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Cryptohermitian Picture of Scattering Using Quasilocal Metric Operators*

Miloslav ZNOJIL

Nuclear Physics Institute ASCR, 250 68 Řež, Czech Republic
E-mail: *znojil@ujf.cas.cz*
URL: `http://gemma.ujf.cas.cz/~znojil/`

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Abstract. One-dimensional unitary scattering controlled by non-Hermitian (typically, $\mathcal{PT}$-symmetric) quantum Hamiltonians $H \neq H^\dagger$ is considered. Treating these operators via Runge–Kutta approximation, our three-Hilbert-space formulation of quantum theory is reviewed as explaining the unitarity of scattering. Our recent paper on bound states [Znojil M., *SIGMA* **5** (2009), 001, 19 pages, arXiv:0901.0700] is complemented by the text on scattering. An elementary example illustrates the feasibility of the resulting innovative theoretical recipe. A new family of the so called quasilocal inner products in Hilbert space is found to exist. Constructively, these products are all described in terms of certain non-equivalent short-range metric operators $\Theta \neq I$ represented, in Runge–Kutta approximation, by $(2R-1)$-diagonal matrices.

Key words: cryptohermitian observables; unitary scattering; Runge–Kutta discretization; quasilocal metric operators

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1 Introduction and summary

In paper I [1] we summarized the situation in which certain very complicated quantum bound-state Hamiltonians $\mathfrak{h} = \mathfrak{h}^{(\mathrm{P})} = \mathfrak{h}^\dagger$ (acting in the usual physical Hilbert space $\mathcal{H}^{(\mathrm{P})}$) were assumed solvable via a Dyson-inspired transition to their non-Hermitian but perceivably simpler isospectral partners $H = \Omega^{-1}\mathfrak{h}\Omega \neq H^\dagger$. The latter auxiliary operators were assumed acting in a doublet of the first auxiliary and the second auxiliary Hilbert spaces $\mathcal{H}^{(\mathrm{F,S})}$, respectively. The latter space $\mathcal{H}^{(\mathrm{S})}$ was finally assumed endowed with an unusual inner product $(a,b)^{(\mathrm{S})}$ defined by the formula $(a,b)^{(\mathrm{S})} := (a,\Theta b)^{(\mathrm{F})}$ in terms of the usual Dirac's inner product $(a,b)^{(\mathrm{F})}$ and of the so called metric operator $\Theta = \Theta^\dagger = \Omega^\dagger\Omega > 0$.

In the present continuation of paper I we shall extend our three-Hilbert-space formulation of quantum theory to a class of models of scattering. For illustrative purposes we shall discretize the axis of coordinates into Runge–Kutta lattice [2]. This discretization is not a mandatory ingredient of the approach but its use will facilitate our explicit constructions. In particular, it will enable us to demonstrate that for a selected sample Hamiltonian H one can construct several alternative metrics Θ which are all compatible with the unitarity of the scattering-state solutions of the underlying Schrödiner equation. This quantification of the ambiguity of Θ will be a core of our message to physicists. Unexpectedly, our unitarity-supporting illustrative Θs will prove "quasilocal", i.e., they will emerge as short-ranged continuous-coordinate limits of $(2R-1)$-diagonal Runge–Kutta approximation matrices $\Theta = \Theta_R$ with integer $R = R(h)$ such that $\lim_{h\to 0} hR(h) = 0$. This will be our main new mathematical result.

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The detailed presentation of this result will be preceded by a short review of motivation (Section 2) and of the currently well-established theoretical understanding of non-Hermitian models of bound states (Section 3). The current status of extension of this version of quantum theory to scattering scenario will be summarized in Section 4.

In Section 5 we pick up one of the elementary concrete models [3] and use it to outline our method applicable in the dynamical regime of scattering. The core of our message is formulated in this section. We fix there the level of approximation given by the Runge–Kutta lattice-spacing $h > 0$ and describe the construction of metric operators $\Theta = \Theta(H)$. For our toy model H, in particular, we list the first few explicit samples of $\Theta = \Theta_R(H)$ possessing the $(2R-1)$-diagonal matrix structure. These matrices are constructed by computerized symbolic manipulations at $R = 1, 2, \ldots, 7$. Our knowledge of these solutions enables us to conjecture (and, subsequently, prove) formula which defines all the eligible quasilocal metrics $\Theta_R(H)$ at any R in closed form.

In complementary and concluding Sections 6 and 7 we construct underlying Dyson operators Ω and discuss some of their potentially most relevant descriptive properties as well as several possible consequences of their use in model-building.

