\textit{CPT–symmetric discrete square well.}

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Abstract

In an addendum to the recent systematic Hermitization of certain $N$ by $N$ matrix Hamiltonians $H(N)(\lambda)$ \[1\] we propose an amendment $H(N)(\lambda, \lambda)$ of the model. The gain is threefold. Firstly, the updated model acquires a natural mathematical meaning of Runge-Kutta approximant to a differential $\mathcal{P}\mathcal{T}$–symmetric square well in which $\mathcal{P}$ is parity. Secondly, the appeal of the model in physics is enhanced since the related operator $\mathcal{C}$ of the so called “charge” (the requirement of observability of which defines the most popular Bender’s metric $\Theta = \mathcal{P}\mathcal{C}$) becomes also obtainable (and is constructed here) in an elementary antidiagonal matrix form at all $N$. Last but not least, the original phenomenological energy spectrum is not changed so that the domain of its reality [i.e., the interval of admissible couplings $\lambda \in (-1, 1)$] remains the same.
1 Introduction

In paper [1] (to be cited as paper I in what follows) we felt inspired by the recently revealed formal merits of an exceptionally easy non-trivial-metric-mediated Hermitizations of boundary-condition interactions [2]. We turned attention there to the simplified, discrete, real and manifestly asymmetric tridiagonal $N \times N$ matrix Hamiltonians

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

We studied these models under an additional, more or less randomly selected simplification with $\mu \to -\lambda$ where we abbreviated $H^{(N)}(\lambda, -\lambda) = H^{(N)}(\lambda)$.

In the present brief complement of paper I we intend to demonstrate that in spite of certain inessential complications of mathematics, the alternative simplifying choice of $\mu = +\lambda$ leads to an enhanced appeal of the physics described by the alternative (and, incidentally, isospectral) toy model $H^{(N)}(\lambda, \lambda)$.

After a very compact summary of the state of the art relocated to Appendices A and B below, the detailed presentation of our new results is split in section 2 (explaining certain practical aspects of the difference between the concepts of $\mathcal{PT}$–symmetry and $\mathcal{P}$–pseudohermiticity), section 3 (clarifying the mathematical and physical meaning of the Bender’s [3] special operator of “charge” $C$) and section 4 (where we show that for our updated Hamiltonians $H^{(N)}(\lambda, \lambda)$ the “charge” $C$ proves obtainable in an extremely elementary closed matrix form).

Section 5 will summarize our results re-emphasizing that our construction of $C$ guarantees the physical acceptability of the model. We shall point out that the availability of compact formula for $C$ renders our amended Hamiltonian $H^{(N)}(\lambda, \lambda)$ fully compatible with all of the postulates of standard quantum theory. In comparison with the model of paper I, it is also better understood in the continuous limit of $N \to \infty$. 
2 Parity \( \mathcal{P} \)

The initial encouragement to our present study stemmed from a few observations as made in paper I. Without repeating the details here we may merely recall the definition of the \( \mathcal{PT} \)-symmetry of \( H \) (cf. also Eq. (12) in Appendix A below) and rewrite it in its fully explicit equivalent matrix form

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

In paper I we revealed that there exists the whole set of sparse-matrix pseudometrics \( \mathcal{P} = \mathcal{P}_k^{(N)} \) with \( k = 1, 2, \ldots, N \), none of which appeared to be a rigorous discrete approximant to the parity. At the same time, our ability of finding all matrices \( \mathcal{P} \) compatible with \( H \) via Eq. (2) facilitated significantly our discussion and construction of the metrics.

The difficulty of the search for solutions \( \mathcal{P} \) of Eq. (2) is one of the main obstacles of an exhaustive understanding of physics which can potentially be covered by any given Hamiltonian, Hermitian or not \( \mathcal{H} \). In parallel, the search for the auxiliary, sparse-matrix solutions \( \mathcal{P} \) of Eq. (2) (we may call it Dieudonné’s equation \[5\]) may be perceived as one of the key mathematical conditions of practical applicability of the vast majority of non-Hermitian \( H \neq H^\dagger \).

The particular minus-sign model \( H^{(N)}(\lambda) \equiv H^{(N)}(\lambda, -\lambda) \) of paper I admitted a complete solution of Eq. (2). From our present point of view the serious drawback and weakness of the model lies in the fact that all operators \( \mathcal{P} \) compatible with the Dieudonné’s equation proved manifestly coupling-dependent.

