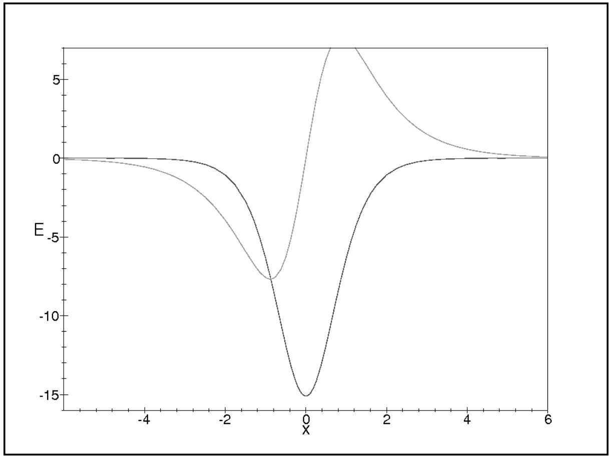
Normalizable if $\quad n^{(q)} < -[\mathrm{Re}(q\alpha + \beta) + 1]/2$

The second set corresponds to resonances in the Hermitian setting $(\alpha^* = \beta)$

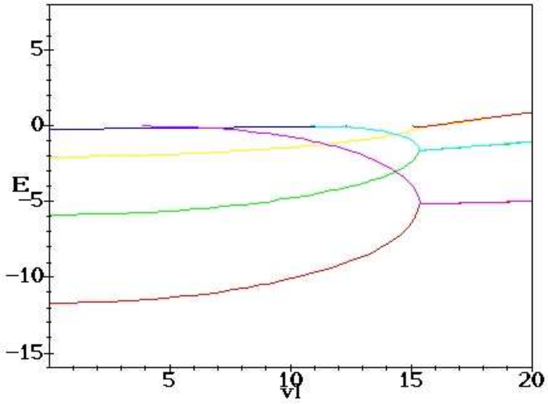
$$E_n^{(q)} = -\left(n + \frac{q\alpha + \beta + 1}{2}\right)^2$$

Complex conjugate pairs if α is imaginary Spontaneous breakdown of $\mathcal{PT}$ symmetry

The transition to complex energy eigenvalues



$v_r = 15.1,\ v_i = 12.7$

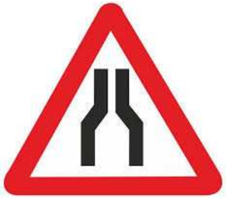


$v_i = 0 \rightarrow 20$

Complexification occurs for $|v_i| > v_r + 1/4$ for all n

Sudden mechanism of $\mathcal{PT}$ symmetry breaking

Real energy with $E_n^{(+)}$ and $E_n^{(-)}$ eigenvalues merge at the same v_i



Note: $\psi_0^{(-)}(x)$ normalizable for $v_i \geq 3.886$, $\psi_1^{(-)}(x)$ for $v_i \geq 10.858$, $\psi_2^{(-)}(x)$ for $v_i \geq 15.083$, $\psi_3^{(+)}(x)$ for $v_i \leq 12.325$

The Rosen–Morse II potential

G. Lévai, E. Magyari, J. Phys. A **42** (2009) 195302

$$V(x) = -v_r \frac{1}{\cosh^2(x)} + \mathrm{i} v_i \tanh(x) \ , \qquad v_r = s(s+1) \ , \quad v_i = 2\lambda$$

$\mathcal{PT}$ symmetry: $\Longrightarrow$ $s(s+1)$, λ are real

Only one solution can be regular at the same time take $\psi^{(+)}(x)$ to get bound states

$$E_n = -(s-n)^2 + \frac{\lambda^2}{(s-n)^2} \ , \qquad n = 0,\ 1,\ \ldots n_{\max} < s \ .$$

