Complete set of inner products for a discrete $\mathcal{PT}$–symmetric square-well Hamiltonian

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Abstract

A discrete $N$–point Runge-Kutta version $H^{(N)}(\lambda)$ of one of the simplest non-Hermitian square-well Hamiltonians with real spectrum is studied. A complete set of its possible hermitizations (i.e., of the eligible metrics $\Theta^{(N)}(\lambda)$ defining its non-equivalent physical Hilbert spaces of states) is constructed, in closed form, for any coupling $\lambda \in (-1,1)$ and any matrix dimension $N$. 

1 Introduction

1.1 Bound states in Runge-Kutta approximation

The concept of the solvability of a dynamical model in physics is rather vague. Its definition is usually adapted to the range of expected applications. By some authors even the single-particle motion along a finite one-dimensional interval would be called solvable only if the underlying ordinary differential Schrödinger equation for bound states

\[-\frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x) , \quad \psi(\pm L) = 0 \quad (1)\]

proved reducible to the Gauss’ or confluent hypergeometric equation. Remarkably enough, even this extremely narrow specification of solvability finds very plausible physical reasons in the related shape invariance of potentials $V(x)$ and/or in their close relationship to supersymmetry [1].

In what follows we shall rather accept different terminology in which one treats virtually any sufficiently smooth and real potential $V(x)$ in Eq. (1) as exactly solvable, i.e., solvable, in principle, with arbitrary precision, in a purely numerical setting at least. Typically, the Runge-Kutta (RK, [2]) discrete approximation of the above equation, viz.,

\[- \frac{\psi(x_{k-1}) - 2 \psi(x_k) + \psi(x_{k+1})}{h^2} + V(x_k) \psi(x_k) = E \psi(x_k) , \quad (2)\]

$x_k = k h , \ k = 0, \pm 1, \ldots, \pm K , \ x_{\pm K} = \pm L , \ \psi(x_{\pm(K+1)}) = 0$

may be used to reduce the original bound-state problem to a routine computer-assisted diagonalization of the finite-dimensional RK matrix Hamiltonian

\[
H = \begin{pmatrix}
\ddots & \ddots & \ddots \\
\ddots & 2 + h^2 V(x_{-1}) & -1 \\
-1 & 2 + h^2 V(x_0) & -1 \\
-1 & 2 + h^2 V(x_1) & \ddots \\
\ddots & \ddots & \ddots
\end{pmatrix} . \quad (3)
\]

The choice of the lattice distance $h \ll 1$ is only dictated by the required precision of reproduction of the original energies and/or wave functions.

1.2 $\mathcal{PT}$–symmetric Runge-Kutta models

The standard formalism of quantum theory admits Schrödinger Eqs. (1) and/or (2) which generate the real bound-state spectra from certain complex
potentials $V(x)$. Conventionally, these potentials are called \(PT\)-symmetric (cf. reviews [3, 4] or Appendix A for more details). For a sensible extension of the concept of solvability to this new context it is most important that the \(PT\)-symmetric models are characterized by the Hamiltonian-dependence of their physical Hilbert spaces \(\mathcal{H}^{(S)}\). Although the superscript \(^{(S)}\) stands here for “standard”, the inner product is defined in a nonstandard manner in this space, by a formula containing an \(ad\ hoc\) metric operator \(\Theta = \Theta(H) \neq I\) (cf. Eq. (27) in Appendix A below).

In spite of the existence of several powerful techniques of reconstruction of \(\Theta\) for differential Eq. (1) [3, 5] one can rarely find a closed-form result (for illustration check a few samples in Refs. [6, 7]). Many successful constructions rely upon various assumptions requiring, e.g., the existence of a charge of the system \([8, 9]\) or of some other additional and/or complementary observable(s) \(\mathcal{O} [10]\). Moreover, people are mostly able to obtain \(\Theta\) just in an approximate form, say, of perturbation series [11].

Some of these difficulties have been addressed in our papers [12]. We restricted our attention to the discrete Schrödinger Eq. (2) considered at a pre-determined precision, i.e., at a fixed spacing constant \(h > 0\). This enabled us to broaden the scope of the theory and to consider certain nonlocal generalizations of interaction terms. More explicitly, we complemented the diagonal elements \(V(x_k)\) in the RK matrix Hamiltonian \(H\) by a set of real chain-coupling constants \(u_k\) in a way which still left the resulting asymmetric real matrix \(H\) tridiagonal,

\[
H = \begin{pmatrix}
  \ddots & \ddots & \ddots & \ddots \\
  \ddots & 2 + h^2 V(x_{-1}) & -1 - u_0 & -1 - u_1 \\
  -1 + u_0 & 2 + h^2 V(x_0) & -1 - u_1 & \ddots \\
  \ddots & -1 + u_1 & 2 + h^2 V(x_1) & \ddots \\
  \ddots & \ddots & \ddots & \ddots
\end{pmatrix}
\] (4)

For several special cases of this family of Hamiltonians we then constructed particular diagonal-matrix metrics \(\Theta \neq I\) in closed form.

This partial success of the project encouraged us to re-open the question of a \textit{complete} solvability of a \(PT\)-symmetric model in our subsequent paper [13]. In the cryptohermitian scenario characterized by the nontriviality of the metrics \(\Theta \neq I\) we found a complete set of metrics for a special case of Eq. (4) with \(V(x_k) = 0\) (i.e., without any complex local force) and with \(u_1 = u_2 = \ldots = 0\) and \(u_{-1} = u_{-2} = \ldots = 0\), i.e., with the single off-diagonal real coupling constant \(g = u_0 \neq 0\) representing a nonlocal, manifestly non-Hermitian potential.

In spite of the feasibility of such a construction we still felt disappointed not only by the necessity of the really lengthy calculations but also by the
comparatively complicated structure of matrix elements of metrics Θ. Although these elements were expressible in terms of closed-form polynomials in \( g \), the degree of these polynomials grew quickly with the cut-off dimension \( N \) of the \( g \)-dependent Hilbert space \( H^{(S)} \). In this sense the results of Ref. [13] proved discouraging, especially in the light of a really extreme simplicity of the underlying single-center interaction.

In our present paper we intend to report a return to optimism. Firstly, in a preparatory Sec. 2 we shall introduce a double-center model and show that its more complicated dynamics does not worsen the feasibility of calculations nor a guarantee of the reality of the energy spectra. Next, we shall formulate our project of construction of all the eligible metrics for this model in Sec. 3. In contrast to the similar results of Ref. [13] we shall be able to show here that the present version of the \( \mathcal{PT} \)-symmetric discrete square-well model is much more friendly since the related menu of metrics \( \Theta \) exhibits a paradoxical decrease of complexity during the increase of dimension \( N \). In Sec. 4 (dealing with exceptional, one- or two-diagonal metrics) and Sec. 5 (describing all the remaining metrics) this fact will enable us to find and prove results valid at all \( N \). A compact rigorous proof will be delivered confirming the validity of our closed and elementary explicit formulae for metrics \( \Theta^{(N)}(\lambda) \) at any given dimension \( N \) and coupling \( \lambda \in (-1, 1) \).