This is an unpleasant feature. For illustration let us recall equation Nr. (15) of paper I which defines the most natural (viz., antidiagonal) candidate for the parity-reminding operator compatible with Eq. (12). It possesses the indefinite-matrix closed form

\[
\mathcal{P} = \mathcal{P}_k^{(N)}(\lambda) = \begin{bmatrix}
0 & 0 & \ldots & 0 & \alpha \\
0 & \ldots & 0 & 1 & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & 1 & 0 \\
\alpha & 0 & \ldots & 0 & 0
\end{bmatrix}, \quad \alpha = \frac{1 - \lambda}{1 + \lambda} \tag{3}
\]

which varies with \( \lambda \). In the continuous limit \( N \to \infty \) (viz., Runge-Kutta
limit, see paper I) this matrix cannot be interpreted as a standard, coupling-independent operator of parity, therefore. Strictly speaking, Hamiltonian $H^{(N)}(\lambda, -\lambda)$ remains out of the scope of $\mathcal{PT}$–symmetric quantum mechanics. This observation motivated our present study.

In a search for a manifestly $\mathcal{PT}$–symmetric model with better properties we were rather lucky when we turned attention to the next simplest choice of the parameters and inserted $\mu = +\lambda$ in Eq. (1). The core of the success lied in the emergence and verification of the coupling-independence of the most natural candidate

$$P = P^{(N)}(0) = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & \cdots & 0 & 1 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

(4)

for the pseudometric operator entering Eq. (2) and/or Eq. (12) below.

3 The operator of charge

A hidden root of success of $\mathcal{PT}$–symmetric models in physics may be seen in the decisive simplification of the theory using a specific form of the third, “superfluous” representation space $\mathcal{H}^{(S)} = \mathcal{H}^{(S)}_{(\mathcal{CP}T)}$. The metric $\Theta = \Theta_{(\mathcal{CP}T)}$ is only considered in a specific factorized form $\Theta_{(\mathcal{CP}T)} \equiv \mathcal{CP}$. Under such a simplifying assumption one reveals the equivalence of Eq. (13) of Appendix A and the formula representing the Hermiticity of the model in space $\mathcal{H}^{(S)}$. In its matrix form this equation reads

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

(5)

is linear in $\Theta$ and very similar to Eq. (2) of preceding section. Thus, one may make use of the $N$–parametric ansatz

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

(6)

where just the positivity of $\Theta^{(N)}$ must be required and guaranteed (cf. [6]).
In the above-outlined context the reconstruction of the charges might proceed via the knowledge of the sums

\[ \Theta = \sum_k \kappa_k^2 \langle k \rangle \langle k \rangle, \quad \mathcal{P}^{-1} = \sum_m \nu_m \langle m \rangle \langle m \rangle \]

where the single-ketted and double-ketted symbols \( |k\rangle \) and \( |k\rangle \langle k\rangle \) denote the \( k \)-th eigenvectors of \( H \) and \( H^\dagger \), respectively. This strategy (employed, say, in Refs. \([2, 7]\)) will be used also in what follows. In more detail, once the real parameters \( \kappa_k \) and \( \nu_m \) stay variable and virtually arbitrary (cf. \([8]\) for details) one can postulate, in our biorthogonal basis, the spectral formula

\[ \mathcal{C} = \sum_n |n\rangle \omega_n \langle \langle n \rangle . \]

The (in general, complex) values of overlaps \( \mu_n = \langle \langle n | n \rangle \) may be considered known. Constraints \( \mathcal{C} = \mathcal{P}^{-1} \Theta \) and \( \mathcal{C}^2 = I \) then merely imply that we have to demand that

\[ \omega = \mu_n^* \nu_n \kappa_n^2, \quad \mu_n \omega_n^2 = 1/\mu_n. \]

For a given set of “input” data \( \mu_n \) and \( \nu_n \) this determines all the coefficients \( \kappa_n^2 > 0 \) so that only a change in our choice of parity \( \mathcal{P} \) may lead to a different version of \( \mathcal{C} \) and of the metric.

In this sense, the undeniable phenomenological as well as theoretical appeal of \( \mathcal{PT} \)-symmetric models lies in the existence of a straightforward recipe for suppression of the well known ambiguity of the assignment of the metric \( \Theta \) to a given \( \mathcal{PT} \)-symmetric Hamiltonian. In matrix models the operator \( \mathcal{C} \) is not a sparse matrix while it \textit{proved to be} a sparse in our present, exceptional model \( H^{(N)}(\lambda, \lambda) \).

