Singular perturbations and solvable models in one-dimensional quantum mechanics

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Outline of talk

- General remarks on point interactions in one dimension.
- Discussion on 1D Schrödinger equation with $\delta'(x)$ potential.
- Resonant tunneling through one-point (singular) potentials.
- Existence of bound states in $\delta'(x)$ potential.
- Point approximation of well-shaped potential revisited.
- Conclusions.

Point interactions in one dimension

Advantages of point interactions (PIs):

- Shrinking a system to isolated points (set of Lebesgue's measure zero) leads to exactly solvable models.
- These models are referred to as 'point' (contact or zero-range) interactions (PIs).
- Resolvents and spectra of Schrödinger operators, scattering coefficients and other characteristics can analytically be computed.

Connection matrix

1D Schrödinger equation:

$$-\psi''(x) + V(x)\psi(x) = E\psi(x).$$

If a PI is located at $x = 0$, it is identified by the two-sided boundary conditions: $\psi(\pm 0)$ and $\psi'(\pm 0)$.

Example

$V(x) = \alpha\delta(x)$ potential, $\delta(x)$ is Dirac's delta function:

$$\psi(+0) = \psi(-0) =: \psi(0), \quad \psi'(+0) - \psi'(-0) = \alpha\psi(0).$$

These boundary conditions can be written through a connection Λ-matrix:

$$\begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = \Lambda \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 1 & 0 \\ \alpha & 1 \end{pmatrix}.$$

Point interactions in one dimension

- All non-trivial PIs (at $x = \pm 0$) can be described by coupling (four-parametric) conditions (non-separated):

$$\begin{pmatrix} \psi(+0) \\ \psi'(+0) \end{pmatrix} = \Lambda \begin{pmatrix} \psi(-0) \\ \psi'(-0) \end{pmatrix}, \quad \Lambda = \mathrm{e}^{\mathrm{i}\chi} \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix},$$

$$\chi \in [0, \pi), \ \lambda_{ij} \in \mathbb{R}, \ \lambda_{11}\lambda_{22} - \lambda_{12}\lambda_{21} = 1.$$

- Trivial PIs (acting as a fully reflecting wall) are called separated.
- Example: $\lambda_{12} = 0$, λ_{11} and λ_{22} are finite but $|\lambda_{21}| = \infty$.
- Boundary conditions are $\psi(\pm 0) = 0$.

Albeverio S, Dabrowski L and Kurasov P 1998 *Lett. Math. Phys.* **45** 33.

Some literature:

- F.A. Berezin and L.D. Faddeev, *Dokl. Akad. Nauk SSSR* **137**, 1011 (1961) [*Sov. Math. Dokl.* **2**, 372 (1961)].
- Y.N. Demkov and V.N. Ostrovskii, *Zero-Range Potentials and their Applications in Atomic Physics* (Leningrad University Press, 1975) [Plenum Press, NY, 1988].
- S. Albeverio, F. Gesztesy, R. Høegh-Krohn, and H. Holden, *Solvable Models in Quantum Mechanics* (Springer, Berlin, 1988).
- S. Albeverio and P. Kurasov, *Singular Perturbations of Differential Operators: Solvable Schrödinger-Type Operators* (Cambridge University Press, Cambridge, 2000).
- S. Albeverio *et al.*, *Solvable Models in Quantum Mechanics (With an Appendix Written by Pavel Exner)*, 2nd revised ed. (AMS Chelsea Publishing, Providence, RI, 2005).

Some historical remarks on the δ'-problem

In *Phys. Scripta* (1994), for 1D Schrödinger equation

$$-\psi''(x) + V(x)\psi(x) = E\psi(x),\ E > 0,$$

Patil computed transmission probability for

$$V(x) = \gamma\delta'(x), \quad \gamma \in \mathbb{R},$$

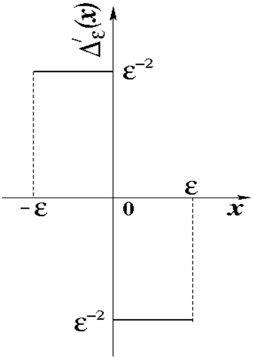
and found that the probability was identically zero.

Regularization of $\delta'(x)$ distribution has been done through Dirac's delta function $\delta(x)$:

$$\frac{\delta(x+\varepsilon) - \delta(x-\varepsilon)}{2\varepsilon} \to \delta'(x).$$

Patil S H 1994 *Phys. Scripta* **49** 645.

