\( \mathcal{PT} \)-symmetric model with an interplay between kinematical and dynamical non-localities

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Abstract
A new family of non-Hermitian \( \mathcal{PT} \)-symmetric quantum models is proposed in which the Hamiltonians \( H = T + V \) are finite-dimensional and in which the dynamical-input potential \( V \) is multi-parametric and non-local. The choice is supported by the exact solvability of Schrödinger equation and by the well known fact that in \( \mathcal{PT} \)-symmetric models a non-locality is already present due to the generic kinematical non-diagonality of the Hermitizing metrics \( \Theta \). For a subfamily of our \( H \), also all of the eligible metrics \( \Theta \) appear obtainable in closed form.

Keywords: non-Hermitian long-range interactions, closed-form constructions of bound states, physical inner products

1. Introduction and summary

In 1998, Bender and Boettcher [1] turned attention to \( \mathcal{PT} \)-symmetric (i.e., parity times time-reversal invariant) ordinary differential operators of the form

\[
H = -\frac{d^2}{dx^2} + V(x) \neq H^\dagger,
\]

and conjectured that in spite of manifest non-Hermiticity, these operators could still play the role of bound state Hamiltonians for certain unconventional quantum systems. Almost ten years later Hugh Jones [2] recalled this conjecture (which had been developed, in between, into a consistent branch of quantum theory [3, 4]) and tried to extend its applicability to scattering. His results forced him to conclude that one is only allowed ‘to treat the non-Hermitian scattering potential as an effective one, and work in the standard framework of quantum mechanics, accepting that this effective potential may well involve the loss of unitarity’ [5]. Fortunately, almost immediately the threatening crisis has been averted by the
observation [6] that the fundamental theory status of the whole $\mathcal{PT}$-symmetric quantum theory (PTSQT) may be reestablished (i.e., the necessary unitarity of the scattering process may be reinstalled) via a replacement of the traditional local-interaction potentials $V(x)$ by their smeared, $ad$ hoc non-local forms such that in the coordinate basis $\{|x\rangle\}$ (or rather, for the sake of simplicity, in the discretized grid-point basis $\{|x_j\rangle\}$) one has $\langle x|V|x'\rangle \neq 0$, at some $x \neq x'$ at least.

In our present paper we shall return to the related conceptual questions and reanalyze the role of non-local interactions in the bound-state PTSQT context. The key purpose of our study is to demonstrate, via a family of examples, that one must be very careful with the use of the traditional concept of locality, for reasons which were thoroughly explained by Ali Mostafazadeh (see e.g., his papers [4, 7]) and which are also summarized briefly in appendix below. Besides this global reminder our specific toy-model analysis is intended to support the use of dynamically non-local $\mathcal{PT}$-symmetric quantum models. Via the description of our schematic examples we shall show, in particular, that the introduction of the dynamical non-locality via interaction $V$ need not spoil the solvability. We shall see that in such a case the model may prove exactly solvable even in a stronger, PTSQT-related sense meaning that also the obligatory construction of the physical inner product (or even of all of the eligible physical inner products) may remain feasible by non-numerical means.

The presentation of our results will start in section 2 where we shall introduce the terminology and a concrete family of simple toy models. We shall characterize there the non-locality of a quantum system as split into its dynamical and kinematical components. For a large subfamily of our models, moreover, the kinematical non-locality will be found obtainable, by non-numerical recurrent means, in explicit form. In section 3, such a constructive kinematics-related result will be then followed by its dynamics-related parallel in which the wave functions will be found forming two families, with both of which being obtainable in closed form. The subsequent section 4 will offer a deeper, numerically supported insight into certain characteristic features of the parameter-dependence and, in particular, of the occurrence of the domains of reality or, alternatively, of the Kato’s [8] exceptional points (EPs) of complexification of the bound state energies. Besides the direct localization of the latter points we shall also emphasize that and how their alternative, indirect localization could be based on the constructive analysis of the metrics in which these boundaries of stability of the quantum system acquire the form of the points of the loss of positivity of the sophisticated [9] physical Hilbert-space metric $\Theta \neq I$. Finally, a few historical and contextual comments will be added in the last section nr. 5.

2. New $\mathcal{PT}$-symmetric toy-model Hamiltonians

In [6], during the PTSQT-applicability restoration the decisive progress has been achieved due to a purely technical simplification based on a non-perturbative replacement of the continuous axis of $x \in \mathbb{R}$ by its discretized equidistant version with $x = x_k \sim k$ and $k \in \mathbb{Z}$. This simplification (which will also be used in what follows and which may be removed, in principle at least, in the zero-distance grid point limit) was accompanied by the more or less standard replacement of the one-dimensional kinetic-energy operator $T = -d^2/dx^2$ by its difference-operator analogue.

We did—and also shall—use the doubly-infinite tridiagonal-matrix version of the discretized kinetic energy $T$ with elements $T_{kk} = 2$ (or, in a shifted-energy regime, $T_{kk} = 0$) and $T_{k+1,k} = T_{k,k+1} = -1$ in suitable units. Another assumption of our constructive considerations in [6] was the restriction of attention to the most elementary version of the non-locality of the
interaction \(V\). Indeed, in the grid-point representation matrix \(\langle x_k | V | x_m \rangle\) contained, in its simplest version, just the four non-vanishing matrix elements which lied at the pairs of subscripts \((k, m) = (k_0 - 1, k_0), (k_0, k_0 - 1), (k_0, k_0 + 1)\) and \((k_0 + 1, k_0)\). In what follows we shall feel inspired by the mathematical as well as physical user-friendly nature of such a four-parametric toy model.