### 4 Charge \( \mathcal{C} \) for Hamiltonian \( H^{(N)}(\lambda, \lambda) \)

The privileged metrics of the form \( \Theta = \mathcal{PC} \) are usually accepted on the purely pragmatic grounds of simplicity. In general, one still must get through complicated calculations before arriving at any concrete \( \mathcal{C} \) or \( \Theta = \mathcal{PC} \). An exception has been found in paper I where a systematic construction of all the eligible \( \Theta \)s has been shown feasible due to a maximal friendliness of the model \( H = H^{(N)}(\lambda, -\lambda) \).

Beyond the framework of \( \mathcal{PT} \)-symmetric quantum mechanics which requires the observability of charge the formal assignment of the metric to a
Hamiltonian requires an alternative specification of the menu of required observables \([4, 9]\). In this sense, the additional requirement of the existence of charge \(C\) may be perceived as one of the most compact recipes for making the model unambiguous.

In our present letter we accepted such a research project, made use of the symbolic-manipulation algorithms developed in paper I and applied them to the alternative model \(H = H^{(N)}(\lambda, +\lambda)\). As long as the updated equations (2) exhibit now much less symmetries, we were really surprised by revealing that our rather naive strategy gave us an affirmative answer of an unexpectedly elementary form. The resulting charge has been found in the following, purely antidiagonal and manifestly involutive form

\[
C^{(N)}(\lambda) = \begin{bmatrix}
0 & 0 & \ldots & 0 & 1/\alpha(\lambda) \\
0 & \ldots & 0 & 1 & 0 \\
\vdots & \ddots & \ddots & \vdots & \vdots \\
0 & 1 & 0 & \ldots & 0 \\
\alpha(\lambda) & 0 & \ldots & 0 & 0
\end{bmatrix}, \quad \alpha(\lambda) = \frac{1 - \lambda}{1 + \lambda}, \quad (10)
\]

This corresponds to the safely positive and purely diagonal metric

\[
\Theta_0^{(N)}(\lambda) = \begin{bmatrix}
\alpha(\lambda) & 0 & \ldots & 0 & 0 \\
0 & 1 & 0 & \ldots & 0 \\
\vdots & \ddots & \ddots & \ddots & \vdots \\
0 & \ldots & 0 & 1 & 0 \\
0 & 0 & \ldots & 0 & 1/\alpha(\lambda)
\end{bmatrix}, \quad \alpha(\lambda) = \frac{1 - \lambda}{1 + \lambda}, \quad (11)
\]

The latter metric is only unessentially more complicated than its maximally symmetric diagonal analogue as specified by equation Nr. (14) in paper I.

5 Summary

In a brief conclusion let us emphasize that the exact solvability of models exhibiting hidden Hermiticity must involve not only the feasibility of diagonalization of the Hamiltonian but also the feasibility of construction and selection of an optimal metric \(\Theta\). There exist not too many quantum models which would satisfy both these criteria. Among them we were inspired by the models with \(N = \infty\) in which the unitarity of the quantum scattering has been achieved \([10]\).
We paid attention just to bound states here. Naturally, our work has significantly been simplified by the results of paper I because due to the easily demonstrated isospectrality relationship between Hamiltonians $H^{(N)}(\lambda) = H^{(N)}(\lambda, -\lambda)$ and $H^{(N)}(\lambda, +\lambda)$ the spectrum of energies $E_n^{(N)}(\lambda)$ remains real and non-degenerate for the same set of couplings lying inside the same open and $N$–independent interval of $\lambda \in (-1, 1)$.

In the updated calculations devoted to $H^{(N)}(\lambda, +\lambda)$ we succeeded in satisfying both the constraints of $\mathcal{PT}$–symmetry and $\mathcal{CPT}$–symmetry exactly, in non-perturbative manner. We may summarize that

- our Hamiltonians $H^{(N)}(\lambda, \lambda)$ are $\mathcal{PT}$–symmetric in the narrow sense, satisfying relation (12) of Appendix A below with $\lambda$–independent parity (11);
- for the same model there exists the operator of charge $\mathcal{C}$ such that $\mathcal{C}^2 = I$ which is represented by an extremely elementary matrix (10).

In the spirit of review [3] and Refs. [9] [11] [12], our explicit construction of charge makes the corresponding amended toy model manifestly $\mathcal{CPT}$–symmetric, i.e., compatible with the constraint (13) of Appendix A below. This means that every Hamiltonian $H^{(N)}(\lambda, \lambda)$ with the not too strong coupling $\lambda \in (-1, 1)$ is assigned an exceptional physical Hilbert space $\mathcal{H}_{(\mathcal{CPT})}^{(S)}$ in which the metric is defined as product $\Theta_{(\mathcal{CPT})}^{(N)} = \mathcal{PC}$.