Resonant tunneling through a $\gamma\delta'(x)$ potential



- Finite barrier-well approximation (P. L. Christiansen *et al.*): $\Delta'_\varepsilon(x) \to \delta'(x)$,
- Countable set of values $\gamma \in \mathbb{R}$ in

$$-\psi''(x) + \gamma\delta'(x)\psi(x) = E\psi(x), \quad E > 0,$$

  where transmission was non-zero.
- These values form a resonance set $\Sigma := \{\gamma_n\}_{n\in\mathbb{Z}}$ with γ_n's being the roots of equation

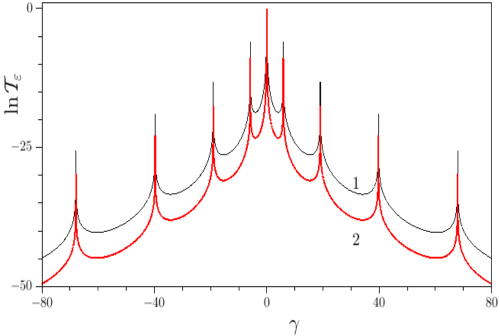
$$\tan\sqrt{\gamma} = \tanh\sqrt{\gamma}\,.$$

Beyond Σ ($\gamma \notin \Sigma$), transmission was shown to be zero.

Christiansen P L, Arnbak N C, Zolotaryuk A V, Ermakov V N and Gaididei Y B 2003 *J. Phys. A: Math. Gen.* **36** 7589.

Spire-like scenario of appearance of resonant tunneling

Convergence of transmission probability $\mathcal{T}_\varepsilon$ as $\varepsilon \to 0$ (numerical result):



$\mathcal{T}_\varepsilon \to 0$ occurs almost everywhere in the γ-space, but not everywhere!

$\varepsilon = 0.01$ (1, black),
$\varepsilon = 0.001$ (2, red).

P.L. Christiansen, N.C. Arnbak, A.Z., V.N. Ermakov and Y.B. Gaididei 2003 *J. Phys. A: Math. Gen.* **36** 7589.
A.Z. & Y.Z. 2015 *J. Phys. A: Math. Theor.* **48** 035302.

Šeba's theorem

In *Rep. Math. Phys.* , Šeba proved the theorem saying that for any regular function $\mathcal{V}(\xi)$ such that

$$\Delta'_\varepsilon(x) = \varepsilon^{-2}\mathcal{V}(x/\varepsilon) \to \delta'(x) \text{ as } \varepsilon \to 0,$$

the following norm resolvent convergence:

$$\text{N.R.} \lim_{\varepsilon \to 0} \left[H_0 + \gamma \Delta'_\varepsilon(x)\right] = H_0^- \oplus H_0^+$$

took place with boundary conditions $\psi(\pm 0) = 0$. This means zero transmission for all $\gamma \in \mathbb{R}$.

Šeba P 1986 *Rep. Math. Phys.* **24** 111.

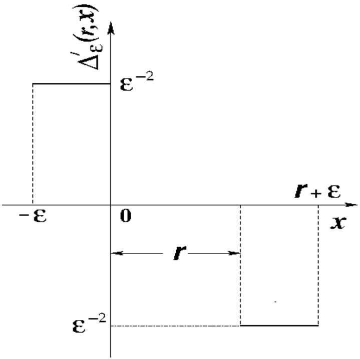
Clear discrepancy with our results!

Resolved in: Golovaty Y D and Hryniv R O 2010 J. Phys. A: Math. Theor. 43 155204.

However, Patil's result where, using the approximation

$$\frac{\delta(x+\varepsilon)-\delta(x-\varepsilon)}{2\varepsilon} \to \delta'(x),$$

he obtained zero transmission for all $\gamma \in \mathbb{R}$, appeared to be correct!



This mismatch can be explained using separated barrier and well.