2 Discrete non-Hermitian square wells

The key motivation of the present paper resulted from our study of Refs. [14] and [7] where the differential version (1) of a square-well Schrödinger equation has been analyzed with a \( \mathcal{PT} \)-symmetric point interaction localized in the origin (i.e., at \( x = 0 \)) and at the two distant points \( (x = \pm L) \), respectively. The former, simpler, single-center arrangement found its discrete RK analogue in the models of Ref. [13]. Our present paper will offer the discrete RK complement to the latter, more ambitious study [7].

2.1 Hamiltonians

We shall analyze the two-center boundary-interaction \( N \)-dimensional models \( H^{(N)}(\lambda) \) which form the family

\[
H^{(3)}(\lambda) = \begin{bmatrix}
2 & -1 - \lambda & 0 \\
-1 + \lambda & 2 & -1 + \lambda \\
0 & -1 - \lambda & 2
\end{bmatrix},
\]
$$H^{(4)}(\lambda) = \begin{bmatrix}
2 & -1 - \lambda & 0 & 0 \\
-1 + \lambda & 2 & -1 & 0 \\
0 & -1 & 2 & -1 + \lambda \\
0 & 0 & -1 - \lambda & 2
\end{bmatrix}$$

$$H^{(5)}(\lambda) = \begin{bmatrix}
2 & -1 - \lambda & 0 & 0 & 0 \\
-1 + \lambda & 2 & -1 & 0 & 0 \\
0 & -1 & 2 & -1 & 0 \\
0 & 0 & -1 & 2 & -1 + \lambda \\
0 & 0 & 0 & -1 - \lambda & 2
\end{bmatrix}$$

(etc) and which have the following tridiagonal $N$ by $N$ matrix form in general,

$$H^{(N)}(\lambda) = \begin{bmatrix}
2 & -1 - \lambda & 0 & \ldots & 0 & 0 \\
-1 + \lambda & 2 & -1 & 0 & \ldots & 0 \\
0 & -1 & 2 & \ddots & \ddots & \vdots \\
\vdots & 0 & \ddots & \ddots & -1 & 0 \\
0 & \vdots & \ddots & -1 & 2 & -1 + \lambda \\
0 & 0 & \ldots & 0 & -1 - \lambda & 2
\end{bmatrix}.$$  \hspace{1cm} (5)

We intend to pay attention to these models in bound-state regime. Hence, we have to clarify, first of all, the structure of the domain of couplings $\lambda$ for which the energy spectrum remains real.

### 2.2 The reality of the spectra of energies

![Figure 1: Real spectrum and its degeneracy and complexification at $N = 4$.](image)

In the first step, at $N = 3$ we obtain the three easily evaluated eigenvalues

$$E_0 = 2, \quad E_{\pm 1} = 2 \pm (2 - 2 \lambda^2)^{1/2}$$
which are all real and non-degenerate inside the interval of \( \lambda \in (-1, 1) \). Next, at \( N = 4 \) we arrive at the four eigenvalues

\[
E_{\pm 1/2} = 3/2 \pm 1/2 (5 - 4 \lambda^2)^{1/2}, \quad E_{\pm 3/2} = 5/2 \pm 1/2 (5 - 4 \lambda^2)^{1/2}
\]

which stay real within a \textit{larger} interval of \( \lambda \in (-\sqrt{5}/2, \sqrt{5}/2) \). This may seem to indicate that the domain of the admissible values of \( \lambda \) may vary with the dimension. Fortunately, it is not so. Figure 1 clarifies the apparent puzzle by showing that the condition of non-degeneracy gets violated precisely at the boundary of the same, dimension-independent interval \( \lambda \in (-1, 1) \).

![Figure 2: The \( \lambda \)-dependence of energies at \( N = 5 \).](image)

Proceeding to \( N = 5 \) we reveal that the five eigenvalues

\[
E_0 = 2, \quad E_{\pm 1} = 2 \pm (1 - \lambda^2)^{1/2}, \quad E_{\pm 2} = 2 \pm (3 - \lambda^2)^{1/2}
\]

are all real and non-degenerate inside the same interval of \( \lambda \in (-1, 1) \). Our Figure 2 displays the coupling-dependence of these energies in full detail.

In the next case, at \( N = 6 \), the closed formulae for the energies become clumsy. Still, Figure 3 demonstrates clearly that the six eigenvalues behave in expected manner at all \( \lambda \in (-1, 1) \). At \( N = 7 \) (cf. Figure 4) the formulae become, paradoxically, simpler, defining all the spectrum by the compact equations

\[
E_0 = 2, \quad E_{\pm 1} = 2 \pm 1/2 \sqrt{8 - 2 \lambda^2 - 2 \sqrt{8 + \lambda^4}}, \quad E_{\pm 2} = 2 \pm \sqrt{2 - \lambda^2},
\]

\[
E_{\pm 3} = 2 \pm 1/2 \sqrt{8 - 2 \lambda^2 + 2 \sqrt{8 + \lambda^4}}.
\]

Next, two separate and rather complicated equations of fourth order de-
termine the spectrum at even $N = 8$ (cf. Figure 5). In contrast, our last illustration at $N = 9$ (cf. Figure 6) yields closed formulae again,

$$E_0 = 2, \quad E_{\pm 1} = 2 \pm 1/2 \sqrt{6 - 2 \lambda^2 - 2 \sqrt{\lambda^4 - 2 \lambda^2 + 5},}$$

$$E_{\pm 2} = 2 \pm 1/2 \sqrt{10 - 2 \lambda^2 - 2 \sqrt{\lambda^4 + 2 \lambda^2 + 5},}$$

$$E_{\pm 3} = 2 \pm 1/2 \sqrt{6 - 2 \lambda^2 + 2 \sqrt{\lambda^4 - 2 \lambda^2 + 5},}$$

$$E_{\pm 4} = 2 \pm 1/2 \sqrt{10 - 2 \lambda^2 + 2 \sqrt{\lambda^4 + 2 \lambda^2 + 5}.}$$

This indicates that the secular polynomials are simpler at odd dimensions. In all the Figures 1-6 the interval of the allowed couplings $\lambda \in (-1, 1)$ does not
vary with the growth of the dimension $N$. An independent confirmation of this feature of our model will follow, later, from the existence and invertibility conditions imposed upon the metric $\Theta$ at any $N$.

Our pictures illustrate that the extreme values of $\lambda = \pm 1$ correspond to the triple confluence of the energies $E_{\pm 1}$ with $E_0$ at odd $N$ and, in our notation, to the incidental degeneracy of $E_{+1/2}$ with $E_{-3/2}$ at even $N$. In the language of Refs. [15] one can conclude that at any dimension $N \geq 4$ our model possesses strictly four fragile energies which complexify during the transition from the Hermitian limit $\lambda = 0$ to the asymptotic, strongly non-Hermitian regime under very large $|\lambda| \gg 1$. 

Figure 5: The $\lambda$–dependence of energies at $N = 8$.

Figure 6: The $\lambda$–dependence of energies at $N = 9$. 

