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Discrete \mathcal{PT} -symmetric models of scattering**Miloslav Znojil**

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Online at stacks.iop.org/JPhysA/41/292002**Abstract**

One-dimensional scattering mediated by non-Hermitian Hamiltonians is studied. A schematic set of models is used which simulates two point interactions at a variable strength and distance. The feasibility of the exact construction of the amplitudes is achieved via the discretization of the coordinate. By direct construction it is shown that in all our models the probability is conserved. This feature is tentatively attributed to the space- and time-reflection symmetry (also known as \mathcal{PT} -symmetry) of our specific Hamiltonians.

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1. Introduction

In the absence of an external potential, the motion of a quantum particle is described by the kinetic-energy Hamiltonian $H_0 = -d^2/dx^2$ in one dimension ($\hbar = 2m = 1$). This operator is Hermitian and, incidentally, symmetric with respect to the space and time reflection (i.e., \mathcal{PT} -symmetric, $H_0\mathcal{PT} = \mathcal{PT}H_0$, cf many relevant comments on such a type of symmetry in [1]).

In an approximation where the real line is replaced by the mere discrete lattice of coordinates with some sufficiently small stepsize $h > 0$,

$$x_k = kh, \quad k = 0, \pm 1, \dots$$

the role of the kinetic energy is often being played by the doubly infinite tridiagonal matrices

$$H'_0 = \begin{bmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 2 & -1 & & & \\ & & -1 & 2 & -1 & & \\ & & & -1 & 2 & \ddots & \\ & & & & & \ddots & \ddots \end{bmatrix} \quad \text{or} \quad H_0 = \begin{bmatrix} \ddots & & & & & & \\ & \ddots & & & & & \\ & & 0 & -1 & & & \\ & & -1 & 0 & -1 & & \\ & & & -1 & 0 & \ddots & \\ & & & & & \ddots & \ddots \end{bmatrix}$$

which differ just by a trivial shift of the energy scale. Whenever we treat \mathcal{P} as the parity ($\mathcal{P}x_k = x_{-k}$) and the antilinear operator \mathcal{T} as the time reversal (i.e., in our present setting, transposition plus complex conjugation), we may represent the product-operator symmetry of our real matrices H_0 by the antidiagonal unit matrix

$$\mathcal{PT} = \begin{bmatrix} & & & \ddots & & & \\ & & & & 1 & & \\ & & & & & 1 & \\ & & & & & & 1 \\ \ddots & & & & & & \\ & & & & & & \end{bmatrix}. \tag{1}$$

Using this definition we shall demand that also all the nontrivial, doubly infinite discrete Hamiltonians $H = H_0 + W$ possessing a nonvanishing interaction term W will be required to be real and \mathcal{PT} -symmetric.

The matrix dimension of the interaction matrix W (i.e., the ‘range’ of the interaction) will be assumed finite. One expects that then the scattered states could stay asymptotically undistorted. In the mathematical terminology such an expectation means that we feel allowed to search for the solutions of the discrete and \mathcal{PT} -symmetric Schrödinger equations

$$(H_0 + W)\psi = E\psi \tag{2}$$

complemented by the *standard, undistorted* boundary conditions

$$\psi_m = \begin{cases} e^{im\varphi} + R e^{-im\varphi}, & m \leq -M, \\ T e^{im\varphi}, & m \geq M. \end{cases} \tag{3}$$

We should remind the readers that the standard re-parametrization of the energy $E = (2 - 2 \cos \varphi)/h^2$ in terms of the real angle $\varphi \in (0, \pi)$ should be used [2].

Our study has been inspired by a few papers on the scattering in a non-Hermitian scenario [3–5] and, in particular, by the Jones’ paper [6]. Unfortunately, its author worked in the differential-equation limit $h \rightarrow 0$ which made the detailed analysis perceptibly hindered by the non-Hermiticity of the equations. In effect, the feasibility requirements (cf [8]) restricted his attention to the mere \mathcal{PT} -asymmetric delta-function interactions, therefore.