Compare both the repeated limits of transmission $\mathcal{T}_\varepsilon(r)$:

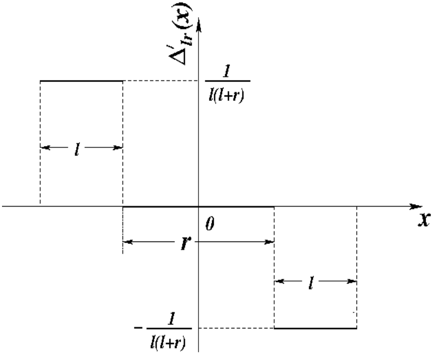
$$\lim_{\varepsilon\to 0}\lim_{r\to 0}\mathcal{T}_\varepsilon(r) \neq \lim_{r\to 0}\lim_{\varepsilon\to 0}\mathcal{T}_\varepsilon(r).$$

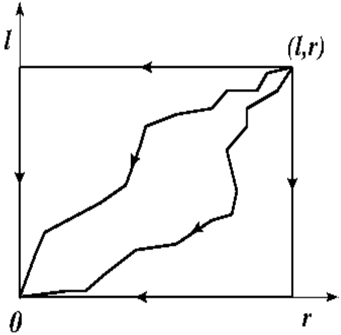
$\lim_{\varepsilon\to 0}\lim_{r\to 0}\mathcal{T}_\varepsilon(r) \to 0$ almost everywhere, while $\lim_{r\to 0}\lim_{\varepsilon\to 0}\mathcal{T}_\varepsilon(r) \to 0$ everywhere.

Two-scale regularization of $\delta(x)$ potential

Consider an antisymmetric regularization in the form of separated barrier and well:

$$\Delta'_{lr}(x) = \frac{1}{l(l+r)} \begin{cases} 1 & \text{for } -r/2 - l < x < -r/2, \\ -1 & \text{for } r/2 < x < r/2 + l, \\ 0, & \text{otherwise}, \end{cases} \qquad \to \quad \delta'(x).$$





Transmission matrix

Transmission matrix connecting $\psi(x)$ and $\psi'(x)$ at $x = \pm(l + r/2)$:

$$\begin{pmatrix} \psi(l+r/2) \\ \psi'(l+r/2) \end{pmatrix} = \Lambda_{lr} \begin{pmatrix} \psi(-l-r/2) \\ \psi'(-l-r/2) \end{pmatrix}, \quad \Lambda_{lr} = \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix}.$$

The Λ_{lr}-matrix can be computed as the product

$$\Lambda_{lr} = \Lambda^+ \Lambda_0 \Lambda^-,$$

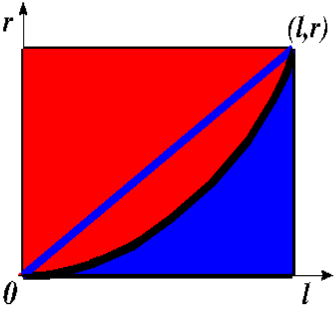
$$\Lambda^\pm = \begin{pmatrix} \cos(q^\pm l) & (1/q^\pm)\sin(q^\pm l) \\ -q^\pm \sin(q^\pm l) & \cos(q^\pm l) \end{pmatrix}, \quad \Lambda_0 = \begin{pmatrix} \cos(kr) & k^{-1}\sin(kr) \\ -k\sin(kr) & \cos(kr) \end{pmatrix}$$

$$q^\pm := \sqrt{E \pm \frac{\gamma}{l(l+r)}}, \quad \gamma \in \mathbb{R}.$$

Transmission matrix in the squeezing limit

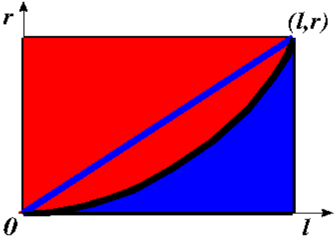
Specify the squeezing limit on pencil $r = cl^{\tau}$, $c > 0$, $\tau > 0$.
Asymptotically ($\gamma > 0$), $q^{+}l \sim \sigma$, $q^{-}l \sim \mathrm{i}\sigma$, $\sigma := \sqrt{\frac{\gamma}{1+cl^{\tau-1}}}$.
In the $l \to 0$ limit, $\lambda_{12} \to 0$, λ_{11} and λ_{22} are finite constants,

$$\frac{\lambda_{21}}{\cos\sigma\cosh\sigma} \sim \frac{\sigma}{l}(\tanh\sigma - \tan\sigma) - \frac{\sigma^2 r}{l^2}\tan\sigma\ \tanh\sigma.$$



- In red region ($0 < \tau < 1$, $1 < \tau < 2$), $|\lambda_{21}| \to \infty \quad \Rightarrow \psi(\pm 0) = 0$.
- In blue region ($\tau = 1$, $2 < \tau < \infty$), $\lambda_{21} \to 0$.
- On boundary black line ($\tau = 2$), $\lambda_{21} \to -c\gamma\ \sin\sqrt{\gamma}\ \sinh\sqrt{\gamma} =: \alpha$.