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3 Hermitization

The study of non-Hermitian Hamiltonians $H$ with real spectra is easier whenever there exists an invertible map $\Omega$ of $H$ upon an isospectral operator (say, upon $\mathfrak{h} = \Omega H \Omega^{-1}$) which is Hermitian (it is, sometimes, called Dyson’s map). The latter operator $\mathfrak{h}$ (acting in some abstract physical Hilbert space $\mathcal{H}^{(P)}$, cf. [4, 10, 16]) may be assumed prohibitively complicated (otherwise, there would exist no good reason for studying $H$). The space $\mathcal{H}^{(P)}$ may be assumed endowed with the usual Dirac’s trivial metric $\Theta^{(P)} = I$. By definition, the latter space must be unitarily equivalent to its equally acceptable physical alternative $\mathcal{H}^{(S)}$ [17].

In applications, the role of the Dyson map $\Omega$ degenerates to the introduction of the elementary product $\Theta = \Omega^\dagger \Omega$ called metric in $\mathcal{H}^{(S)}$. For this reason we shall only be interested here in the constructions of the matrices $\Theta = \Theta(H)$.

3.1 The matrices of metrics

In the theoretical setting outlined in Appendix A below, the key questions to be answered in connection with the analysis of models sampled by Eq. (5) result from the ambiguity of the assignment of the metric $\Theta$ to a given Hamiltonian $H$ [5, 10]. For the purposes of clarification of the roots and forms of this ambiguity the Runge-Kutta discretized Hamiltonians prove particularly suitable. Indeed, in the related finite-dimensional (i.e., $N$–dimensional) standard physical Hilbert spaces $\mathcal{H}^{(S)}$ the admissible metrics $\Theta = \Theta(H)$ do only form a finite, strictly $N$–parametric family. Thus, we may decompose

$$\Theta^{(N)} = \sum_{k=1}^{N} \mu_k \mathcal{P}_k^{(N)}$$

and require that the individual Hermitian components $\mathcal{P}_k^{(N)}$ of our metric are some extremely simple pseudometric (i.e., not necessarily positive definite) matrices with, presumably, sparse-matrix structure.

From the purely algebraic point of view the correspondence between $H$ and $\Theta(H)$ is exclusively specified by Eq. (25) of Appendix A which can be rewritten in the explicit linear algebraic form

$$\sum_{k=1}^{N} \left[(H^\dagger)_{jk} \Theta_{kn} - \Theta_{jk} H_{kn}\right] = 0, \quad j, n = 1, 2, \ldots, N.$$  

At the first sight, the direct use of such a systems of $N^2$ equations for the determination of the matrix elements of $\Theta = \Theta(H)$ looks discouragingly difficult. Fortunately, not all of these equations are linearly independent. The
number of unknowns is also lowered by the necessary Hermiticity of acceptable matrices $\Theta = \Theta^\dagger$. Still, for any given Hamiltonian $H$, an encouragement and insight into the generic structure of the solutions $\Theta = \Theta(H)$ may only be acquired step by step, by the patient solution of Eq. (7) starting from the smallest dimensions $N$.

Our first nontrivial real and asymmetric, i.e., $\mathcal{PT}$—symmetric and non-Hermitian Hamiltonian $H^{(3)}(\lambda)$ has already been studied in the different context (viz., in connection with the cryptounitary description of scattering, cf. section 2.1 of Ref. [18]). In the present, bound-state version of this model we may expect that any eligible $H^{(3)}(\lambda)$—dependent metric $\Theta^{(3)}(\lambda)$ compatible with Eq. (7) will have the real and symmetric six-parametric matrix form

$$\Theta = \begin{bmatrix} a & b & c \\ b & f & g \\ c & g & m \end{bmatrix}.$$  

The values of its six free real parameters $a - m$ are only restricted by the sequence of nine linear relations (7) and by the positivity requirement $\Theta > 0$. It is easy to verify that the six nontrivial items of Eq. (7) number 2, 3, 4, 6, 7 and 8 read, respectively,

- $-f + f\lambda + a + a\lambda + c + c\lambda = 0$,
- $-a - a\lambda - c - c\lambda + f - f\lambda = 0$,
- $-c - c\lambda - m - m\lambda + f - f\lambda = 0$,
- $-b + b\lambda + g - g\lambda = 0$,
- $-c - c\lambda + c\lambda + m + m\lambda = 0$.

At $\lambda \in (-1, 1)$, both the items number 3 and 7 give $b = g$ while the comparison of items number 2 and 8 gives $m = a$. The remaining four nontrivial equations all coincide with the constraint $f(1 - \lambda) = (a + c)(1 + \lambda)$. We may summarize that the complete solution of Eq. (7) has the three-parametric form

$$\Theta^{(3)}_{(a,b,c)}(\lambda) = \begin{bmatrix} a & b & c \\ b & \frac{(a+c)(1+\lambda)}{1-\lambda} & b \\ c & b & a \end{bmatrix}.$$  

At $c = 0$ we get the tridiagonal matrix

$$\Theta^{(3)}_{(a,b,0)}(\lambda) = \begin{bmatrix} a & b & 0 \\ b & \frac{a(1+\lambda)}{1-\lambda} & b \\ 0 & b & a \end{bmatrix}$$

which becomes strictly diagonal at $b = 0$ where one could also set, without any loss of generality, $a = \alpha = (1 - \lambda)/(1 + \lambda)$ yielding

$$\Theta^{(3)}_{(\alpha,0,0)}(\lambda) = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad \alpha = \frac{1 - \lambda}{1 + \lambda}. \tag{9}$$

At any nonvanishing $\lambda \in (-1, 1)$ the latter, diagonal metric is safely positive and manifestly non-Dirac, $\Theta \neq I$. At the same time, the positivity of its non-diagonal predecessors must be guaranteed by an explicit (and not too easy)
specification of the admissible domain of parameters $a$, $b$ and $c$. Without this guarantee we may only speak about potentially non-invertible or indefinite pseudometrics replacing, accordingly, also the symbol $\Theta^{(N)}_{(a,b,c,...)}(\lambda)$ for the metric, say, by a less specific symbol $\mathcal{Q}^{(N)}_{(a,b,c,...)}(\lambda)$ whenever appropriate (cf., e.g., Appendix B).

3.2 The set of simplified pseudometrics

We shall see below that the feasibility of transition to higher dimensions $N > 3$ will be rendered possible by the Runge-Kutta algebraization of the Hamiltonian as well as by our localization of interaction far from the origin. We shall reveal that these features of our model open the path toward an enhancement of efficiency of the construction of $\Theta$ via expansion (6) where the individual pseudometric components $P$ may be sought in certain simplified sparse-matrix forms. Naturally, Eq. (7) may be required to be satisfied also by every individual component matrix $P = P^{(N)}_{k}$,

$$\sum_{i=1}^{N} \left[ (H^\dagger)_{ji} P_{in} - P_{ji} H_{in} \right] = 0, \quad j, n = 1, 2, \ldots, N. \quad (10)$$

The explicit solution of the latter, simplified system of equations will be further facilitated by the tridiagonal matrix structure of our Hamiltonians. This can be illustrated at $N = 4$ for which the real, $\mathcal{PT}$-symmetric and non-Hermitian Hamiltonian $H^{(4)}(\lambda)$ admits the following real and symmetric ansatz for the metric

$$\Theta^{(4)}(\lambda) = \Theta^{(4)}_{(a,b,c,d)}(\lambda) = \begin{bmatrix} a & b & c & d \\ b & f & g & h \\ c & g & m & n \\ d & h & n & j \end{bmatrix}. \quad (11)$$