Peculiarities of the spectrum

No quasi-parity

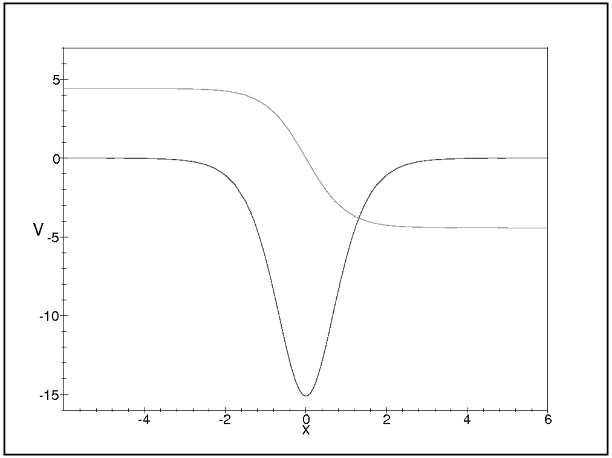
No complex energy eigenvalues **No** spontaneous breakdown of $\mathcal{PT}$ symmetry

But $E_n > 0$ if $s - |\lambda|^{1/2} \leq n < s$ increasing non-hermiticity

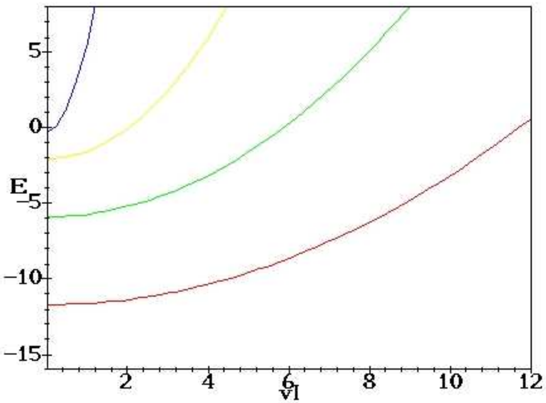
Furthermore for $|\lambda| > s^2$ **all** $E_n > 0$

This is very different from the Scarf II (and other) potentials...

$$V_R(\pm\infty) = 0 \qquad \text{BUT} \qquad V_I(\pm\infty) = \pm 2\mathrm{i}\lambda \neq 0$$



$v_r = 15.1,\ v_i = -4.42$



$-v_i = 0 \rightarrow 12$

Increasing non-hermiticity does not lead to complex energy eigenvalues.

Instead of that, the real energy eigenvalues shift to the positive domain.

It is somewhat similar to the $V(x) = \mathrm{i}x^3$ *potential*

But a real potential component is needed to have bound states

Note: v_i has no effect on the normalizability of the states

The finite $\mathcal{PT}$-symmetric square well potential

GL J. Kovács, J. Phys. A **52** *(2019) 025302*

A semi-analytically solvable "model" of the $\mathcal{PT}$-symmetric Rosen–Morse II potential

$$V(x) = \begin{cases} -\mathrm{i}v \ , & x < -a \\ -V_0 \ , & |x| < a \\ \mathrm{i}v \ , & x > a \end{cases}$$

$V_0 > 0$, $a > 0$, $\quad v \to 0$: the real finite square well potential

$$p_{\pm} = \left[\frac{2m}{\hbar^2}(E \mp \mathrm{i}v)\right]^{1/2} \ , \qquad k = \left[\frac{2m}{\hbar^2}(E + V_0)\right]^{1/2}$$

The general solutions:

$$\Psi(x) = \begin{cases} F^-(p_-)\exp(\mathrm{i}p_-x) + F^-(-p_-)\exp(-\mathrm{i}p_-x) \ , & x < -a \\ F^0(k)\exp(\mathrm{i}kx) + F^0(-k)\exp(-\mathrm{i}kx) \ , & |x| < a \\ F^+(p_+)\exp(\mathrm{i}p_+x) + F^-(-p_+)\exp(-\mathrm{i}p_+x) \ , & x > a \ , \end{cases}$$