Two types of cancellation of divergences occur in λ_{21} as $l \to 0$.



$$\frac{\lambda_{21}}{\cos\sigma\cosh\sigma} \simeq \frac{\sigma}{l}(\tanh\sigma - \tan\sigma) - \frac{\sigma^2 r}{l^2}\tan\sigma\,\tanh\sigma.$$

- On blue line $\tau = 1$, resonance equation:

$$\tan\sqrt{\frac{\gamma}{1+c}} = \tanh\sqrt{\frac{\gamma}{1+c}}\left[1 + c\sqrt{\frac{\gamma}{1+c}}\tanh\sqrt{\frac{\gamma}{1+c}}\right]^{-1}, \quad \gamma \in \mathbb{R}.$$

- On black line and in blue region ($2 \le \tau < \infty$), resonance equation:

$$\tan\sqrt{\gamma} = \tanh\sqrt{\gamma}\,.$$

- Resonance sets: $\Sigma := \{\gamma_n\}_{n=-\infty}^{\infty}$.

Bound states for $\gamma\delta'(x)$ potential

Setting

$$\psi(x) = \begin{cases} C_1 \mathrm{e}^{\kappa x} & \text{for } -\infty < x < x_1 , \\ C_2 \mathrm{e}^{-\kappa x} & \text{for } x_2 < x < \infty, \end{cases}$$

one can prove a general equation for bound states:

$$\lambda_{12}\kappa^2 + (\lambda_{11} + \lambda_{22})\kappa + \lambda_{21} = 0,$$

where λ_{ij}-elements in general depend on κ.
Since $\lambda_{12} \to 0$ and on the pencil $r = c\, l^2$, $\lambda_{21} \neq 0$,

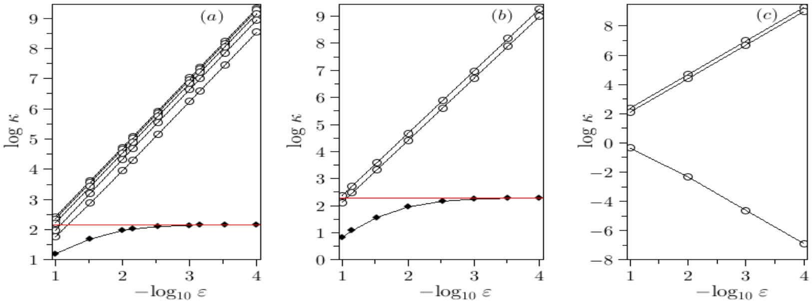
$$\kappa = -\frac{\lambda_{21}}{\lambda_{11} + \lambda_{22}} = -\frac{\alpha}{\theta + \theta^{-1}} = \frac{c}{2}\gamma \tanh^2\sqrt{\gamma} = \frac{c}{2}|\gamma| \tanh^2\sqrt{|\gamma|}\,,$$

where θ is the limit:

$$\lambda_{11} = \lambda_{22}^{-1} \to \theta = \frac{\cosh\sqrt{\gamma}}{\cos\sqrt{\gamma}}\,, \quad \gamma = \gamma_n, n \in \mathbb{Z}.$$

Scenario of appearance of a single bound state

Convergence of bound state levels κ_i's as $\varepsilon \to 0$:



(a) and (b): 'Pinning' of the highest energy level, whereas lower levels escape to $-\infty$; Red lines are analytical solutions.
(c): The highest level tends to zero ($r = c\,l^3$), while the lower one to $-\infty$.

A.Z. & Y.Z. *J. Phys. A: Math. Theor.* **54** (2021) 035201 (29pp).