Out of the sixteen linear relations in (7) only the ones with numbers 1, 6, 11 and 16 are trivially satisfied. Further, items 3 and 13 give $h = c$, items 7 and 10 yield $m = f$ while the comparison of 2 with 15 gives $j = a$ and the comparison of 8 with 9 yields $n = b$. The rest of the set of constraints degenerates to the doublet of requirements $f = \frac{c + a(1+\lambda)}{1-\lambda}$ and $g = \frac{b + d(1+\lambda)}{1-\lambda}$ so that the exhaustive solution of Eq. (7) has the four-parametric form as it should,

$$\Theta^{(4)}_{(a,b,c,d)}(\lambda) = \begin{bmatrix} a & b & c & d \\ b & \frac{c + a(1+\lambda)}{1-\lambda} & \frac{c}{1-\lambda} & \frac{b + d(1+\lambda)}{1-\lambda} \\ c & \frac{b + d(1+\lambda)}{1-\lambda} & \frac{c + a(1+\lambda)}{1-\lambda} & c \\ d & \frac{c}{1-\lambda} & \frac{b}{1-\lambda} & a \end{bmatrix}. \quad (12)$$
At $d = 0$ this matrix becomes pentadiagonal while the additional constraint $c = 0$ makes it tridiagonal. Finally, at $b = 0$ we get the diagonal metric

$$
\Theta^{(4)}(\alpha, 0, 0, 0) (\lambda) = \begin{bmatrix} 
\alpha & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & \alpha 
\end{bmatrix}, \quad \alpha = \frac{1 - \lambda}{1 + \lambda}.
$$

(13)

Up to two elements the latter metric coincides with the most common Dirac’s $\Theta^{(\text{Dirac})} = I$. One can expect (and we shall verify below) that the existence of the similar diagonal metric is a generic feature of our model at all the dimensions $N = 3, 4, \ldots$.

4 Exceptional metrics

The well known ambiguity of the correspondence between Hamiltonian $H$ and metric $\Theta(H)$ [10] seems to be particularly important when one tries to improve the precision of RK approximation and to guess the form of metric $\Theta^{(N+1)}$ from the knowledge of $\Theta^{(N)}$. For such an extrapolation the complete solution of Eq. (7) at the smallest dimensions $N \leq 4$ does not suffice. Moreover, just a marginal help may be extracted from the related mathematical literature (dating back to the early sixties [16]). More insight has only been obtained during the first use of the metrics $\Theta \neq I$ in nuclear physics [9, 10] and during the development of $\mathcal{PT}$-symmetric quantum mechanics. In the latter setting an additional constraint has been accepted and the metric $\Theta$ has been assumed factorized into the product of parity (i.e., of one of the pseudometrics $\mathcal{P}$) with the so called quasiparity [19] or charge [8].

Even under the latter class of additional assumptions the metric $\Theta(H)$ may remain non-unique [5, 9, 10, 20]. This means that the usual choice of the Hamiltonian $H$ should be accompanied by the additional phenomenological or pragmatic considerations, i.e., by the physics-dictated or comfort-dictated specification of some optimal or exceptional hermitizing metrics $\Theta(H)$.

4.1 The strictly diagonal metrics

In section 3 three important generic features of our present square-well model have been revealed. Firstly, the eligible matrices $\Theta$ were found to possess more symmetries than expected. Secondly, the structure of these matrices appeared to simplify when one keeps just single first-line matrix element different from zero. Thirdly, the simplest form of matrix elements seems to be achieved when the first-line matrix elements $a, b, \ldots$ are properly rescaled in a coupling-dependent way.
In practice, the most prominent role will always be played by the matrices \( \Theta \neq I \) which are as close to diagonal ones as possible having \( a(= \Theta_{11}) \neq 0 \) while \( b(= \Theta_{12}) = c(= \Theta_{13}) = \ldots = 0 \). In this sense our first present interesting result is the following one.

**Theorem 4.1.** For any matrix Hamiltonian (5) with coupling \( \lambda \in (-1, 1) \) and dimension \( N = 3, 4, \ldots \) there always exists a diagonal, positive definite metric matrix which differs from the Dirac’s \( \Theta = I \) just at the elements \( \Theta_{kk} \) with \( k = 1 \) and \( k = N \). Its explicit form is

\[
\Theta^{(N)}_{(\alpha,0,\ldots,0)}(\lambda) = \begin{bmatrix}
\alpha & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & 1 & 0 \\
0 & 0 & \ldots & 0 & \alpha \\
\end{bmatrix}, \quad \alpha = \alpha(\lambda) = \frac{1 - \lambda}{1 + \lambda}. \quad (14)
\]

**Proof.** Equation (14) coincides with Eq. (9) at \( N = 3 \) and with Eq. (13) at \( N = 4 \). At any integer \( N > 4 \) the insertion of ansatz (14) converts Eq. (7) into identity.

**Corollary 4.2.** The spectrum of Hamiltonian (5) with coupling \( \lambda \in (-1, 1) \) is real at any dimension \( N = 3, 4, \ldots \).

**Proof.** The existence of the metric guarantees that in the corresponding finite-dimensional Hilbert space the Hamiltonian matrix is Hermitian.

Just an inessential modification of the above construction leads also to the following interesting observation.

**Proposition 4.3.** For any matrix Hamiltonian (5) with coupling \( \lambda \in (-1, 1) \) and dimension \( N = 3, 4, \ldots \) there always exists an antidiagonal, indefinite pseudometric matrix of the form

\[
Q^{(N)}_{(0,0,\ldots,0,\alpha)}(\lambda) = \begin{bmatrix}
0 & 0 & \ldots & 0 & \alpha \\
0 & \ldots & 0 & 1 & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & 1 & 0 \\
\alpha & 0 & \ldots & 0 & 0 \\
\end{bmatrix}, \quad \alpha = \alpha(\lambda) = \frac{1 - \lambda}{1 + \lambda}. \quad (15)
\]

**Proof.** At \( N = 3 \), equation (15) degenerates to formula (8) at \( a = b = 0 \) and \( c = \alpha \). At \( N = 4 \), equation (15) degenerates to formula (12) at \( a = b = c = 0 \) and \( d = \alpha \). At any higher integer \( N > 4 \) the insertion of ansatz (15) converts Eq. (7) into identity. At the same time one can easily verify that matrix (15) is not positive definite at any \( N \geq 2 \).
Remark 4.4. It is worth noticing that before one performs the continuous $h \to 0$ limit of the present Runge-Kutta picture, certain metric operators obtained in Ref. [5] at $\lambda = 0$ may be interpreted as positive definite superpositions of our two one-diagonal matrices (14) and (15).

4.2 The strictly bidiagonal pseudometrics

In our present concrete realization of expansion (6) the general matrix of metric $\Theta^{(N)}_{(a,b,...)}(\lambda)$ will always be written as a linear superposition of the following $N$–plet of specific pseudometric matrices

$$P^{(N)}_1(\lambda) \sim Q^{(N)}_{(a,0,...,0)}(\lambda), \quad P^{(N)}_2(\lambda) \sim Q^{(N)}_{(0,b,0,...,0)}(\lambda), \quad \ldots .$$

Their mutual independence is trivially guaranteed by the presence of the mere single nonvanishing matrix element in their respective first lines.