In our subsequent comment [7] we facilitated the technicalities by the transition to the discretized equation (2). Having preserved the Jones’ philosophy we choose just the \mathcal{PT} -asymmetric models exemplified by the ‘ultralocal’, two-by-two matrix example

$$W^{(UL)} = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix}$$

such that $W^{(UL)}\mathcal{PT} \neq \mathcal{PT}W^{(UL)}$. Due to the discretization approximation $h > 0$ we were able to construct the explicit formulae for the reflection and transmission coefficients R and T , respectively,

$$R^{(UL)} = -\frac{a^2}{\Delta}, \quad T^{(UL)} = \frac{(1-a)(1-e^{2i\varphi})}{\Delta}, \quad \Delta = 1 - (1-a^2)e^{2i\varphi}.$$

We were also able to mimic the key features of the Jones' first-order perturbation results by another entirely exact and compact formula

$$|R^{(UL)}|^2 + |T^{(UL)}|^2 = \frac{1 - a[1 + U(a, \varphi)]^{-1}}{1 + a[1 + U(a, \varphi)]^{-1}}, \quad U(a, \varphi) = \frac{a^4}{2(1 - a)(1 - \cos 2\varphi)}.$$

This formula closely resembled the very similar Jones' perturbation results [6]. Hence, we could also parallel his conclusion that since the predicted sum appears greater than 1 or less than 1 (depending on the sign of the coupling a) it cannot be given the usual probabilistic interpretation. One must rather assume the presence of some respective 'unknown source' or 'unknown absorber' near the origin. Thus, in the effective-theory manner, the mathematical non-Hermiticity of the interaction terms W *precisely reflects* the presence of certain hidden physical mechanisms which violate the conservation of the number of particles.

In the context of the internal physical consistency of many non-Hermitian bound-state models [1] such an effective-theory physical interpretation of the scattering looks rather unsatisfactory. In what follows, for this reason, we shall try to re-install the \mathcal{PT} -symmetry in our matrix model(s) and study the consequences. For this purpose we shall make use of the enhancement of the feasibility of the calculations at a finite $\hbar > 0$. This will make us able to show that the return to the simplest \mathcal{PT} -symmetric discrete models finds its unexpected reward in a *complete* suppression and elimination of the 'unknown' annihilation and creation processes. In the other words we shall reinstall a firmer parallel between a simplifying role of \mathcal{PT} -symmetry in *both* the bound-state and scattering-state hypothetical experimental arrangements.

2. Solvable discrete models of scattering

Let us consider the Hamiltonian $H = H^{(M)}(g) = H_0 + W(g)$ of the doubly infinite matrix form where the non-vanishing part of the matrix $W(g) = gV^{(M)}$ will be linear in the real coupling g and where the matrix $V^{(M)}$ itself will be tridiagonal and formed just by the four off-diagonal nonvanishing matrix elements. These elements will be arranged in such a way that using the definition (1), the \mathcal{PT} -symmetry of the complete Hamiltonian will be guaranteed,

$$V_{1-M, -M}^{(M)} = V_{M-1, M}^{(M)} = 1, \quad V_{-M, 1-M}^{(M)} = V_{M, M-1}^{(M)} = -1. \quad (4)$$

The resulting Hamiltonian H can be interpreted as a discrete kinetic-energy operator complemented by an interaction mimicking the \mathcal{PT} -symmetrized pair of delta functions [9]. At the smallest 'distances' $M = 1, 2, \dots$ our model (4) may also resemble certain solvable short-range square-well differential-operator Hamiltonians [10]. In the free-motion case the above-mentioned connection between our $H(0) = H_0$ and the Runge–Kutta Laplacean may be recalled to explain the origin of the constraint $E \in (0, 4/\hbar^2)$. This is a peculiarity which is well known in the bound-state context [2]. Here this restriction proves equally important for the physical consistency of the scattering boundary conditions (3).

In what follows, we intend to search for the solutions of Schrödinger equation (2) + (3) using the standard matching method. We should emphasize that in the scattering scenario the key specific feature of wavefunctions is that they are constructed at any energy (from the allowed interval with, say, $\varphi \in (0, \pi)$) and that they are *not* \mathcal{PT} -symmetric themselves (this symmetry is broken by the boundary conditions). At the same time, due to the compact nature of the range of our interactions W , the non-compact character of the wavefunctions is fully

leads to the solution in closed form,

$$T = \frac{1}{1 + iA}, \quad R = \frac{-iA}{1 + iA}, \quad A = \frac{x^2}{1 - x^2} \cot \varphi.$$

We may immediately verify that

$$|R|^2 + |T|^2 = 1.$$

This enables us to conclude that in spite of its non-Hermiticity, our scattering model conserves the probability at $M = 1$.