Conclusions:

- Different pathways $\Delta'_\varepsilon(x) \to \delta'(x)$ lead to different PIs with boundary conditions:
  - separated, Dirichlet type: $\psi(-0) = \psi(+0) = 0$ (full reflection);
  - non-separated without bound states:
    $\psi(+0) = \theta_n \psi(-0), \;\; \psi'(+0) = \theta_n^{-1} \psi'(-0),$
    $\theta_n = \frac{\cosh\sqrt{\gamma_n}}{\cos\sqrt{\gamma_n}}, \quad \gamma_n \in \Sigma$ (resonant tunneling);
  - non-separated with bound states:
    $\psi(+0) = \theta_n \psi(-0), \;\; \psi'(+0) = \alpha_n \psi(-0) + \theta_n^{-1} \psi'(-0),$
    $\alpha_n = -\,c\,\gamma_n \sin\sqrt{\gamma_n} \sinh\sqrt{\gamma_n}$ (resonant tunneling).
- Equation $-\psi''(x) + \gamma\delta'(x)\psi(x) = E\psi(x)$ contains a hidden parameter.

Point approximation of a well-shaped potential

$$-\psi''(x) + V(x)V(x) = E\psi(x), \quad E > 0,$$
$$V(x) \equiv \begin{cases} V, & 0 < x < l, \\ 0, & \text{otherwise.} \end{cases}$$

$V > 0$ (barrier), $V < 0$ (well). Transmission probability:

$$\mathcal{T} = \left[1 + \frac{V^2}{4E(E-V)} \sin^2\left(\sqrt{E-V}\, l\right)\right]^{-1},$$

Point approximation: $V = \varepsilon^{-\nu} v$, $\nu > 0$. Only $\nu = 1$ and $\nu = 2$ are appropriate as $\varepsilon \to 0$.

$$\mathcal{T}_{\varepsilon \to 0}(\nu = 1) \to \frac{1}{1 + (\alpha/2k)^2}, \quad \alpha = vl(\text{strength of}\delta(x)), \alpha \in \mathbb{R}.$$

$$\mathcal{T} = \mathcal{T}_w = \lim_{\varepsilon \to 0} \mathcal{T}_{w,\varepsilon} = \begin{cases} 1 & \text{if } \sqrt{d}\, a = n\pi, \\ 0 & \text{if } \sqrt{d}\, a \neq n\pi, \end{cases} \qquad n = 1, 2, \ldots.$$

$$\Sigma := \{d, a \mid \sqrt{d}\, a = n\pi, \; n = 1, 2, \ldots\}.$$

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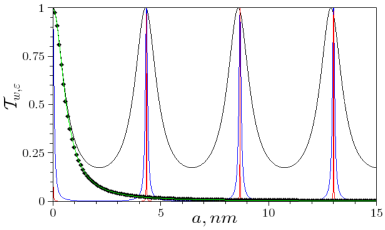
The point approximation of a well-shaped potential



- $\varepsilon = 1$ (black), unsqueezed (realistic);
- $\nu = 2$, $\varepsilon = 0.1$ (blue);
- $\nu = 2$, $\varepsilon = 0.01$ (red);
- $\nu = 1$, $\varepsilon = 0.01$ (green), δ-approximation.

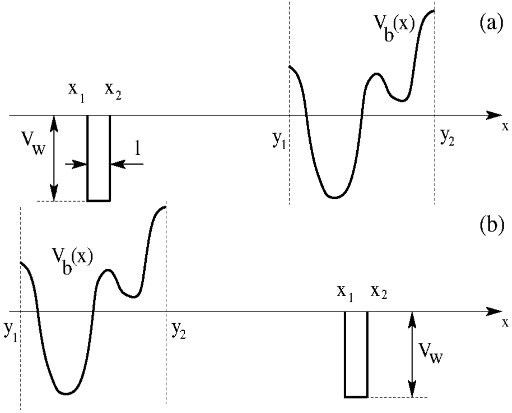
Conclusion: Both limits: $\lim_{\varepsilon\to 0} \mathcal{T}_{w,\varepsilon}(\nu = 1) = \left[1 + (\alpha/2k)^2\right]^{-1}$,

$$\lim_{\varepsilon\to 0} \mathcal{T}_{w,\varepsilon}(\nu = 2) = \begin{cases} 1 & \text{if } \sqrt{d}\, a = n\pi, \\ 0 & \text{if } \sqrt{d}\, a \neq n\pi, \end{cases} \quad n = 1, 2, \ldots,$$

are possible for a well. However, limit with $\nu = 2$ is more physically realistic. Resonance set is $\Sigma := \{d, a \mid \sqrt{d}\, a = n\pi,\ n = 1, 2, \ldots\}$. Potential $\varepsilon^{-2} V(x/\varepsilon)$ has no limit as $\varepsilon \to 0$, not even in the sense of (Schwartz) distributions.