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Appendix A: The concepts of $\mathcal{PT}$ and $\mathcal{CPT}$ symmetries

During the recent developments of quantum mechanics of (stable) bound states as initiated by Bender and Boettcher [13] it became increasingly popular to select a suitable phenomenological potential $V(x)$ in an innovative non-selfadjoint version. In such a purely theoretical setting (as reviewed, e.g., in Refs. [3]) as well as in its very recent experimental verifications [14] it makes sense to choose $V(x)$ in an exactly solvable and simplest possible form, say, of a square well [15] or of a point interaction [16] or of their perturbations [17].

In all of the similar non-selfadjoint models it is generically difficult to complement the “easy” results concerning energies by the “difficult” predictions of the role and physical interpretation of any other observable quantity (like, e.g., of the coordinate [18]). In the context of nuclear physics, for example, this problem of interpretation has already been addressed almost twenty years ago [4] but it still waits for a final satisfactory resolution [19, 6].

One of the most widely accepted transient strategies lies in the use of constructions of a single additional observable $\mathcal{C}$ with eigenvalues one or minus one. In accord with the original proposal by authors of Ref. [11] we may call it a charge. In general, even such a simplified strategy need not imply its easy implementation (cf., e.g., Ref. [20] for an illustration). One has to feel satisfied by any partial success.

A sample of such a success has been described in Ref. [2] where the operator $\mathcal{C}$ was constructed as a product of parity $\mathcal{P}$ and of the so-called metric $\Theta$. The feasibility of the construction (based on a resummation of infinite series) required a maximal simplicity of the interaction. Thus, the deep one-dimensional square-well potential $V_0(x)$ was assumed perturbed just by a user-friendly point interaction $V_1(x) = \lambda V_-(x) + \mu V_+(x)$ acting at the two boundaries of the well. Even after such a comparatively drastic simplification (after which the interaction proved equivalent to a mere redefinition of boundary conditions) the analysis of the model still remained quite difficult (cf. also its amended version in [7]).

A technically less difficult approach to the construction of $\mathcal{C}$ has been found after a further transition from the differential Hamiltonian operators to their discrete approximants and analogues [21]. A new broad and interesting class of tractable quantum models emerged. Even the extremely
schematic $N$–dimensional matrix models with $N = 2$ proved of value for our understanding of certain theoretical subtleties [22, 23, 24].

Once one restricts attention to Jacobi-matrix models exemplified by Eq. (1) and possessing a nontrivial interaction terms solely near the ends of the main diagonal, the first important merit of the resulting matrix toy Hamiltonian appears to be the reality of the energy spectrum inside a non-empty domain $\mathcal{D}$ of parameters $\lambda$ and $\mu$. In Figures 1 - 6 of paper I a few characteristic samples of the rich and flexible parametric dependence of this spectrum were displayed. Under additional restriction $\mu = \pm \lambda$ domains $\mathcal{D}$ were shown $N$–independent and specified as a sufficiently large interval of $\lambda \in (-1, 1)$. Within the latter interval we proceeded in a constructive manner, selected a definite (viz., minus) sign in $H = H^{(N)}(\lambda, -\lambda)$ and constructed an exhaustive list of $N$–dimensional, not necessarily positive definite pseudometrics $\mathcal{P} = \mathcal{P}^\dagger$. In the spirit of review papers [25] these operators were interpreted as alternative generalized parities.

In the light of an older mathematical study [26] the latter operators $\mathcal{P}$ need not even be required invertible. Nevertheless, all of them were designed as compatible with the $\mathcal{PT}$—symmetry constraint imposed upon the Hamiltonian and written in the form

$$\mathcal{PT} H^{(N)}(\lambda, \mu) = H^{(N)}(\lambda, \mu) \mathcal{PT}$$

(12)

Although operator $\mathcal{T}$ is intended to simulate time reversal, a vivid debate in the literature [12] indicated that some of its technical aspects are nontrivial. The net result of this debate may be summarized as a conclusion that the existence of symmetry (12) facilitates a safe return to the traditional textbook formalism of quantum theory.