$\Psi(x)$ and $[\Psi(x)]'$ have to be continuous at $x = \pm a$

These conditions will indirectly determine the discrete energy eigenvalues

Consider first the case of real E

$$p_- = [p_+]^* \ , \qquad k \quad \text{real}$$

Solutions with definite $\mathcal{PT}$ parity can be defined

$$\Psi_e(x) = \begin{cases} f^-(p_-)\exp(\mathrm{i}p_-x) + f^-(-p_-)\exp(-\mathrm{i}p_-x) \ , & x < -a \\ \alpha\cos(kx) + \mathrm{i}\beta\sin(kx) & |x| < a \ , \\ f^+(p_+)\exp(\mathrm{i}p_+x) + f^-(-p_+)\exp(-\mathrm{i}p_+x) \ , & x > a \ , \end{cases}$$

$$[f^-(p_-)]^* = f^+(p_+) \ , \quad [f^-(-p_-)]^* = f^+(-p_+) \ , \quad \alpha* = \alpha \ , \quad \beta^* = \beta$$

$$\Psi_o(x) = \begin{cases} g^-(p_-)\exp(\mathrm{i}p_-x) + g^-(-p_-)\exp(-\mathrm{i}p_-x) \ , & x < -a \\ \alpha\cos(kx) + \mathrm{i}\beta\sin(kx) & |x| < a \ , \\ g^+(p_+)\exp(\mathrm{i}p_+x) + g^-(-p_+)\exp(-\mathrm{i}p_+x) \ , & x > a \ , \end{cases}$$

$$[g^-(p_-)]^* = -g^+(p_+) \ , \quad [g^-(-p_-)]^* = -g^+(-p_+) \ , \quad \alpha* = -\alpha \ , \quad \beta^* = -\beta$$

Defining $\xi = ka$ and $\mu_\pm = p_\pm a$

$$f^+(p_+) = \frac{1}{2\mathrm{i}\mu_+}\left[\mathrm{i}\cos(\xi)(\alpha\mu_+ + \beta\xi) + \sin(\xi)(\beta\mu_+ + \alpha\xi)\right]\exp(-\mathrm{i}\mu_+)$$

with α and β real

$g^+(p_+)$ is the same, with α and β imaginary

Care should be taken in identifying waves travelling to left and right

The problem lies in the complex square root and in the imaginary component of $p_\pm$

$$p_\pm = \left[\frac{2m}{\hbar^2}(E \mp \mathrm{i}v)\right]^{1/2} = p_{\pm R} + \mathrm{i}p_{\pm I}$$

$$\exp(\pm\mathrm{i}p_\pm x) = \exp(\pm\mathrm{i}p_{\pm R}x)\exp(\mp p_{\pm I}x)$$

$$p_{+I} > 0 \quad \text{for} \quad v < 0, \qquad p_{-I} < 0 \quad \text{for} \quad v < 0$$

How to find normalisable solutions for real E?

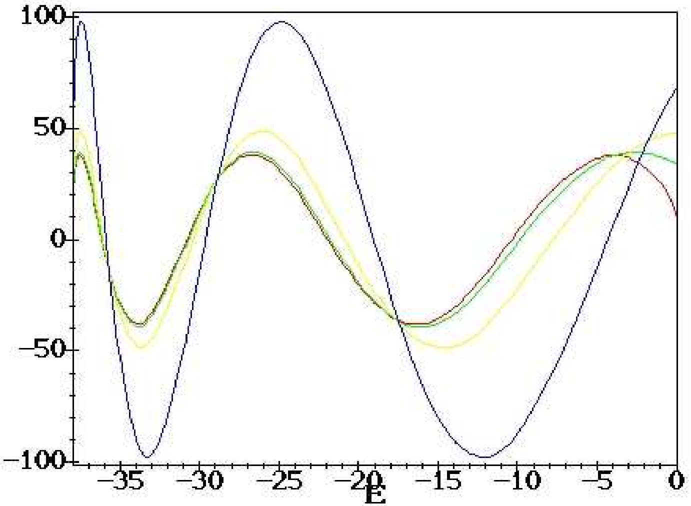
1. Take $[f(-p_-)]^* = f^+(-p_+) = 0$, and separate the real and imaginary components
2. Solve the resulting algebraic system of equations

$$\begin{aligned}(\xi \sin(\xi) - \mu_{+I}\cos(\xi))\alpha - \mu_{+R}\sin(\xi)\beta &= 0\\ \mu_{+R}\sin(\xi)\alpha - (\xi\cos(\xi) + \mu_{+I}\sin(\xi))\beta &= 0\end{aligned}$$