2.2. $M = 2$

At the next integer index $M = 2$ the set of matching conditions comprises the following five items,

$$\begin{bmatrix} -1 & 2 \cos \varphi & -1 - x & 0 & 0 & 0 & 0 \\ 0 & -1 + x & 2 \cos \varphi & -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 \cos \varphi & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 \cos \varphi & -1 + x & 0 \\ 0 & 0 & 0 & 0 & -1 - x & 2 \cos \varphi & -1 \end{bmatrix} \begin{bmatrix} e^{-3i\varphi} + R e^{3i\varphi} \\ e^{-2i\varphi} + R e^{2i\varphi} \\ e^{-i\varphi} + R e^{i\varphi} + \chi_{-1} \\ \psi_0 \\ T e^{i\varphi} + \chi_1 \\ T e^{2i\varphi} \\ T e^{3i\varphi} \end{bmatrix} = 0.$$

From the first and last lines we get

$$(1 + x)\chi_{-1} = -x(e^{-i\varphi} + R e^{i\varphi}), \quad (1 + x)\chi_1 = -xT e^{i\varphi}.$$

This enables us to consider just the three modified matching conditions

$$\begin{bmatrix} -1 + x^2 & 2 \cos \varphi & -1 & 0 & 0 \\ 0 & -1 & 2 \cos \varphi & -1 & 0 \\ 0 & 0 & -1 & 2 \cos \varphi & -1 + x^2 \end{bmatrix} \begin{bmatrix} e^{-2i\varphi} + R e^{2i\varphi} \\ e^{-i\varphi} + R e^{i\varphi} \\ (1 + x)\psi_0 \\ T e^{i\varphi} \\ T e^{2i\varphi} \end{bmatrix} = 0.$$

The first row gives

$$(1 + x)\psi_0 = 1 + x^2 e^{-2i\varphi} + (1 + x^2 e^{2i\varphi})R$$

while the third row offers

$$(1 + x)\psi_0 = (1 + x^2 e^{2i\varphi})T$$

so that we may eliminate ψ_0 and obtain the first rule for R and T ,

$$T = R + \frac{1 + x^2 e^{-2i\varphi}}{1 + x^2 e^{2i\varphi}} = R + \frac{1 - i\lambda}{1 + i\lambda}, \quad \lambda = \frac{x^2 \sin 2\varphi}{1 + x^2 \cos 2\varphi}.$$

The remaining middle row leads to the third independent formula for

$$(1 + x)\psi_0 = \frac{1 + (R + T) e^{2i\varphi}}{1 + e^{2i\varphi}}.$$

We may combine all three representations of $(1 + x)\psi_0$ and extract the second rule for R and T . In the light of the above representation of the difference $T - R$ we shall complement it by the

second rule which determines the sum $R + T$. Such a recipe leads to the particularly compact final result,

$$2R = \frac{1 - i\alpha}{1 + i\alpha} - \frac{1 - i\beta}{1 + i\beta},$$

$$2T = \frac{1 - i\alpha}{1 + i\alpha} + \frac{1 - i\beta}{1 + i\beta},$$

where

$$\alpha = \frac{x^2 \cos 2\varphi \cot \varphi}{1 - 2x^2 \cos^2 \varphi}, \quad \beta = \frac{\sin 2\varphi}{1 + x^2 \cos 2\varphi}.$$

Since both α and β are real, it is immediate to prove that

$$|R|^2 + |T|^2 = 1.$$

We see that in the model with $M = 2$ the flow of probability is conserved as well. One feels tempted to expect such a unitary-type behavior of the amplitudes at all the integer ‘interaction distances’ M .

Let us test such a conjecture on the next version of our model.

2.3. $M = 3$

Let us abbreviate $U_{-m} = e^{-mi\varphi} + R e^{mi\varphi}$ and $L_n = T e^{ni\varphi}$ and partition the seven matching conditions at $M = 3$ as follows:

$$\begin{bmatrix} 2 \cos \varphi & -1 - x & & & & & \\ -1 + x & 2 \cos \varphi & -1 & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 \cos \varphi & -1 + x & \\ & & & & -1 - x & 2 \cos \varphi & \end{bmatrix} \begin{bmatrix} U_{-3} \\ U_{-2} + \chi_{-2} \\ U_{-1} + \chi_{-1} \\ \psi_0 \\ L_1 + \chi_1 \\ L_2 + \chi_2 \\ L_3 \end{bmatrix} = \begin{bmatrix} U_{-4} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ L_4 \end{bmatrix}.$$