2.1. Dynamical non-locality

In a way explained in review paper [4] the Bender’s physics-inspired requirement of the \(PT\)-symmetry of a Hamiltonian \(H\) (i.e., formal relation \(PH = HPT\) [3]) may be perceived as equivalent to the standard mathematical requirement

\[
P = H^TP, \tag{2}
\]

of the \(P\)-pseudo-Hermiticity alias Krein-space Hermiticity of \(H\). In other words, the usual time-reversal operator \(T\) may be perceived as acting on the matrices exemplified by the potential \(\langle x_k | V | x_m \rangle\) as an antilinear operator of transposition plus complex conjugation. Concerning the second, parity-type involution operator \(P\) such that \(P^2 = I\), one may decide to make a choice among several standard indefinite self-adjoint matrix forms of this operator. In our present paper we shall choose and work with the most common discrete version of the operator of parity represented by antidiagonal \(N\) by \(N\) matrix

\[
P = P^{(N)} = \begin{pmatrix}
1 & 
& 
& 

& 1 & 
& 

& 
& 1 &

& 

& & & 1
\end{pmatrix}, \tag{3}
\]

It is rather straightforward to verify that the requirement of \(PT\)-symmetry allows us to work with the \(N = 2M + 1\)-dimensional Hamiltonians

\[
\hat{H}^{(PT)} = \begin{pmatrix}
-w_1 & 
& w_1
-w_2 & 
& w_2 \\
& \ddots & 
& 

& \ddots & \ddots
\end{pmatrix}^{\top}
\begin{pmatrix}
-v_M & \ldots & v_2 & v_1 \\
& w_M & \ldots & w_2 & w_1 \\
& u & w_M & \ldots & w_2 & w_1 \\
& v_M & \ldots & v_2 & v_1 \end{pmatrix}, \tag{4}
\]

which degenerate immediately to their predecessors of [6] in the four-parametric special case. The general, multiparametric version (4) seems particularly suitable for our present purposes because it combines a specific dynamical long-range-interaction non-locality with a formal simplicity (reflected by the thee-by-three partitioning) and, at the same time, flexibility (besides a real parameter \(u\), the models vary with as many as \(2M\) complex parameters collected in two \(M\)-dimensional vectors).

One of the most useful special cases of model (4) will be obtained in a maximally asymmetric case with, say, \(v_1 = -1\) and trivial subdiagonal long-range couplings.
Moreover, the remaining $M$-plet of parameters $w_j$ will be chosen real. A nontrivial matrix model is then obtained, with

$$
\hat{H}^{(MA)} = \begin{bmatrix}
-1 & w_1 \\
-1 & \ddots & w_2 \\
& \ddots & \ddots & \ddots \\
-1 & \ddots & \ddots & -1 \\
-1 & \ddots & \ddots & w_M \\
& \ddots & \ddots & \ddots & -1 \\
& & \ddots & \ddots & \ddots & -1 \\
& & & \ddots & \ddots & \ddots & \ddots & -1 \\
& & & & \ddots & \ddots & \ddots & \ddots & \ddots & -1 \\
\end{bmatrix}
$$

(5)

offering a simplified picture of the long range interaction which is characterized by its maximal asymmetry.

2.2. Kinematical non-localities

In review paper [4] the author reminded his readers that the $PT$-symmetry alias Krein-space Hermiticity (2) of quantum Hamiltonians $H$ plays in fact just a useful but purely auxiliary heuristic role. The correct physical interpretation may only be deduced from the hidden-Hermiticity relations

$$
H^\dagger \Theta = \Theta H,
$$

(6)
in which a suitable operator $\Theta$ of a physical Hilbert space metric is positive definite (see a compact review of the whole formalism as well as a more detailed discussion of this point in appendix below).

Naturally, with the trivial choice of $\Theta^{(\text{Dirac})} = I$ one would immediately return back to the conventional Hermiticity requirement $H^\dagger = H$ of textbooks. In particular, in a way illustrated by the purely kinetic choice of $H_0 = T = -d^2/dx^2 = H_0^\dagger$ one could then still speak about a 'kinematical non-locality' related, in the above discrete-coordinate picture, to the 'residual non-diagonality' of matrices (4) or (5) even in the complete absence of interaction couplings $v_j$ and $w_k$.

In what follows, we shall strictly speak about a 'kinematical non-locality' in another sense in which the genuinely non-dynamical, potential-independent non-locality becomes introduced via the non-diagonal-matrix nature of the inner-product metric $\Theta \neq I$ (see appendix once more). In such a setting, an important consequence of the choice of special toy model (5) with a nontrivial dynamical part lies in the related thorough simplification of equation (6). Purely formally, these relations may be then interpreted as an underdetermined linear algebraic system of equations

$$
\mathcal{M}_{ij} = (H^\dagger \Theta - \Theta H)_{ij} = 0, \quad i, j = 1, 2, \ldots, N,
$$

(7)

which define all of the eligible metrics which would make a given Hamiltonian (5) self-adjoint in the related sophisticated physical Hilbert space $\mathcal{H}^{(F)}$. Indeed, the main reason for our restriction of attention to matrix $\hat{H}^{(MA)}$ which is so extremely non-Hermitian in the friendly but false Hilbert space $\mathcal{H}^{(F)} = \mathbb{R}^N$ lies in the emergent and unexpected feasibility of construction of all of the related eligible Hermitizing metrics at arbitrary matrix dimensions $N = 2M + 1$. 