3. Set the 2×2 determinant to 0 to get

$$2\xi\mu_{+I}\cos(2\xi) + (\mu_{+R}^2 + \mu_{+I}^2 - \xi^2)\sin(2\xi) = 0$$

4. Find the roots in $E \in [-V_0, 0]$
$V_0 = 38$, $a = 1$, $v = 0$, -10, -30, -90



5. Determine β/α

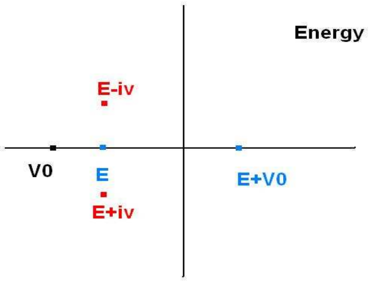
6. Combine it with the normalization condition

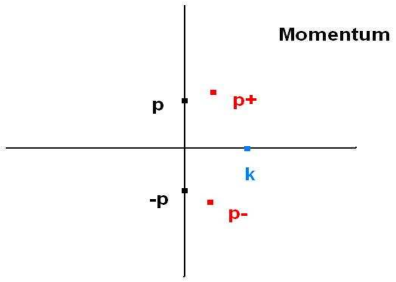
$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \Psi_e(x)[\mathcal{PT}\Psi_e(x)]\mathrm{d}x \\ &= -\mathrm{Im}([f^+(p_+)]^2 \exp(2\mathrm{i}\mu_+)a/\mu_+) + a(\alpha^2 - \beta^2) + a(\alpha^2 + \beta^2)\sin(2\xi)/(2\xi) \end{aligned}$$

7. Use real α and β to evaluate $f^+(p_+) = [f^-(p_-)]^*$

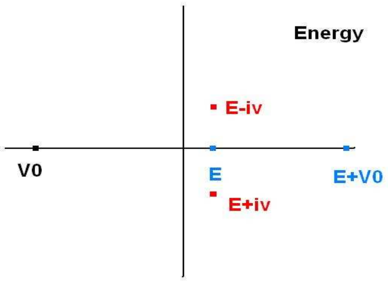
8. Construct $\Psi_e(x)$ ($\Psi_o(x)$ *can be obtained in the same way with imaginary* α *and* β*)*

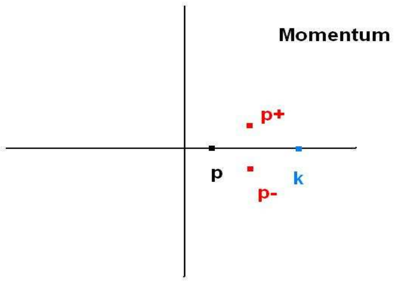
But what happens for $E > 0$?





$E < 0 \quad \Longrightarrow \quad E > 0$



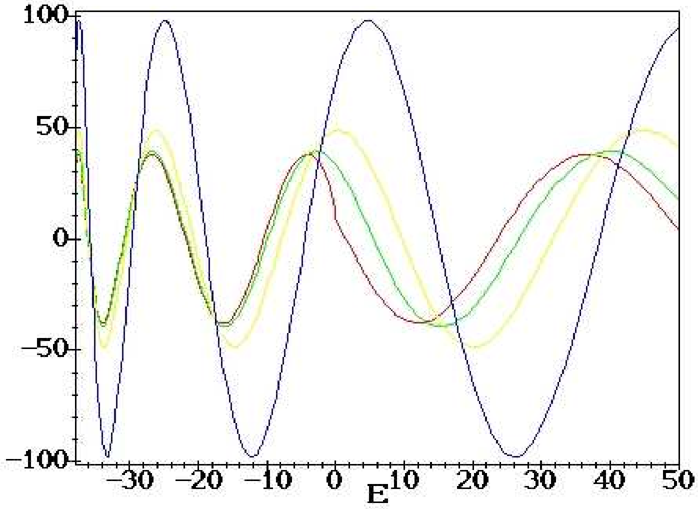


For the real case, $v = 0$, $p = E^{1/2}$ turns real from imaginary $\Longrightarrow$ **no bound states**

BUT in the $\mathcal{PT}$ case everything remains qualitatively the same: **bound states survive!**

Like in the Rosen–Morse II case

What does $[f(-p_-)]^* = f^+(-p_+) = 0$ mean in this case?