On the level of our above-mentioned $N \leq 4$ experience and constructions we just managed to guess and prove the generic form of the diagonal and antidiagonal pseudometrics $P_1(\lambda)$ [cf. Eq. (14)] and $P_N(\lambda)$ [cf. Eq. (15)]. Further insight must be built using the next, $N = 5$ ansatz for the real and symmetric metric $\Theta^{(5)}$. Using symbolic manipulations we managed to reveal that without any loss of generality this ansatz may be written in the simplified, symmetrized nine-parametric form

$$\Theta^{(5)}_{(a,b,c,d,e)}(\lambda) = \begin{bmatrix} a & b & c & d & e \\ b & f & g & h & d \\ c & g & m & g & c \\ d & h & g & f & b \\ e & d & c & b & a \end{bmatrix} .$$

Out of the twenty five independent relations (7) we managed to eliminate nine trivial ones yielding the four quadruplets of equations which enabled us to eliminate $m = f + h - c(1+\lambda)$ (from items 8, 12, 14 and 18), $g = (b+d)/(1-\lambda)$ (from items 3, 11, 15 and 23), $h = (c + e(1+\lambda))/(1-\lambda)$ (from items 4, 10, 16 and 22) and $f = (c + a(1+\lambda))/(1-\lambda)$ from items 2, 6, 20 and 24. Thus, we arrived at the complete five-parametric solution $\Theta^{(5)}_{(a,b,c,d,e)}(\lambda)$ of Eq. (7),

$$\begin{bmatrix} a & b & c & d & e \\ b & f & g & h & d \\ c & g & m & g & c \\ d & h & g & f & b \\ e & d & c & b & a \end{bmatrix} .$$

At $e = 0$ this matrix is seven-diagonal. After we set $d = 0$ it becomes pentadiagonal while the next constraint $c = 0$ makes it tridiagonal. The
last, \( b = 0 \) item in the list of simplifications is the diagonal matrix which is compatible with Eq. (14) and non-Dirac, \( \Theta_{(a,0,0,0,0)}^{(5)}(\lambda) \neq I \) at \( \lambda \neq 0 \).

The most important consequence of our “brute-force” calculations performed at \( N = 5 \) lies in the highly desired clarification of certain higher-\( N \) tendencies exhibited by nondiagonal metrics. In the light of this experience we were able to formulate and prove the following

**Proposition 4.5.** At any dimension \( N = 3, 4, \ldots \) and coupling \( \lambda \in (-1, 1) \), pseudo-Hermiticity relation (14) is satisfied by Hamiltonian (5) and by the bidiagonal pseudometric matrix

\[
P^{(N)}_2(\lambda) = Q^{(N)}_{(0,0,0,0)}(\lambda) = \begin{bmatrix}
0 & \beta & 0 & 0 & \ldots & 0 \\
\beta & 0 & 1 & 0 & \ldots & 0 \\
0 & 1 & \ddots & \ddots & \ddots & \vdots \\
0 & \ddots & \ddots & 0 & 1 & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \ldots & 0 & 1 & 0 & \beta \\
0 & \ldots & 0 & \beta & 0 & 0 
\end{bmatrix}
\]  \hspace{1cm} (17)

containing two pairs of \( \lambda \)-dependent elements \( \beta = \beta(\lambda) = 1 - \lambda \) connected by two unit diagonals.

**Proof.** Equation (17) is compatible with Eq. (8) at \( N = 3 \) and with Eq. (12) at \( N = 4 \). At any integer \( N > 4 \) the insertion of ansatz (17) converts Eq. (10) into identity. \( \square \)

**Proposition 4.6.** At any dimension \( N = 3, 4, \ldots \) and coupling \( \lambda \in (-1, 1) \), Hamiltonian (5) and pseudometric matrix

\[
P^{(N)}_{N-1}(\lambda) = Q^{(N)}_{(0,0,\ldots,0,\beta,0)}(\lambda) = \begin{bmatrix}
0 & \ldots & 0 & 0 & \beta & 0 \\
0 & \ldots & 0 & 1 & 0 & \beta \\
\vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & 1 & \ddots & \ddots & \ddots & \vdots \\
\beta & 0 & 1 & 0 & \ldots & 0 \\
0 & \beta & 0 & 0 & \ldots & 0 
\end{bmatrix}
\]  \hspace{1cm} (18)

with two antidiagonals and four elements \( \beta = 1 - \lambda \) satisfy the pseudo-Hermiticity relation (14).

**Proof.** Equation (18) is compatible with Eq. (8) at \( N = 3 \) and with Eq. (12) at \( N = 4 \). At any integer \( N > 4 \) the insertion of ansatz (18) converts Eq. (10) into identity. \( \square \)

We see that at \( N > 3 \) the same simplification of the interior matrix elements to units or zeros occurs in both the bidiagonal and antibidiagonal cases. Similar phenomenon will characterize also the structure of all the remaining elements of our set of pseudometrics \( P^{(N)}_k = P^{(N)}_k(\lambda) \).
5 The complete set of pseudometrics

The simplest pseudometric matrices $\mathcal{P}^{(N)}_k(\lambda)$ entering expansion (6) were defined by Eq. (14) (where we have to set $k = 1$), by Eq. (17) (where $k = 2$), by Eq. (15) (where $k = N$), and by Eq. (18) (where $k = N - 1$). On the basis of inspection of metrics $\Theta^{(N)}$ evaluated at dimensions $N \leq 5$ we are now prepared to guess and prove the explicit form of the remaining pseudometrics $\mathcal{P}^{(N)}_k(\lambda)$ at all the subscripts $k$ such that $3 \leq k \leq N - 2$. Our $N$ by $N$ candidates $\mathcal{C}^{(N)}_k$ for these pseudometrics will be sparse matrices with the property

$$
\left(\mathcal{C}^{(N)}_k\right)_{mn} = 0 \quad \text{whenever} \quad m + n \equiv k \pmod{2}.
$$

This means that on a sufficiently large chessboard the nonvanishing matrix elements of each of these matrices would only occupy either black or white fields. Secondly, all of these “colored” (i.e., black or white) ansatz matrices will share the following two-parametric form of their upper segment,

$$
\mathcal{C}^{(N)}_k = \mathcal{C}^{(N)}_k(z, v) = 
\begin{bmatrix}
\ldots & 0 & 0 & z & 0 & 0 & \ldots & 0 \\
\ldots & 0 & v & 0 & v & 0 & \ldots \\
\ldots & v & 0 & 1 & 0 & v & \ldots \\
\ldots & 0 & 1 & 0 & 1 & 0 & \ldots \\
\ldots & 1 & 0 & 1 & 0 & 1 & \ldots \\
\ldots & 0 & 1 & 0 & 1 & 0 & \ldots \\
\ldots & \ldots & \ldots & \vdots & \ldots & \ldots & \ldots \\
\end{bmatrix}
$$