Let us add here also the well known fact that the non-Hermiticity of Hamiltonians with real spectra may be treated as just a misinterpretation or rather a price paid for a wrong choice of the Hilbert space. In one of the most popular resolutions of the apparent paradox Carl Bender with coauthors [3] introduced the concept of charge $\mathcal{C}$ with the only (i.e., multiply degenerate) eigenvalues equal to +1 or −1. The availability of this charge enabled them to introduce an amended, standard Hilbert space where the input Hamiltonian $H$ becomes self-adjoint. The recipe has been shown equivalent to the additional symmetry requirement

$$\mathcal{CPT} H^{(N)}(\lambda, \mu) = H^{(N)}(\lambda, \mu) \mathcal{CPT}.$$ 

(13)
The important role of this constraint contrasts with the scarcity of the available known pairs of mutually compatible observables $H$ and $C$. In this sense our present paper partially fills the gap.

**Appendix B. Hidden Hermiticity**

The abstract formalism of quantum theory is frequently being explained via concrete descriptions of a point particle moving in a confining one-dimensional potential well $V(x)$ [27]. In the notation of our review [19] one prefers the use of a specific, “friendly” realization $H^{(F)}$ of the abstract Hilbert space of states. In it, the measurable coordinate $q \in \mathbb{R}$ (i.e., strictly speaking, the eigenvalue of operator $Q^{(F)}$ of observable position) coincides with the argument $x$ of the normalized bound-state wave function $\psi_n = \psi_{n}^{(F)}(x)$ (cf. also a longer exposition of this subtlety in [28]). In the Dirac’s compact notation one prefers working with the ket vectors $|\psi_n^{(F)}\rangle \in H^{(F)} \equiv L^2(\mathbb{R})$.

For non-local potentials $V(x, x')$ one may turn attention to an alternative, momentum representation $|\psi_n^{(P)}\rangle \in H^{(P)} \equiv L^2(\mathbb{R})$ of the same states. The Fourier-like mapping $\mathcal{F}$ between spaces $H^{(F)}$ and $H^{(P)}$ is postulated unitary, $\mathcal{F}^\dagger \mathcal{F} = I$. The physical meaning of the real line $\mathbb{R}$ is now different but the physical contents of the theory remains the same.

In a generalization of this picture one replaces operators $\mathcal{F}$ by non-unitary maps $\Omega$ and defines

$$|\psi_n^{(P)}\rangle = \Omega |\psi_n^{(F)}\rangle, \quad \Omega^\dagger \Omega = \Theta \neq I. \quad (14)$$

Taken, originally, as a mere mathematical curiosity [26, 29] the latter trick proved unexpectedly useful and fruitful in nuclear physics where the first non-unitary version of the boson-fermion map $\Omega$ has been proposed by Dyson (cf. review [4]). Its mathematical essence may most easily be interpreted as an introduction of certain third representation space $H^{(S)}$ where superscript $(S)$ may stand for “standard” or, if you wish, “sophisticated”.

By construction, the two Hilbert spaces $H^{(S)}$ and $H^{(P)}$ must be unitarily equivalent. Similar requirement does not apply to the two spaces $H^{(S)}$ and $H^{(F)}$ which may only be allowed to coincide as Banach spaces formed by the identical vector spaces $V^{(F)} = V^{(S)}$ of kets, with their inner products not yet specified. In the latter pair the differences only emerge between the dual (i.e., representation-dependent and, in standard notation, primed) Banach
spaces of bra-vectors. The first space \( (\mathcal{V}^{(F)})' \) of linear functionals in \( \mathcal{H}^{(F)} \) must be different from the second space \( (\mathcal{V}^{(S)})' \) of linear functionals in \( \mathcal{H}^{(S)} \).

In order to avoid confusion we would recommend the use of the full-fledged notation of Ref. [30]. In it, the respective operations of Hermitian conjugation \( T = T^{(F,P,S)} \) are defined as the most common vector (or matrix) transposition plus complex conjugation in \( \mathcal{H}^{(F)} \),

\[
T^{(F)} : |\psi^{(F)}_n\rangle \rightarrow \langle \psi^{(F)}_n| \in (\mathcal{V}^{(F)})'
\]

and in \( \mathcal{H}^{(P)} \),

\[
T^{(P)} : |\psi^{(P)}_n\rangle \rightarrow \langle \psi^{(P)}_n| \in (\mathcal{V}^{(P)})'
\]

and as the more complicated prescription valid in \( \mathcal{H}^{(S)} \),

\[
T^{(S)} : |\psi^{(S)}_n\rangle \rightarrow \langle \psi^{(S)}_n| = \langle \psi^{(F)}_n| \Theta \equiv \langle \psi^{(F)}_n| \in (\mathcal{V}^{(S)})'.
\]

A more extensive discussion of such a version of quantum theory in its triple Hilbert-space representation may be found in Ref. [19].