For $v = 0$: $p_- = p_+ = p$ real

$$\Psi(x) = \begin{cases} f^-(p)\mathrm{e}^{\mathrm{i}px}\,, & x < -a \\ \cos/\sin(kx)\,, & |x| < a\,, \\ f^+(p)\mathrm{e}^{\mathrm{i}px}\,, & x > a\,, \end{cases}$$

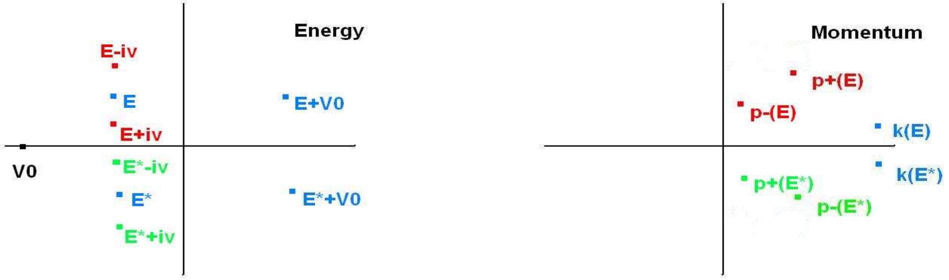
$T = 1$, perfect transition

For $v < 0$: $p_{+I} > 0$, $p_{-I} < 0$

$$\Psi(x) = \begin{cases} f^-(p_-)\mathrm{e}^{\mathrm{i}p_{-I}x}\mathrm{e}^{-p_{-I}x}\,, & x < -a \\ \alpha\cos(kx) + \mathrm{i}\beta\sin(kx) & |x| < a\,, \\ f^+(p_+)\mathrm{e}^{\mathrm{i}p_{+R}x}\mathrm{e}^{-p_{+I}x}\,, & x > a\,, \end{cases}$$

Normalizable states: $\lim_{x\to\pm\infty}|\Psi(x)| \to 0$

And what about complex E?



The relation between p_+ and $(p_-)^*$ does not hold anymore.

BUT new relations arise:

$$p_-(E) = [p_+(E^*)]^* \ , \qquad p_+(E) = [p_-(E^*)]^* \ , \qquad k(E) = [k(E^*)]^*$$

$$\mathcal{PT}\Psi(x,E) = \Psi(x,E^*)$$

Definite $\mathcal{PT}$-parity is lost

Are there normalizable complex-energy levels?

$\longrightarrow$ Does the $D(E)$ determinant have zeros off the real E axis?

If you like beer and sausages, then...

... you should try to avoid seeing how they are prepared.

The proof is presented in GL J. Kovács, J. Phys. A **52** (2019) 025302

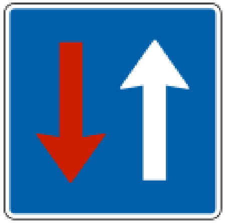
Assuming $\mathrm{Im}(E) \neq 0$ leads to contradiction.

Transmission and reflection for a wave arriving from the Right

Take real E

$$
\begin{aligned}
T_{R} &= \frac{f^{-}(-p_{-})g^{-}(p_{-}) - f^{-}(p_{-})g^{-}(-p_{-})}{f^{+}(-p_{+})g^{-}(p_{-}) - f^{-}(p_{-})g^{+}(-p_{+})} \\
&= \frac{2\mathrm{i}\xi\mu_{+}}{\mathrm{i}\xi(\mu_{+} + \mu_{+}^{*})\cos(2\xi) + (\xi^{2} + \mu_{+}\mu_{+}^{*})\sin(2\xi)} \exp[-\mathrm{i}(\mu_{+} + \mu_{+}^{*})] \ .
\end{aligned}
$$