(20)

copied and shared also by the $\pi/2$—rotated left segment, lower segment and right segment. In compact notation we are led to the left-right as well as up-down asymmetric arrays of matrix elements,

$$
\mathcal{C}^{(N)}_k(z, v) = 
\begin{bmatrix}
0 & 0 & \ldots & 0 & z & 0 & 0 & \ldots & 0 \\
0 & \ldots & 0 & v & 0 & v & \ldots & \vdots \\
\vdots & \ldots & 1 & \ldots & \ldots & \ldots & \ldots & 0 \\
0 & v & \ldots & \ldots & \vdots & \ldots & \ldots & v & 0 \\
z & 0 & 1 & \ldots & 1 & 0 & \ldots & 1 & 0 & z \\
0 & v & \ldots & \ldots & \vdots & \ldots & \ldots & v & 0 \\
\vdots & \ldots & 1 & \ldots & \ldots & \ldots & \ldots & \vdots \\
0 & \ldots & 0 & v & 0 & v & \ldots & \vdots \\
0 & 0 & \ldots & 0 & z & 0 & \ldots & 0 & 0 \\
\end{bmatrix}
$$

(21)
In these two-parametric matrices the uppermost item \( z \) sits in the \( k \)-th place of the first row of our matrix while the bottom line contains \( z \) in the \( (N + 1 - k) \)-th place. Together with the other two \( z \)'s we obtain the quadruplet of vertices connected by the four diagonal rows of elements \( v \) forming a parallelogram. Keeping still in mind the chessboard visualization of matrices \( C_k^{(N)}(z, v) \) we require that this parallelogram separates the outside domain (filled just by zeros) from the rhomboidal interior filled by “equal color” units and “opposite color” zeros. A few illustrative samples of explicitly computed matrices \( P \) possessing this structure may be found in Appendix B below. We are now prepared to prove our final result.

**Theorem 5.1.** Pseudometric matrices \( P_k^{(N)}(\lambda) \) with \( 3 \leq k \leq N - 2 \) which would be compatible with Hamiltonian (2) via condition (10) may be identified with the \( \lambda \)-dependent matrices \( C_k^{(N)}(\gamma, \delta) \) where

\[
\gamma = \gamma(\lambda) = \frac{1 - \lambda}{1 + \lambda^2}, \quad \delta = \delta(\lambda) = \frac{1}{1 + \lambda^2}.
\]

**Proof.** The inspection of concrete examples using small fixed dimensions \( N \) (obtainable by the algorithm outlined in Appendix B) indicates that all our elementary pseudometrics \( P_k(\lambda) \) may be expected to exhibit the above-mentioned fourfold symmetry. This expectation is easily verified by immediate insertions confirming that in our algebraic manipulations with Eq. (10) it is sufficient to work just with the not too large submatrices (20) glued, if necessary, to their rotated neighbors. In this sense, the role of the position of the subscript \( k \) in interval \([3, N - 2]\) remains inessential.

In the next preparatory step of our proof let us recall the detailed form of our generic ansatz (20) and visualize it also as written on the black-and-white chessboard. Obviously, the color of fields with nonvanishing matrix elements will be fixed as “white” or “black” for each subscript \( k \). At the same time, our tridiagonal Hamiltonian \( H \) will be both “white” (= its main diagonal, \( H^{(w)} := 2I \)) and “black” (= its upper diagonal, \( H^{(b+)}(\lambda) \), as well as its lower diagonal, \( H^{(b-)}(\lambda) \)). This type of coloring simplifies our argumentation because in our fundamental Eq. (10) we may use any \( P_k(\lambda) = C_k(\gamma, \delta) \) and decompose \( H = H(\lambda) = H^{(w)} + H^{(b+)}(\lambda) + H^{(b-)}(\lambda) \) and \( H^\dagger = H(-\lambda) = H^{(w)} + H^{(b+)}(-\lambda) + H^{(b-)}(-\lambda) \). Obviously, the “color” of any selected \( C_k(\gamma, \delta) \) will be shared by its products with \( H^{(w)} \) and it will differ from its products with \( H^{(b\pm)}(\pm \lambda) \). Using this idea we may very quickly deduce that starting from Eq. (20) we shall always obtain product \( CH \) in the form characterized...
by its upper segment
\[
\begin{bmatrix}
\ldots & 0 & 0 & -\gamma & 2\gamma & -\gamma & 0 & 0 & \ldots \\
0 & -\delta & 2\delta & -2\delta & 2\delta & -\delta & 0 & \ldots \\
-\delta & 2\delta & -1 - \delta & 2 & -1 - \delta & 2\delta & -\delta & \ldots \\
2\delta & -1 - \delta & 2 & -2 & 2 & -1 - \delta & 2\delta & \ldots \\
-1 - \delta & 2 & -2 & 2 & -2 & 2 & -1 - \delta & \ldots \\
2 & -2 & 2 & -2 & 2 & \ldots & \ldots & \ldots \\
\end{bmatrix}
\]

Similarly, the product $H^\dagger C$ will be specified by its very similar upper segment
\[
\begin{bmatrix}
\ldots & 0 & -\delta(1 - \lambda) & 2\gamma & -\delta(1 - \lambda) & 0 & \ldots \\
-\delta & 2\delta & -1 - \gamma(1 + \lambda) & 2\delta & -\delta & \ldots \\
2\delta & -1 - \delta & 2 & -1 - \delta & 2\delta & \ldots \\
-1 - \delta & 2 & -2 & 2 & -1 - \delta & \ldots \\
2 & -2 & 2 & -2 & 2 & \ldots & \ldots & \ldots \\
\end{bmatrix}
\]

The difference between these two upper-part matrix structures only involves the underlined matrix elements. It is easy to check that the coincidence of these two remaining triplets of underlined matrix elements is guaranteed since it follows from definition (22) of quantities $\gamma = \gamma(\lambda)$ and $\delta = \delta(\lambda)$.

The symmetries of our pseudometrics imply that the same coincidence of matrix elements will take place for the two lower parts of products $CH$ and $H^\dagger C$. In contrast, the rotation of the upper-part matrices by the mere $\pm \pi/2$ changes the picture. Different pattern emerges causing, fortunately, just an exchange of the underlined matrix elements between the respective left or right parts of products $CH$ and $H^\dagger C$. In this way we arrive at another, equivalent matrix representation of equation $H^\dagger C = CH$. Indeed, in its new form this representation can be made explicit, say, via its left-part embodiment
\[
\begin{bmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & -\delta & \ldots \\
0 & -\delta & 2\delta & \ldots \\
-\gamma & 2\delta & -1 - \delta & \ldots \\
2\gamma & -2\delta & 2 & \ldots \\
-\gamma & 2\delta & -1 - \delta & \ldots \\
0 & -\delta & 2\delta & \ldots \\
0 & 0 & -\delta & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{bmatrix}
= 
\begin{bmatrix}
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & -\delta & \ldots \\
0 & -\delta & 2\delta & \ldots \\
-\delta(1 - \lambda) & 2\delta & -1 - \delta & \ldots \\
2\gamma & -1 - \gamma(1 + \lambda) & 2 & \ldots \\
-\delta(1 - \lambda) & 2\delta & -1 - \delta & \ldots \\
0 & -\delta & 2\delta & \ldots \\
0 & 0 & -\delta & \ldots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\end{bmatrix}
\]
We see that the modifications are inessential and that the rotated recipe leads to the same identities. We may conclude that the products $H^\dagger C$ and $\mathcal{C} H$ coincide. This completes the proof of eligibility of our ansatz (20) + (22) for independent non-exceptional sparse-matrix components $\mathcal{P}_k^{(N)}(\lambda)$ of the general $N$–parametric metric at any dimension $N$. □

6 Summary and discussion

We can summarize that for our square-well model (5) the $N$–term decomposition (6) of all the existing metrics $\Theta^{(N)}(\lambda)$ may be written in terms of the non-exceptional closed-form pseudometrics of Theorem 5.1 complemented by the exceptional closed-form metric $\mathcal{P}_1^{(N)}(\lambda)$ [defined by Eq. (14)] and closed-form pseudometrics $\mathcal{P}_2^{(N)}(\lambda)$ [defined by Eq. (17)], $\mathcal{P}_N^{(N)}(\lambda)$ [defined by Eq. (18)] and $\mathcal{P}_N^{(N)}(\lambda)$ [defined by Eq. (15)].