The first and last lines give

$$(1 + x)\chi_{-2} = -xU_{-2}, \quad (1 + x)\chi_2 = -xL_2$$

and the elimination of the left-hand-side expressions gives the following reduced set of the five matching conditions,

$$\begin{bmatrix} 2 \cos \varphi & -1 & & & & \\ -1 & 2 \cos \varphi & -1 & & & \\ & -1 & 2 \cos \varphi & -1 & & \\ & & -1 & 2 \cos \varphi & -1 & \\ & & & -1 & 2 \cos \varphi & \end{bmatrix} \begin{bmatrix} U_{-2} \\ (1 + x)(U_{-1} + \chi_{-1}) \\ (1 + x)\psi_0 \\ (1 + x)(L_1 + \chi_1) \\ L_2 \end{bmatrix} = \begin{bmatrix} (1 - x^2)U_{-3} \\ 0 \\ 0 \\ 0 \\ (1 - x^2)L_3 \end{bmatrix}.$$

From the first and last equations we eliminate

$$(1 + x)\chi_{-1} = -xU_{-1} + x^2U_{-3}, \quad (1 + x)\chi_1 = -xL_1 + x^2L_3$$

and insert these expressions in the remaining three equations, with the result

$$\begin{bmatrix} -1 & 2 \cos \varphi & -1 & 0 & 0 \\ 0 & -1 & 2 \cos \varphi & -1 & 0 \\ 0 & 0 & -1 & 2 \cos \varphi & -1 \end{bmatrix} \begin{bmatrix} U_{-2} \\ U_{-1} + x^2U_{-3} \\ (1 + x)\psi_0 \\ L_1 + x^2L_3 \\ L_2 \end{bmatrix} = 0.$$

Let us rewrite these equations again as the three non-equivalent definitions of ψ_0 ,

$$\begin{aligned}(1+x)\psi_0 &= U_0 + 2x^2 \cos \varphi U_{-3}, \\ (1+x)\psi_0 &= L_0 + 2x^2 \cos \varphi L_3, \\ (1+x)\psi_0 &= \frac{1}{2 \cos \varphi} [L_1 + x^2 L_3 + U_{-1} + x^2 U_{-3}]\end{aligned}$$

and eliminate ψ_0 in two alternative ways which define the difference

$$T - R = \frac{1 + 2x^2 e^{-3i\varphi} \cos \varphi}{1 + 2x^2 e^{3i\varphi} \cos \varphi} = \frac{1 - iy}{1 + iy},$$

and the sum

$$T + R = -e^{-2i\varphi} \frac{1 - e^{i\varphi} \cos \varphi - x^2 e^{-2i\varphi} \cos 2\varphi}{1 - e^{-i\varphi} \cos \varphi - x^2 e^{2i\varphi} \cos 2\varphi}.$$

From these formulae it is again easy to derive

$$|R|^2 + |T|^2 = 1$$

i.e., the desirable conservation-of-probability law at $M = 3$.

2.4. $M = 4$

Out of the nine lines of the $M = 4$ matching conditions

$2 \cos \varphi$	$-1 - x$	-1	
$-1 + x$	$2 \cos \varphi$	-1	
	\ddots	\ddots	\ddots
	-1	$2 \cos \varphi$	$-1 + x$
		$-1 - x$	$2 \cos \varphi$

U_{-4}
$U_{-3} + \chi_{-3}$
$U_{-2} + \chi_{-2}$
$U_{-1} + \chi_{-1}$
ψ_0
$L_1 + \chi_1$
$L_2 + \chi_2$
$L_3 + \chi_3$
L_4

 $=$

U_{-5}
0
0
0
0
0
0
0
0
L_5

we may eliminate the first and last lines using the general formula

$$(1+x)\chi_{1-M} = -xU_{1-M}, \quad (1+x)\chi_{M-1} = -xL_{M-1}.$$

Also the rest of the solution can be perceived as a guide to the construction of the amplitudes R and T at any higher M . Indeed, once we return to the remaining seven matching conditions at $M = 4$,

$2 \cos \varphi$	-1			
-1	$2 \cos \varphi$	-1		
	\ddots	\ddots	\ddots	
	-1	$2 \cos \varphi$	-1	
		-1	$2 \cos \varphi$	

U_{-3}
$(1+x)(U_{-2} + \chi_{-2})$
$(1+x)(U_{-1} + \chi_{-1})$
$(1+x)\psi_0$
$(1+x)(L_1 + \chi_1)$
$(1+x)(L_2 + \chi_2)$
L_3