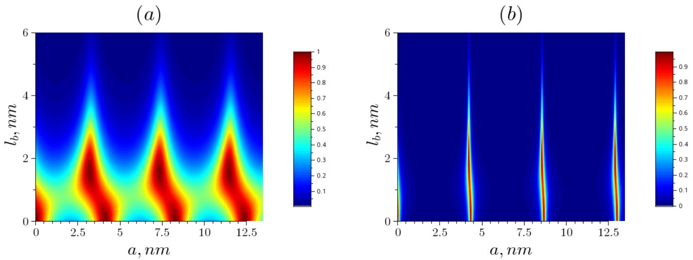
Y.Z & A.Z. *Annals of Physics* (to appear), arXiv:2407.01156 [quant-ph].

Bilayer = rectangular well + arbitrary barrier



$\rho \geq 0$ (distance)2

Influence of a squeezed prewell on tunneling



$\varepsilon = 1$ $\qquad$ $\varepsilon = 0.1$

$$\boxed{\mathcal{T} = \lim_{\varepsilon \to 0} \mathcal{T}_{w,\varepsilon} \cdot \mathcal{T}_b.}$$

Conclusions:

- Controlling of tunneling with tuning parameters of a well.
- “Quantization of Tunneling”.
- $V(x) = V_-(x) + V_+(x) \to \varepsilon^{-2} V_-(x/\varepsilon) + \varepsilon^{-1} V_+(x/\varepsilon)$.

Y.Z & A.Z. *Annals of Physics* (to appear), arXiv:2407.01156 [quant-ph].

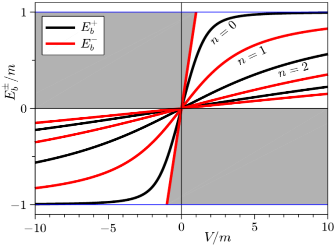
Dirac-like pseudospin-one structures

The 1D pseudospin-one Hamiltonian $H = H_0 + V(x)$:

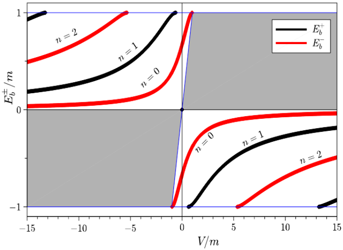
$$H_0 = -\mathrm{i} S_y \frac{d}{dx} + m S_z\,, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$V(x) = \begin{pmatrix} V_{11}(x) & 0 & 0 \\ 0 & V_{22}(x) & 0 \\ 0 & 0 & V_{33}(x) \end{pmatrix}.$$

$$\begin{pmatrix} 0 \\ V \\ 0 \end{pmatrix}$$



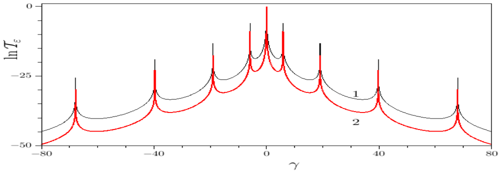
$$\begin{pmatrix} V \\ 0 \\ V \end{pmatrix}$$



A.Z., Y.Z., V.P. Gusynin, Bound states and point interactions of the one-dimensional pseudospin-one Hamiltonian, *J. Phys. A: Math. Theor.* **56** (2023) 485303 (33pp).

More conclusions

- Resonant tunneling through one-point (singular) potentials is a new phenomenon in the domain of point interactions.
- Enhancement of resonance properties with shrinking a nanosystem. This might be used for fabricating electronic devices. Spire-like picture is remarkable.



More conclusions

- Different regularizations of $\delta'(x)$ distribution produce different transmission properties of equation

$$-\psi''(x) + \gamma\delta'(x)\psi(x) = E\psi(x).$$

  Therefore this equation does not make any physical sense if considered alone (warning for physicists!), contrary to equation

$$\psi''(x) + \alpha\delta(x)\psi(x) = E\psi(x).$$

  The equation with $\delta'(x)$ distribution contains a hidden parameter. Family of regularization pathways can be considered as this parameter.
- Squeezed regular potentials themselves may or not may have a shrinking limit, even in the sense of distributions.

Vielen Dank
für Ihre Aufmerksamkeit!