In a broader perspective, the existence of remarkable parallels as well as differences between the standard and $\mathcal{PT}$–symmetric models of bound states has been reconfirmed. It has been emphasized that in the former case one works, as a rule, solely with the most elementary Dirac metric $\Theta = I$. In the majority of $\mathcal{PT}$–symmetric models, on the contrary, the technically most difficult task concerns the construction of the appropriate metric or metrics $\Theta \neq I$. For this reason, the work with the difference (rather than with the more current differential) $\mathcal{PT}$–symmetric Schrödinger equations has been preferred and may be recommended as easier in technical terms.

In our present paper we intended to address and formulate the problem of solvability in $\mathcal{PT}$–symmetric context. We felt inspired by one of the simplest differential square-well Hamiltonians where a “minimal” non-Hermiticity has been introduced via boundary conditions and where an exceptionally elementary metric $\Theta$ has been found in Ref. [7]. On this background we selected and analyzed the difference-equation version (5) of this model.

A supplementary reason for our choice of model (5) has been provided by Refs. [15] and [21] where several physical and dynamical assumptions (say, about a large distance between interaction centers, etc) have been made in the technically more difficult differential-equation context. In our study of the discrete sample (5) of a generic boundary-condition model some of the empirical observations made in these references (concerning, e.g., the correspondence between the fragile and robust energy levels [15]) reappeared and have been illustrated by a few pictures.

The most interesting conclusions may be extracted from the comparison of our present results with their predecessors described in Ref. [13]. In both these cases point-like interactions were used. Still, the decisive advantage of their present version has been found in their consequent localization in the closest vicinity of the boundaries. Formally, this feature of our $H$ has been
reflected by an enormous simplification of the structure of all of the related matrices $\mathcal{P}$ (= pseudometrics) and $\mathcal{\Theta}$ (= metrics).

The latter merit of our model was quite unexpected and its explanation also forms a mathematical core of our present message. A posteriori we may conclude that the simplification of our matrix equations for $\mathcal{P}$ and $\mathcal{\Theta}$ resulted from a “hidden” possibility of their split in the “white” and “black” components. This is also a deeper reason why the simplicity of the metrics attached to our present model is in a sharp contrast with the complicated recurrent nature of the analogous matrices in the older model of Ref. [13].

In connection with this feature of our model the core of feasibility as well as of the rigorous form of our constructions may be seen in the availability of appropriate ansatzs. They were found by extrapolation from investigative constructions performed, at the smallest dimensions, by the brute-force linear-algebraic techniques. A posteriori we must appreciate, therefore, the drastic reduction of the large set of algebraic quasihermicity conditions (7) or (10) to the mere double definition (22) of functions $\gamma(\lambda)$ and $\delta(\lambda)$. This reduction seems to have been caused by a certain purely formal interplay between the tridiagonality of $H$ and its free-motion character preserved near the origin. It was precisely this fine-tuned dynamical input which suppressed the computational difficulties and which facilitated, decisively, the explicit interactive and extrapolative analysis of $\Theta(H)$.

Our closed formulae appear transparent, especially if one decides to work, say, with just a few terms in the general series (6). In this way even the very pragmatic users of the discretized norm or inner product

$$\langle\langle \psi|\phi \rangle := \langle \psi|\phi \rangle^{(S)} = \sum_k \sum_n \psi_k^{*}(x_k)\Theta_{k,n} \phi(x_n) \quad \text{in} \quad \mathcal{H}^{(S)}$$

might employ not only the diagonal matrix metric of Eq. (14) but also, say, a Sobolev-space resembling discretized inner product with tridiagonal $\Theta^{(N)} = 2\mathcal{P}_1^{(N)} - \gamma\mathcal{P}_2^{(N)}$ where, even at large $N$, the obligatory guarantee of positive definiteness would just require that $|\gamma| < 1$.

In a more general framework of study of mutually non-equivalent possible physical Hilbert spaces $\mathcal{H}^{(S)}$ assigned to a given Hamiltonian $H$ we believe that a deeper insight if not classification could be obtained in the nearest future, especially on the ambitious level aiming at the less elementary interactions and/or more complicated combinations of independent components in the positive definite matrices of metrics.
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Appendix A: $\mathcal{PT}$–symmetric models

One of the most common tacit assumptions which lies at the very heart of the correct physical interpretation of Eqs. (1) and/or (2) is that the real variables $x$ and/or $x_k$ represent an experimentally measurable quantity (most often, a coordinate or momentum of a point particle). This type of postulate has been declared redundant in the so called $\mathcal{PT}$–symmetric models where all $x$ or $x_k$ are allowed complex (cf. Refs. [3] for a full account of the theory). The endpoints $\pm L$ may be then chosen as any left-right symmetric pair of points, finite or infinite, in complex plane of $x$.

This is a new freedom. It implies, e.g., that the “wrong-sign” potential $V(x) = -x^4$ becomes tractable as a fully legal source of a discrete and real spectrum of bound-state energies which is bounded from below. One only has to complexify the points of boundary in an appropriate left-right symmetric (called, for historical reasons, $\mathcal{PT}$–symmetric) manner. In a typical replacement $+L \rightarrow \rho \exp(-i\phi)$ and $-L \rightarrow -\rho \exp(+i\phi)$ one uses a very large (or infinite) real $\rho \gg 1$ and some safely nonvanishing real angle $\phi$ (cf., e.g., Refs. [22] for more details).