4
Proposition 2.1. For the whole \((M + 1)\)-parametric family of our real and maximally asymmetric \(N = (2M + 1)\)-dimensional and \(PT\)-symmetric Hamiltonian matrices (5) the construction of the necessary Hermitian (i.e., real and symmetric) candidates for a positive-definite Hermitizing metric

\[
\Theta^{(\text{candidate})} = \begin{bmatrix}
\theta_{11} & \theta_{12} & \ldots & \theta_{1N} \\
\theta_{12} & \theta_{22} & \ldots & \theta_{2N} \\
\vdots & \vdots & \ddots & \vdots \\
\theta_{1N} & \theta_{2N} & \ldots & \theta_{NN}
\end{bmatrix}
\]  

may proceed via recurrent solution of linear algebraic system (6).

Proof. Once one starts from equation (7) and decides to treat the first row of matrix \(\Theta^{(\text{candidate})}\) as the \(N\)-plet of independent variable parameters, the closed-form recurrent construction of the further matrix elements may proceed row-wise, leading to the exhaustive sequence of definitions of

\[
\theta_{22}, \theta_{23}, \ldots, \theta_{2N}, \theta_{33}, \theta_{34}, \ldots, \theta_{NN},
\]

which are provided, respectively, by the independent linear equations

\[
\mathcal{M}_{12} = 0, \mathcal{M}_{13} = 0, \ldots, \mathcal{M}_{1N} = 0, \mathcal{M}_{23} = 0, \mathcal{M}_{24} = 0, \ldots, \mathcal{M}_{N-1N} = 0
\]

ordered and selected out of the redundant system (7). This property is a consequence of the extremely friendly sparsity of the Hamiltonian. Due to the Hermiticity of matrix \(\mathcal{M}\), the verification of the recurrent-relation correspondence between the linear equations (10) and their solutions (9) is provided by the insertion of \(H\) and of the Hermitian-matrix ansatz (8) in the system of \(N^2\) linear algebraic equations (7). \(\square\)

Let us add a remark that the possibility of using the first row of matrix \(\Theta^{(\text{candidate})}\) as free parameters implies that one may treat all metrics as linear superpositions of their simpler-matrix components. It makes sense to emphasize here that these components are in general different from the components provided by the well known alternative spectral-like expansion of the metric [10].

\[
\Theta = \Theta(\kappa_1^2, \kappa_2^2, \ldots, \kappa_{2M+1}^2) = \sum_{j=1}^{2M+1} \left| \Psi_j \right\rangle \kappa_j^2 \left\langle \Psi_j \right|.
\]

In the real- and non-degenerate-spectrum case the necessary \((2M + 1)\)-plet of input vectors \(\left| \Psi_j \right\rangle \in \mathcal{H}^{(F)}\) must be made available here in the form of a complete set of non-orthogonal, arbitrarily normalized eigenvectors of the Hermitian conjugate of our non-Hermitian input Hamiltonian,

\[
\left( \tilde{H}^{(PT)} \right)^\dagger \left| \Psi_j \right\rangle = \epsilon_j \left| \Psi_j \right\rangle, \quad j = 1, 2, \ldots, 2M + 1.
\]

The techniques of solution of such a conjugate form of Schrödinger equation are to be discussed below.
3. Wave functions

3.1. Right eigenvectors of the Hamiltonian

Our tilded toy-model Hamiltonians (4) are triply partitioned,

\[
\tilde{H}^{(PT)} = \begin{bmatrix}
D & \vec{w} & 0 \\
\vec{v}^T P & u & \vec{v}^T P \\
0 & \vec{v} & D
\end{bmatrix}.
\]

The real and symmetric tridiagonal matrix \(M \times M\) submatrix \(D\) has the non-degenerate real spectrum [11] and obeys the symmetry relation \(D = D_{MM}(\tilde{D})\). In terms of a unitary \(M \times M\) matrix \(U\) with known, Chebyshev-polynomial elements [12] this matrix may be diagonalized non-numerically,

\[
D = U D_{U} U^\dagger D_{U} U^\dagger.
\]

Hence, we may replace our Hamiltonian \(\tilde{H}^{(PT)}\) by its simpler, untilded form \(\tilde{H}^{(PT)} = U \tilde{H}^{(PT)} U^\dagger\) where

\[
U = \begin{bmatrix}
U_D P & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & U_D
\end{bmatrix}.
\]

Using abbreviations \(\vec{a} = U_D P \vec{w}\) and \(\vec{b} = U_D \vec{v}\), the \((2M + 1)\)-plet of bound states of our present quantum model becomes now defined by the partitioned Schrödinger equation

\[
H^{(PT)} \begin{bmatrix}
\vec{x} \\
\vec{z} \\
\vec{y}
\end{bmatrix} = \epsilon \begin{bmatrix}
\vec{x} \\
\vec{z} \\
\vec{y}
\end{bmatrix}, \quad H^{(PT)} = \begin{bmatrix}
\tilde{\epsilon} & \vec{a} & 0 \\
\vec{b}^T & u & \vec{a}^T \\
0 & \vec{b} & \tilde{\epsilon}
\end{bmatrix}.
\]