$$
\begin{aligned}
R_{R} &= \frac{f^{+}(p_{+})g^{-}(p_{-}) - f^{-}(p_{-})g^{+}(p_{+})}{f^{+}(-p_{+})g^{-}(p_{-}) - f^{-}(p_{-})g^{+}(-p_{+})} \\
&= \frac{\mathrm{i}\xi(\mu_{+} - \mu_{+}^{*})\cos(2\xi) - (\xi^{2} - \mu_{+}\mu_{+}^{*})\sin(2\xi)}{\mathrm{i}\xi(\mu_{+} + \mu_{+}^{*})\cos(2\xi) + (\xi^{2} + \mu_{+}\mu_{+}^{*})\sin(2\xi)} \exp(-2\mathrm{i}\mu_{+})
\end{aligned}
$$



$$
T_{L} = \frac{p_{-}}{p_{+}} T_{R}
$$

$$
R_{L} = \frac{(\xi^{2} - \mu_{+}\mu_{+}^{*})\sin(2\xi) + \mathrm{i}\xi(\mu_{+} - \mu_{+}^{*})\cos(2\xi)}{(\xi^{2} - \mu_{+}\mu_{+}^{*})\sin(2\xi) - \mathrm{i}\xi(\mu_{+} - \mu_{+}^{*})\cos(2\xi)} \exp[2\mathrm{i}(\mu_{+} - \mu_{+}^{*})] R_{R} \ .
$$

Consistency check: $\mathcal{PT}$-symmetric Dirac-δ plus step potential

J. Kovács, GL: Acta Polytechnica **57** *(2017) 412*

$$V(x) = \gamma\delta(x) + \mathrm{i}2\Lambda\mathrm{sgn}(x)$$

One bound state at :

$$E_0 = -\frac{\gamma^2}{4} + \frac{4\Lambda^2}{\gamma^2}$$

$$\psi_0(x) = \begin{cases} C_0 \exp(-\kappa_+ x) & x > 0 \\ C_0 \exp(\kappa_- x) & x < 0 \end{cases}, \quad \kappa_\pm = -\frac{\gamma}{2} \mp \mathrm{i}\frac{2\Lambda}{\gamma} ,$$

Both potentials can be reduced to this system:

Rosen-Morse II: $x \to cx$, $c \to \infty$

$$\delta(x) = \lim_{c\to\infty} \frac{c}{2\cosh^2(cx)}$$

$$\mathrm{sgn}(x) = \lim_{c\to\infty} \tanh(cx) \ .$$

Finite square well potential:

$$V_0 = -\frac{\gamma}{2a} , \quad \Lambda = \frac{\nu}{2} \quad a \to 0$$

The results are reproduced in both limits

An interesting difference in the behavior of normalizable states

E is real and increases rapidly with increasing non-hermiticity

These states can be related to transmission resonances in the hermitian limits

Rosen-Morse II $\longrightarrow -s(s+1)\cosh^{-2}(x)$

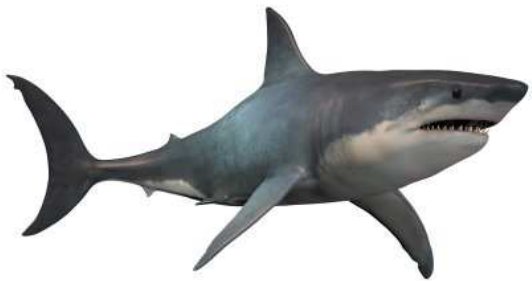
$T = 1$ for
all $E > 0$ and
specific depths: $s =$integer

SUSY partner of the free motion

Finite square well potential:

$T = 1$ for
all depths and
specific $E > 0$: $2ka = N\pi$

waves fit into the box



The global looks are smilar, but some details (e.g. the tailfins) are different.

Summary and conclusions

The Rosen–Morse II potential has real spectrum...

...with E_n that fly away as non-Hermiticity is increased

Perhaps due to the asymptotically non-vanishing $\mathrm{i}\tanh(x)$ term?

We constructed a "model" of the $\mathcal{PT}$-symmetric Rosen–Morse potential:

The finite $\mathcal{PT}$-symmetric square well potential *semi-analytically solvable*

Similar shape $\Longrightarrow$ *similar physics despite different mathematics*

Its main features were indeed found to mimic the Rosen–Morse II results:

Levels with real E_n stay normalizable for $E_n > 0$ and climb rapidly for increasing v

We proved that there are **NO** normalizable complex-energy solutions

Consistency check: the Dirac-δ + imaginary step potential, as a common limit