In the $\mathcal{PT}$–symmetric scenario the role of the variable $x$ (and, mutatis mutandis, of $x_k$) is purely auxiliary. In principle, this variable does not represent an eigenvalue of any operator of observable even when it remains real. Mathematically one speaks about a “false” Hilbert space $\mathcal{H}(F)$ equipped with the most common definition of the inner product of wave functions,

$$\langle \psi_a | \psi_b \rangle \equiv \langle \psi_a | \psi_b \rangle^{(F)} = \int_{-L}^{L} \psi_a^*(x) \psi_b(x) \, dx \quad \text{in} \quad \mathcal{H}(F). \quad (23)$$

Hamiltonians are represented there, typically, by non-self-adjoint differential or difference operators,

$$H = -\frac{d^2}{dx^2} + V(x) \neq H^\dagger \quad \text{in} \quad \mathcal{H}(F). \quad (24)$$

As long as they have to generate a unitary time evolution, we must change the definition of Hermitian conjugation in order to make them properly Hermitian in the resulting “standard”, i.e., physical Hilbert space $\mathcal{H}(S)$,

$$H = -\frac{d^2}{dx^2} + V(x) = H^\dagger \equiv \Theta^{-1} H^\dagger \Theta \quad \text{in} \quad \mathcal{H}(S). \quad (25)$$

The auxiliary operator $\Theta = \Theta^\dagger > 0$ responsible for such a change of the definition of Hermitian conjugation in $\mathcal{H}(S)$ is called “metric” [10]. All the other operators $\mathcal{O}$ of observables must be “cryptohermitian”, i.e., Hermitian in the same space,

$$\mathcal{O} = \mathcal{O}^\dagger \equiv \Theta^{-1} \Theta^\dagger \Theta \quad \text{in} \quad \mathcal{H}(S). \quad (26)$$
The latter requirement (or a set of requirements if necessary) specifies the physics of the system in question. In opposite direction, the set of all the “hidden hermiticity” requirements (25) + (26) may be understood as a practical recipe for the explicit determination of the correct and unique metric operator $\Theta$ assigned to given $H$ and $O$ \cite{10,17}.

An immediate consequence of the latter formulation of the theory is that the two Hilbert spaces $H^{(F)}$ and $H^{(S)}$ coincide as vector spaces composed of the same wavefunction elements. The main and only difference between them lies in the update of the inner product in the latter space. In Ref. \cite{17} a compactified notation using a double-bra symbol has been recommended,

$$\langle \psi_a | \psi_b \rangle \Rightarrow \langle \psi_a | \Theta | \psi_b \rangle \quad \text{(27)}$$

Our Hamiltonian $H$ and Schrödinger Eq. (1) (or, \textit{mutatis mutandis}, Eq. (2), plus all the other operators $O$ of observables) find their physical probabilistic interpretation in the Hilbert space $H^{(S)}$ with a nontrivial metric $\Theta$. Thus, the internally consistent concept of the solvability of the model should, in principle, involve \textit{not only} the feasible construction of all the wave functions $\psi(x)$ and of all the related bound-state spectrum of energies $E$ \textit{but also} the practical feasibility of the assignment of the metric $\Theta$ to our system. This is a challenging problem, addressed in our present paper.

Appendix B: The sample of computation of all the pseudometrics in the six-dimensional square-well model (5) using the linear set of Eqs. (10)

The twelve unknown parameters entering the symmetry-reduced $N = 6$ ansatz for the pseudometric

$$Q_{(a,b,c,d,e,j)}^{(6)}(\lambda) = \begin{bmatrix}
a & b & c & d & e & j \\
b & f & g & h & k & e \\
c & g & m & n & h & d \\
d & h & n & m & g & c \\
e & k & h & g & f & b \\
j & e & d & c & b & a
\end{bmatrix}$$

must be shown compatible with the thirty six quasi-Hermiticity requirements represented by Eq. (10). The reduced set of six items of these equations (say, number 2, 9, 3, 10 and 4) offers the affirmative answer. Indeed, this sextuplet
of equations

\[-f + f \lambda + a + a \lambda + c = 0\]
\[-c - c \lambda - m + f + h = 0\]
\[-g + g \lambda + b + d = 0\]
\[-n - d - d \lambda + g + k = 0\]
\[-h + h \lambda + c + e = 0\]
\[-k + k \lambda + d + j + j \lambda = 0\]

leaves six parameters unconstrained and, with abbreviations

\[U = \frac{c + a (1 + \lambda)}{1 - \lambda} + \frac{c + e}{1 - \lambda} - c (1 + \lambda) = \frac{a (1 + \lambda)}{1 - \lambda} + \frac{c (1 + \lambda^2)}{1 - \lambda} + \frac{e}{1 - \lambda}\]

and

\[V = \frac{b + d}{1 - \lambda} + \frac{d + j (1 + \lambda)}{1 - \lambda} - d (1 + \lambda) = \frac{j (1 + \lambda)}{1 - \lambda} + \frac{d (1 + \lambda^2)}{1 - \lambda} + \frac{b}{1 - \lambda}\]

it specifies the following complete solution of Eq. (10) at \(N = 6\),

\[Q_{(a,b,c,d,e,j)}^{(6)}(\lambda) = \begin{bmatrix} a & b & c & d & e & j \\ b & c + a (1 + \lambda) & b + d & c + e & d + j (1 + \lambda) & j \\ c & b & 1 - \lambda & U & V & 1 - \lambda \\ d & c + e & 1 - \lambda & V & U & 1 - \lambda \\ e & d + j (1 + \lambda) & c + e & b & a \\ j & e & d & c & b & a \end{bmatrix} \]

At \(j = 0\) this matrix is nine-diagonal. It further becomes seven-diagonal with \(e = 0\), pentadiagonal after fixing \(d = 0\) while the next constraint \(c = 0\) makes it tridiagonal. Finally, at \(b = 0\) we arrive at the simplest, diagonal metric predicted by Eq. (14). Due to the symmetries of our problem we may infer that, in parallel, there also exists a very similar antidiagonal metric (15) containing, again, all units up to the endpoint exceptions.

The similar simplifications of the “interior” matrix elements in \(P_{(a,b,c,d,e,j)}^{(6)}(\lambda)\) may be noticed to appear in the tridiagonal and antitridiagonal cases where the two particularly elementary special pseudometrics given by the respective Eqs. (17) and (18) with \(\beta = 1 - \lambda\) are reproduced,

\[P_{2}^{(6)}(\lambda) = \begin{bmatrix} 0 & \beta & 0 & 0 & 0 & 0 \\ \beta & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & \beta \\ 0 & 0 & 0 & 0 & \beta & 0 \end{bmatrix}, \quad P_{5}^{(6)}(\lambda) = \begin{bmatrix} 0 & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & 1 & 0 & \beta \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ \beta & 0 & 1 & 0 & 0 & 0 \\ 0 & \beta & 0 & 0 & 0 & 0 \end{bmatrix}. \]
The remaining two independent components of the set of pseudometrics come out as parametrized via \( \gamma = (1 - \lambda)/(1 + \lambda^2) \) and \( \delta = 1/(1 + \lambda^2) \) yielding

\[
\mathcal{P}_3^{(6)}(\lambda) = \begin{bmatrix} 0 & 0 & \gamma & 0 & 0 & 0 \\ 0 & \delta & 0 & \delta & 0 & 0 \\ \gamma & 0 & 1 & 0 & \delta & 0 \\ 0 & \delta & 0 & 1 & 0 & \gamma \\ 0 & 0 & \delta & 0 & \delta & 0 \\ 0 & 0 & 0 & \gamma & 0 & 0 \end{bmatrix}, \quad \mathcal{P}_4^{(6)}(\lambda) = \begin{bmatrix} 0 & 0 & 0 & \gamma & 0 & 0 \\ 0 & 0 & \delta & 0 & \delta & 0 \\ 0 & \delta & 0 & 1 & 0 & \gamma \\ \gamma & 0 & 1 & 0 & \delta & 0 \\ 0 & \delta & 0 & \delta & 0 & 0 \\ 0 & 0 & \gamma & 0 & 0 & 0 \end{bmatrix},
\]

in full compatibility with Theorem 5.1.