The process of its solution splits into two parts. Firstly, we assume that \(z = 0\). This reduces the problem to the two trivially solvable diagonal-matrix subproblems \((\tilde{\epsilon} - \epsilon \vec{I}) \vec{x} = 0\) and \((\tilde{\epsilon} - \epsilon \vec{I}) \vec{y} = 0\). Hence, it is easy to prove

**Proposition 3.1.** The first, \(z = 0\) subset of solutions of Schrödinger equation (15) is an \(M\)-plet such that its energies \(\epsilon_j^{(z=0)} = \tilde{\epsilon}_j\) are real and independent of parameters \(\vec{a}\) and \(\vec{b}\). For wave functions we have \(\vec{x}_m = \vec{y}_m = 0\) at all \(m \neq j\) for all \(j = 1, 2, \ldots, M\). The remaining middle-line constraint \(\vec{b}_j^+ \vec{x}_j + \vec{b}_j^+ \vec{y}_j = 0\) just makes the first set of wave functions unique after (arbitrary) normalization.

For the 'missing' second set of \(M + 1\) bound-state solutions we may select \(z = 1\) which fixes their norm. We shall skip the detailed discussion of exceptional cases and assume merely, for the sake of simplicity, that \(\epsilon \neq \tilde{\epsilon}_m\) at all \(m = 1, 2, \ldots, M\). From our Schrödinger equation (15) we may then extract the explicit definition of the wave functions,

\[
\vec{x} = -\frac{1}{\tilde{\epsilon} - \epsilon \vec{I}} \vec{a}, \quad \vec{y} = -\frac{1}{\tilde{\epsilon} - \epsilon \vec{I}} \vec{b}.
\]
Ultimately, the remaining middle-row algebraic-equation remnant

\[ \epsilon_j = u + R(\epsilon_j), \quad R(\epsilon_j) = \sum_{i=1}^{M} \left( \beta_i^* \frac{1}{\epsilon_j - d_i} \alpha_i + \alpha_i^* \frac{1}{\epsilon_j - d_i} \beta_i \right), \quad j = 1, 2, \ldots, M \]  

(16)
of our Schrödinger equation determines the spectrum. Although the explicit solution of the latter equation is, in general, a purely numerical problem, we immediately see that our auxiliary function \( R(\epsilon) \) is real and, up to its singularities at the first subset of energies \( \epsilon = d_i \), continuous, with elementary asymptotics

\[ R(\epsilon) = \frac{G}{\epsilon} + \mathcal{O}\left(\frac{1}{\epsilon^2}\right), \quad G = \sum_{i=1}^{M} \left( \beta_i^* \alpha_i + \alpha_i^* \beta_i \right). \]

Moreover, up to the possible exceptional degenerate cases, the singularities are real and isolated first-order poles. This observation completes the proof of the following result.

**Proposition 3.2.** The second, \( z = 1 \) set (i.e., the ‘missing’ \( (M+1) \)-plet) of the \( \vec{\alpha} \)- and \( \vec{\beta} \)-dependent bound-state energy roots \( \epsilon_m \) is defined by the transcendental secular equation (16). Up to the above-mentioned exceptional degenerate cases these roots are real and ordered,

\[ \epsilon_1 < d_1 < \epsilon_2 < \ldots < d_M < \epsilon_{M+1}, \]

(17)
i.e., separated by the poles of \( R(\epsilon) \), i.e., by the remaining energy levels belonging to the first, \( z = 0 \) set.

### 3.2. Left eigenvectors of the Hamiltonian

A remark is to be added now concerning the parallels between the Schrödinger’s bound-state problem (15) and its conjugate forms needed in preceding section. Naturally, the partitioning may be recalled in conjugate case yielding the relations

\[
\begin{bmatrix}
\vec{d} \\
\vec{\beta}
\end{bmatrix}
\begin{bmatrix}
\alpha \\
\beta
\end{bmatrix}
= \begin{bmatrix}
\epsilon_j \\
0
\end{bmatrix},
\begin{bmatrix}
\alpha \\
\beta
\end{bmatrix}
= \begin{bmatrix}
\vec{X} \\
\vec{Y}
\end{bmatrix}.
\]

(18)
The solution remains analogous to the non-conjugate case so we need not describe it in detail. It is only worth mentioning that the treatment of the new, upper-case Schrödinger equation (18) will be facilitated by our knowledge of the spectrum. The comparison of the lower- and upper-case wave functions reveals that the left and right eigenstates of our Hamiltonians are also closely related by an elementary interchange of the two vectors of the complex parameters \( \vec{\alpha} \leftrightarrow \vec{\beta} \).

One could summarize that at any \( M \), the closed-form construction of the necessary physical Hermitizing metric via expansion (11) is only marginally more complicated than the explicit specification of the bound states themselves. At the same time, the mutual non-orthogonality of vectors \( |\psi_j\rangle \) makes the resulting matrices of the metric cumbersome. Even at the smallest integers \( M \), they can hardly be displayed in print, therefore.

On positive side, a definite advantage of using formula (11) lies in the fact that the domain of the acceptable parameters \( \kappa_j^2 \) keeping the metric positive definite is trivial. In contrast, the use of the recurrent construction of Proposition 2.1 does not provide any
sufficiently general guidance for the choice and/or limitations of variability of the free parameters forming the first row of the real matrix $\Theta^{(\text{candidate})}$. A case-by-case analysis is usually needed.