 $=$

$(1-x^2)U_{-4}$
0
0
0
0
0
$(1-x^2)L_4$

we may repeat the algorithm and eliminate its first and last line. Another general pair of formulae serves the purpose,

$$(1+x)\chi_{2-M} = -xU_{2-M} + x^2U_{-M}, \quad (1+x)\chi_{M-2} = -xL_{M-2} + x^2L_M$$

after one inserts $M = 4$. In the subsequent step of the reduction procedure we arrive at the quintuplet of equations

$$\begin{bmatrix} 2 \cos \varphi & -1 & & & \\ -1 & 2 \cos \varphi & -1 & & \\ & -1 & 2 \cos \varphi & -1 & \\ & & -1 & 2 \cos \varphi & -1 \\ & & & -1 & 2 \cos \varphi \end{bmatrix} \begin{bmatrix} U_{-2} + \chi_{-2} \\ U_{-1} + \chi_{-1} \\ \psi_0 \\ L_1 + \chi_1 \\ L_2 + \chi_2 \end{bmatrix} = \begin{bmatrix} U_{-3}/(1+x) \\ 0 \\ 0 \\ 0 \\ L_3/(1+x) \end{bmatrix}.$$

Using the first and fifth equations again, we specify the last auxiliary quantities.

$$(1+x)\chi_{-1} = -xU_{-1} + 2x^2 \cos \varphi U_{-4}, \quad (1+x)\chi_1 = -xL_1 + 2x^2 \cos \varphi L_4.$$

This exemplifies the last step of the generic recurrent recipe because the next step will already involve the exceptional central element ψ_0 . Thus, our knowledge of the expressions for $\chi_{\pm 1}$ leads to the final triplet of conditions

$$\begin{aligned} (1+x)\psi_0 &= U_0 + x^2(1 + 2 \cos 2\varphi)U_{-4}, \\ (1+x)\psi_0 &= L_0 + x^2(1 + 2 \cos 2\varphi)L_4, \\ (1+x)\psi_0 &= \frac{L_1 + U_{-1}}{2 \cos \varphi} + x^2(L_4 + U_{-4}). \end{aligned}$$

After the two alternative eliminations of ψ_0 we routinely arrive at our last two linear equations for the two unknown quantities $R + T$ and $T - R$. Their elementary though a bit clumsy solution will no longer be displayed here. Whenever asked for, the proof of the conservation law at $M = 4$ as well as the further, more or less routine though increasingly tedious continuation of our construction to the higher ‘distances M between interactions’ are left to the readers.

3. Summary

One of the most pleasant and encouraging observations made during many practical applications of quantum theory is that our basic understanding of experimental data can often be provided by fairly elementary mathematical models. Among them, a prominent role is played by the one-dimensional Schrödinger equation. Of course, the detailed physical interpretation of such a class of models can vary with the experimental setup and may range from the naive fitting scenario up to a schematic reduction of field theory to zero dimensions.

In the latter, highly speculative context Bender and Milton [12] and Bender and Boettcher [13] revealed that phenomenological as well as theoretical purposes could be served very well by complex potentials exemplified by $V(x) = ix^3$ and supporting real spectra of bound states [14]. Later on, it has been clarified that the transition to the complex $V(x)$ does not in fact violate any rules of Quantum Mechanics because even for complex potentials the Hamiltonian can be reinterpreted as self-adjoint after a suitable adaptation of the Hilbert space of states [15].

Jones [6] was probably the first author who analyzed the possibilities of the same adaptation of the Hilbert space in the scattering scenario. Although he chose one of the simplest and best understood potentials, viz, the delta function with a complex coupling, his conclusions concerning both the mathematical feasibility and the physical clarity of the complexified scattering problem were rather discouraging. His construction revealed that in spite of the ultralocal form of his toy model the scattered waves proved perceivably and counterintuitively distorted.

In our present note we reanalyzed the situation by incorporating, in explicit manner, the postulate of the so called \mathcal{PT} -symmetry of the Hamiltonian which is often being implemented

in the constructive description of bound states in unusual Hilbert spaces. For this purpose we introduced and solved an entirely new class of discrete models of scattering. We were really surprised when we revealed that these models behaved *differently* in comparison with their similar \mathcal{PT} -asymmetric predecessors of [6, 7].

The key merit of our present family of models should be seen in the fact that not quite expectedly, they fully conserve the probability and do not seem to exhibit any signs of an asymptotic non-locality. Moreover, since they are simple and exactly solvable, the emerging possibilities of their entirely standard practical applications and/or theoretical probabilistic interpretation do not seem to be an artifact of their present discretized mathematical form.

We believe that on the background of certain pessimistic physics-related perspectives as formulated in [6, 7], our present results could serve as a source of new optimism, needed for the continuation of the search for some new manifestly non-Hermitian models of scattering. One can hope that the user-friendly features of our models will survive their extensions, both in the sense of returning to the continuous limit $\hbar \rightarrow 0$ and in the sense of finding their more-parametric descendants of a greater descriptive flexibility.

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