4. Numerical results

4.1. The domains of reality of the energies

Let us start by considering the first nontrivial $M = 2$ (i.e., five-by-five) matrix (4) in which we assume, for the sake of simplicity, that the interaction part is just real and antisymmetric. This yields the two-parametric toy-model Hamiltonian

$$
\hat{H}^{(PT)}(r, s) = \begin{bmatrix}
0 & -1 & r & 0 & 0 \\
-1 & 0 & -1 + s & 0 & 0 \\
-r & -1 - s & 0 & -1 + s & r \\
0 & 0 & -1 - s & 0 & -1 \\
0 & 0 & -r & -1 & 0
\end{bmatrix}, \tag{19}
$$

in which we further set $r = 1/2$. Then, secular equation

$$
e^5 - 7/2 e^3 + 2 e^3 s^2 - 2 s e^2 + 5/2 e - 2 e s^2 + 2 s = 0
$$

may be solved exactly. Its solution determines the roots which remain all real in an interval of $s \in (-0.5242, 0.5242)$ while a pair of these roots merges and becomes complex everywhere out of such an interval (see figure 1).

Although even a very sketchy inspection of figure 1 immediately confirms that the two spectral-reality-boundary points $s = \pm 0.5242$... are complexification singularities, i.e., EPs in the sense of definition as given by Kato [8], one may feel truly puzzled by the very small distance of these boundary points from the other two points of slightly smaller absolute value at which the curve happens to cross the constant-root lines of $e_s = \pm 1$.

A deeper analysis of these intersections localizes them at $s = \pm 1/2$. Moreover, their determination in closed form enabled us to arrive at a truly surprising observation that these points in the interior of the interval of the spectral reality are no ‘normal crossings with the two straight lines’ but rather that they form another pair of the other two Kato’s EP singularities. In other words, one reveals that for the same toy model the values of $s = \pm 1/2$ at
which the respective pairs of the real eigenvalues collide are also the points at which our matrix $\tilde{H}^{(PT)}(1/2, s)$ ceases to be diagonalizable and, hence, acceptable as a Hamiltonian operator in quantum mechanics. Thus, one arrives at the following counterintuitive, interesting and truly important observation.

**Proposition 4.1.** For our illustrative $M = 2$ Hamiltonian $\tilde{H}^{(PT)}(1/2, s)$ of equation (19) the physical domain of its single free parameter $s$ splits in three open intervals, viz., $D_\pm = (-s_{EP}, -1/2)$, $D_0 = (-1/2, 1/2)$ and $D_\times = (1/2, s_{EP})$ with an empty overlap. In terms of an abbreviation $f = \sqrt{5 + \sqrt{33}}$ we also obtain the exact and closed formula

$$s_{EP} = \frac{2\sqrt{6}f^2 - 15f - f\sqrt{33} + 21 + 5\sqrt{33} - 2\sqrt{2}f}{4\sqrt{f(f^2 - 2)}} \approx 0.524\,210\,6130\ldots$$

(20)

determining our initial, reality-boundary EPs.

**Proof.** The derivation of closed formula (20) is based on the secular equation re-interpreted as a quadratic equation for two functions $s = s_\pm(\epsilon)$. For a completion of the proof the EP property of $s = \pm 1/2$ must be verified via the direct evaluation of the related eigenvectors. At either of the two doubly degenerate eigenvalues one really obtains just a single eigenvector (with, e.g., $x_1 = x_2 = z = 0$ and $y_1 = y_2 = 1$ at $s = 1/2$ and $\epsilon = -1$, etc). Thus, the basis in our friendly Hilbert space $H^{(s)} = \mathbb{R}^5$ must be completed by the fifth, ‘missing’ associated-vector element (with, e.g., $x_1 = 0$, $x_2 = -1/2$, $z = -1$, $y_1 = 0$ and $y_2 = 1/2$ at $s = 1/2$ and $\epsilon = -1$, etc.).

The overall pattern does not vary with the dimension $M$ too much. Thus, in the $M = 3$ toy-model Hamiltonian

![Figure 2. The sample of $s$-dependence of the real eigenvalues of Hamiltonian $\tilde{H}^{(PT)}(q, r, s)$ of equation (21) at $r = 1/2$ and $q = 1/3$.](image-url)
we may set, for illustration purposes, $r = 1/2$ and $q = 1/3$ and get the spectrum sampled in figure 2. It is worth noticing that due to the presence of four EPs, the physical domain $\mathcal{D}$ (in which all energies remain real) is now split into four non-overlapping subdomains. In each of them the set of energies is formed by an $s$-independent triplet and an $s$-dependent quadruplet—we in a way predicted in section 3.

4.2. A gap between domains

With the asymmetry of interaction made maximal let us now apply our numerical sampling also to model (5). As long as we now only have $\beta = U_D \vec{\nu} \neq 0$, it makes sense to start our discussion from the choice of $M = 3$ with $u = 0$ yielding the asymmetric toy-model Hamiltonian

$$
\tilde{H}^{(PT)}(q, r, s) = 
\begin{bmatrix}
0 & -1 & 0 & q & 0 & 0 & 0 \\
-1 & 0 & -1 & r & 0 & 0 & 0 \\
0 & -1 & 0 & -1 + s & 0 & 0 & 0 \\
-q & -r & -1 - s & 0 & -1 + s & r & q \\
0 & 0 & 0 & -1 - s & 0 & -1 & 0 \\
0 & 0 & 0 & -r & -1 & 0 & -1 \\
0 & 0 & 0 & -q & 0 & -1 & 0 \\
\end{bmatrix},
$$

(21)

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$$
\tilde{H}^{(PT)}(q, r, s) = 
\begin{bmatrix}
-1 & q \\
-1 & -1 & r \\
-1 & -1 + s \\
-1 & -1 + s & r & q \\
0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & -r & -1 \\
0 & 0 & 0 & -q & 0 \\
\end{bmatrix},
$$

(21)

First of all, one has to analyze the structure of the physical parametric domain $\mathcal{D}$ and, in particular, of its EP boundaries $\partial \mathcal{D}$. For our present purposes, let us just mention that whenever we follow our preceding strategy and restrict the role of a variable parameter, say, to $s$, the $s$-dependence of the real eigenvalues $\varepsilon_j$ remains qualitatively the same as above.

Naturally, there emerge also several qualitative differences. Firstly, in the two illustrative figures 3 and 4 it is not too well visible that the absolute values of the minimal and maximal
energies grow linearly with the unlimited decrease of $s$. What is better visible in these pictures (where we have $M = 3$) is the survival of the coexistence of the $s$-independent (and real) eigenvalue triplet with the not always real quadruplet which varies with $s$. In the non-asymptotic domain of $|s| \ll \infty$ these functions of $s$ may possess the real EP singularities, i.e., they may intersect their $s$-independent partners and also—pairwise—complexify.

From the point of view of unitary quantum mechanics of stable systems one only has to pay attention to the physical parametric subdomains $\mathcal{D}_j$ in which the spectrum remains all real and non-degenerate. At the fixed values of $r$ and $q$ these subdomains become intervals of admissible $s$. We may find three of these intervals in figure 3, and four of them forming the two adjacent pairs separated by a non-empty gap in figure 4.

4.3. The domains of positivity of the metrics

The weakest point of the recurrent construction of the arbitrary-dimension metrics as described in section 2 lies in the necessity of a purely empirical verification of the positivity of all of the eigenvalues of a given $\Theta^{(\text{candidate})}$. The procedure remains numerical and may be sampled using the $N = 5$ Hamiltonian

$$
\hat{H}^{(\text{MA})}(r, s) = \begin{bmatrix}
0 & -1 & r & 0 & 0 \\
-1 & 0 & -1 + s & 0 & 0 \\
0 & -1 & 0 & -1 + s & r \\
0 & 0 & -1 & 0 & -1 \\
0 & 0 & 0 & -1 & 0 \\
\end{bmatrix}.
$$

(23)

Naturally, a fully general discussion would be too long. Let us therefore illustrate the whole approach and a few of its most relevant aspects via a single sample of the determination of the parametric domain of positive definiteness of the metric using the following special sparse-matrix (SSP) choice of the ansatz with normalization $\Theta_{11}^{(\text{SSP})} = 1$, $\Theta_{12}^{(\text{SSP})} = 0$, $\Theta_{13}^{(\text{SSP})} = \xi$ and $\Theta_{14}^{(\text{SSP})} = \Theta_{15}^{(\text{SSP})} = 0$.

After one applies the above-described recurrent algorithm the candidate for the metric $\Theta = \Theta^{(\text{SSP})}(r, s, \xi)$ is obtained in closed and still sufficiently compact form. In an a posteriori test this matrix proves positive definite for a broad range of its parameters (an illustrative sample is shown in figure 5).

A marginal disadvantage of such a purely pragmatic and non-systematic demonstration of the acceptability of the model in quantum mechanics is that although the fully non-
numerical form of the resulting closed-form metric was still not too complicated, its explicit
display would not certainly fit in a single printed page. For the presentation purposes we,
therefore, choose and fixed parameters $r = r_1^2$ (as usual) and $s = 0$ (taken as lying safely
inside one of the above-discussed physical, real-energy domains $D$). This already enables us
to display a representative sample of the matrix of the metric quite comfortably,
\[
\Theta^{\text{SSP}}(1/2, 0, \xi) = \begin{bmatrix}
1 & 0 & \xi & 0 & 0 \\
0 & 1 + \xi & -1/2 & \xi & -1/2 \xi \\
\xi & -1/2 & 1 + \xi & -1/2 - 1/2 \xi & 1/4 + \xi \\
0 & \xi & -1/2 - 1/2 \xi & 5/4 + \xi & -1 - 1/2 \xi \\
0 & -1/2 \xi & 1/4 + \xi & -1 - 1/2 \xi & 5/4 + 1/4 \xi
\end{bmatrix}
\] (24)

For this particular example we arrived at the following last result.

**Proposition 4.2.** For every Hamiltonian of equation (23) with two free parameters which lie
inside such a physical domain $D$ which contains $r = r_1^2$ and $s = 0$ there exists a non-empty
one-parametric family of the above-specifed sparse-matrix Hermitizing metrics $\Theta^{\text{SSP}}(r, s, \xi)$ which are positive definite in a non-empty interval $\mathcal{I}$ of eligible parameters $\xi$.

**Proof.** For the special model in question the positivity of the eigenvalues $\theta_j = \theta_j(r, s, \xi)$ of
matrix $\Theta^{\text{SSP}}(r, s, \xi)$ has an easy proof. It relies on the smoothness of the parameter-
dependence of the roots of the secular equation, say, in the vicinity of zero $\xi = 0$ and of the
pre-selected values of $r = 1/2$ and $s = 0$. Graphically, this feature of the eigenvalues of our
metric candidate is supported by figure 5. Strictly at $\xi = 0$, $r = 1/2$ and $s = 0$ the explicit
construction of the secular polynomial equation

\[
\det[\Theta^{\text{SSP}}(1/2, 0, 0) - \theta I] = -\frac{9}{32} + \frac{181}{64} \theta - \frac{547}{64} \theta^2 + \frac{21}{2} \theta^3 - \frac{11}{2} \theta^4 + \theta^5 = 0 ,
\]

supports the exact localization of one of its roots (viz., the ‘middle’, closed-form one, $\theta_3 = 1$).
Then, the reduced secular equation
\[64 \theta^4 - 288 \theta^3 + 384 \theta^2 - 163 \theta + 18 = 0\]

is, in principle, non-numerical. In practice, it is sufficient to evaluate the remaining four roots numerically, arriving at the values

\[0.1704659382, 0.4862291155, 1.374374593, 2.468930353\]

which are all safely positive.

5. Discussion

In many PT-symmetric quantum models of bound states the physical Hilbert-space metric $\Theta$ acts at a distance. Its most conventional, kinematically local representation $\langle x | \Theta | y \rangle \sim \delta(x - y)$ is generalized to a non-local expression [7]. This means that there is no physical reason for keeping the dynamical-input Hamiltonians local. In our present paper we supported this abstract observation of admissibility of non-local interactions by a concrete constructive support. Using the coordinates in a discrete-lattice grid-point approximation $x \to x_k$ with $k = 1, 2, \ldots, N = 2M + 1$ we proposed a family of Hamiltonians $H = T + V$ in which the interaction $V$ was strongly non-local but still user-friendly. In particular, the wave functions as well as Hermitizing metrics proved obtainable by algebraic means. Now, we only intend to add a few complementary comments.

Firstly, let us mention that although certain features of non-locality (i.e., in some sense, of an ‘action at a distance’) are deeply encoded in the very formalism of quantum theory, many of their concrete manifestations look suspicious. They evoke doubts which may be best sampled by the famous EPR ‘paradox’ [13] in which the (indeed, deplorable!) incompatibility of quantum mechanics (of systems with the finite number of degrees of freedom) with the kinematical principles of special relativity was interpreted as an obvious ‘disproof of completeness’ of the former theory. The same old locality-involving misunderstanding reemerged, again, in the above-mentioned Jones’ papers [2, 5] as well as in a very recent new round of the revitalized discussion in which the ‘superluminal signaling’ argument was targeted directly against PTSQT. According to the authors, their results ‘kill any hope of PTSQT as a fundamental theory of nature’ [14]. Naturally, this is not true at all.

It is necessary to admit that our present study was partially provoked also by the latter provocative conclusion. Via the description of our dynamically manifestly non-local models we decided to contradict the statement by emphasizing that the currently accepted formalism of quantum theory may really appear strongly counterintuitive and deeply non-local, especially in some of its less common implementations. So in support of the acceptability of similar models we offered an exactly solvable example.

In the light of the various intuitive perceptions of the concept of locality (which form, in fact, a very frequent core of similar misunderstandings), the specific PTSQT implementation of the abstract formalism of quantum theory is particularly vulnerable, indeed. One of the reasons is even purely historical: the variable $x$ in the traditional benchmark PTSQT examples (1) is often called ‘coordinate’ in spite of not being even real in general. In fact, its asymptotic complexity is a strict necessary condition of the reality of the observable bound-state energies for all of the toy-model potentials $V(x) = -(ix)^\delta$ of [1] whenever one selects $\delta \geq 4$.

Another reason of an enhanced sensitivity of PTSQT to misunderstandings may be found to lie in a innovative double meaning of non-locality in this context. Indeed, in addition to the traditional dynamical nonlocalities resulting, say, from a replacement of the conventional potential $V(x)$ by its non-local (i.e., e.g., momentum-dependent) alternatives, one also has to
deal with the purely kinematical non-localities as caused by the necessity of reconstruction of
the inner product with respect to which a given PT-symmetric Hamiltonian \( H \neq H^\dagger \) would
be made Hermitian. In this setting the readers are advised to re-read, once more, appendix
and, in particular, its application—and physics—oriented parts in which \( H \) describes a heavy
atomic nucleus (composed, as we know, of fermions) while using, highly counterintuitively,
the language of bosons.

In the broader context of quantum physics, naturally, the present demonstration of the
theoretical as well as practical acceptability of a combination of the nonstandard (i.e.,
dynamically non-local) interactions \( V \) with the nonstandard (i.e., kinematically non-local)
representations \( \mathcal{H}^{(S)} \) of the physical Hilbert spaces of quantum states may be perceived as an
couragement. We believe that our present constructive mathematical results might be also
read as opening new perspectives in the phenomenological model building.

Appendix. PTSQT in nuce

What is shared by the majority of textbooks on quantum mechanics is the preference of
representations \( \mathcal{H}^{(P)} \) of the physical Hilbert space of states in a mathematically most friendly
form, say, of the space of square-integrable functions \( L^2(\mathbb{R}) \) or \( L^2(\mathbb{R}^3) \) etc. In the conven-
tional quantum theory all of the latter spaces could be also collectively denoted by an
alternative dedicated symbol \( \mathcal{H}^{(F)} \) in which the superscript stands for ‘friendly’. In such a
rigid setting the bound-state Hamiltonians with real spectra must be necessarily assumed self-
adjoint of course. For our present purposes, let us denote them, say, by a dedicated symbol \( \mathfrak{h} \).

In the PTSQT context one weakens the assumptions and requires that a given Hamil-
tonian (let us denote it by a different symbol \( H \)) ceases to be self-adjoint in the preselected
friendly Hilbert space. Then, one has to employ a new theoretical framework called, in our
compact review \[9\], a three-Hilbert-space (THS) representation of quantum theory. In this
new framework the friendly space becomes unphysical and, in terms of physics, ‘false’, with
the consequence that \( \mathcal{H}^{(F)} \neq \mathcal{H}^{(P)} \). The third, ‘standard’ Hilbert space \( \mathcal{H}^{(S)} \) representing
physics must be introduced as another option which remains different from the preceding two.
Thus, the third, \( S \)-superscripted Hilbert space \( \mathcal{H}^{(S)} \) is, in general, constructed as unitarily
equivalent to \( \mathcal{H}^{(P)} \). One can summarize that in the light and from the time of the earliest
applications of the idea by physicists in 1956 \[15\] the introduction of the third, \( S \)-super-
scripted physical Hilbert space is sufficiently strongly motivated by making the calculations
as well as the interpretations of the results perceivable simpler in technical sense (see
also \[16\]).

The requirements of the unitary equivalence of \( \mathcal{H}^{(S)} \) with \( \mathcal{H}^{(P)} \) and, in parallel, of the non-
equivalence between the physical \( \mathcal{H}^{(S)} \) or \( \mathcal{H}^{(P)} \) and the false space \( \mathcal{H}^{(F)} \) may be easily
clarified. It is sufficient to redefine the kets \( |\psi\rangle^{(P)} \in \mathcal{H}^{(P)} \) (treated, typically, as ‘fermionic’ in
nuclear-physics applications \[16\]) as the mere images (called, conveniently, Dyson’s maps \[15\]) of certain ‘bosonic’ kets which remain the same in both of the ‘bosonic’ spaces,
\( |\psi\rangle^{(F)} = |\psi\rangle^{(S)} \),

\[
|\psi\rangle^{(P)} = \Omega |\psi\rangle^{(F)} \equiv \Omega |\psi\rangle^{(S)} \in \mathcal{H}^{(P)}, \ |\psi\rangle^{(F)} \in \mathcal{H}^{(F)}, \ |\psi\rangle^{(S)} \in \mathcal{H}^{(S)}. \tag{25}
\]

Naturally, whenever the Dyson’s map \( \Omega \) itself is admitted to be a non-unitary operator, we
may define a non-trivial Hilbert-space metric \( \Omega^2 \Omega = \Theta \neq I \). The required unitary equivalence
between \( \mathcal{H}^{(P)} \) and \( \mathcal{H}^{(S)} \) (i.e., the postulated coincidence of the results of the respective inner
products) will then acquire, after the mere insertions, the following next-to-elementary metric-
dependent form,
The latter formula should now be interpreted as the definition of the physical, correct inner product in $H^{(S)}$. Alternatively, we may read the latter formula as a metric-mediated representation of the correct, $S$-superscripted inner product when represented inside auxiliary space $H^{(F)}$. Indeed, for the purposes of the mere constructive considerations, one does not need to work with the third, $S$-superscripted space at all. After an explicit use of metric $\Theta$, all of the necessary formulae may be pulled back to the manifestly unphysical, $F$-superscripted space $H^{(F)}$. In the resulting THS setting the Hamiltonian becomes re-interpreted as safely self-adjoint in the correct, $S$-superscripted space. Equivalently, one may write $H = H^\dagger \equiv \Theta^{-1} H^\dagger \Theta$ or $H = \Omega^{-1} \hbar \Omega$ (remember that $\hbar = \hbar^\dagger$) and call operator $H$ self-adjoint with respect to the metric-mediated inner product, or crypto-self-adjoint when studied inside the most friendly auxiliary and unphysical $F$-superscripted Hilbert space.

As a consequence, the unitarity of the evolution in the physical Hilbert space $H^{(S)}$ becomes guaranteed by the quasi-Hermiticity property (6) of the Hamiltonian which is manifestly non-Hermitian in the ‘false’ Hilbert space $H^{(F)}$. The same quasi-Hermiticity feature must necessarily characterize all of the other candidates $\Lambda$ for acceptable physical observables [16],

$$\Lambda^\dagger \Theta = \Theta \Lambda.$$  (27)

In multiple applications, a decisive appeal of such a THS representation terminology (see [9]) is seen in the possibility of an explicit guarantee of a sufficient technical simplicity of Hamiltonians $H$ in $H^{(F)}$ [16]. In our present paper the interpretation of the whole scheme follows [7] and is, therefore, different because the argument $x$ of wave functions $\psi(x) \in L^2(\mathbb{R} \equiv H^{(F,S)})$ does not represent, in general, an observable point-particle position anymore. In this sense, virtually all $\mathcal{PT}$-symmetric quantum models are, by construction, non-local in the physical representation space $H^{(S)}$ because in the conventional delta-function basis in $H^{(F)}$ the operator of the coordinate (if any) is generically non-diagonal (see a few concrete examples in [7]). Thus, one can only conclude that in the PTSQT theoretical framework the origin of any measurable non-locality lies, more or less inseparably, in both of its input-information sources given by the non-Hermitian-potential dynamical input and by the independent, metric-selection-related kinematical input.

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