2 Context: $\mathcal{PT}$-symmetric Hamiltonians

Among all of the simplified phenomenological models used in quantum mechanics a prominent role is played by the families described by Schrödinger equations of ordinary differential form

$$\frac{\hbar^2}{2m}\left[-\frac{d^2}{dx^2}+\frac{L(L+1)}{x^2}\right]\Psi(x)+V(x)\Psi(x)=E\Psi(x). \tag{1}$$

Centrifugal coefficient $L(L+1)$ may be admitted to vanish. Variable x is then interpreted as the one-dimensional coordinate. Requirement $\Psi(x) \in \mathbb{L}_2(\mathbb{R})$ is being imposed upon bound states while the scattering solutions are characterized by asymmetric asymptotic boundary conditions at all real $\kappa = \sqrt{E - V(\infty)}$,

$$\Psi(x) = \begin{cases} e^{i\kappa x} + Re^{-i\kappa x}, & x \ll -1, \\ Te^{i\kappa x}, & x \gg 1. \end{cases} \tag{2}$$

At nonvanishing centrifugal coefficients one demands that $L(L+1) > -1/4$ while variable x is treated as the radial coordinate in D dimensions, $x = |\vec{r}| \in (0,\infty)$. An additional, specific boundary condition must be then imposed in the origin in order to guarantee the regularity of bound-state as well as scattering solutions [4]. Of course, physics represented by equation (1) on half line depends again on the asymptotic behavior of potential $V(x)$.

Usually one distinguishes between the confining, bound-state regime (where $V(x)$ is chosen smooth, real and very large at large $x \to \pm\infty$) and the scattering scenario (where, typically, $V(\pm\infty) = 0$ and where wave functions $\Psi(x)$ are selected as free waves at large $x \to \pm\infty$). Recently, several authors emphasized the existence of another, unusual quantization of the ordinary differential Schrödinger equation (1) which is assumed integrated along a non-standard, *complex* contour of "pseudocoordinates" $x = x(s) \in \mathbb{C}$ where $s \in \mathbb{R}$ is a parameter (cf., e.g., Sibuya [5] or Bender and Turbiner [6]).

The early attempts in this direction were treated and accepted as a mere mathematical curiosity. For illustration we may recall paper [7] by Buslaev and Grecchi who studied anomalous potentials $V(x) \sim -x^4 + \mathcal{O}(x^3)$. Equation (1) with these "wrong-sign" potentials has been considered along a shifted line of $x = x^{(\mathrm{BG})}(s) = s - \mathrm{i}\varepsilon$. By this trick, the potential (which looks asymptotically repulsive) has been made manifestly confining. In parallel, the usual requirement of Hermiticity has been replaced by $\mathcal{PT}$-symmetry, i.e., by left-right symmetry in the complex plane of x (cf. also [8] for more comments).

During the last ten years we witnessed a quick growth of interest in $\mathcal{PT}$-symmetric models. Within physics community this interest has been inspired by Bender's and Boettcher's influential letter [9] where the authors emphasized the deeply physical appeal of the combination of the parity-reversal symmetry (mediated by the operator $\mathcal{P}$) with the time-reversal symmetry (cf. operator $\mathcal{T}$). They conjectured and demonstrated, by approximate methods, the reality (i.e., in principle, measurability) of the bound-state spectra for the whole family of specific $\mathcal{PT}$-symmetric toy potentials

$$V^{(\mathrm{BB})}(x) = x^2(\mathrm{i}x)^{4\delta}, \qquad \delta \geq 0. \tag{3}$$

A few years later the validity of the conjecture has rigorously been proved by Dorey, Dunning and Tateo [10] and by Shin [11]. This clarified, for bound states, the mathematics of complexification of the argument x of wave functions $\psi(x)$ and/or of potential $V(x)$.

The questions emerging in scattering regime have temporarily been left open.

3 New horizons: cryptohermitian observables

The success of the latter generalization of the class of quantum bound-state models opened several new theoretical directions of research since in many concrete examples the complex value of "coordinate" x ceased to be tractable as a measured or measurable quantity. For this reason the theoretical as well as practical acceptance of the internal mathematical consistency of apparently non-Hermitian models exemplified by equations (1) + (3) took some time in physics community (cf., e.g., review paper [12] for historical comments). The paradoxes seem to be clarified at present and, for bound states, a new pattern is established for implementation of the formalism of textbook quantum mechanics.

The key to the safe return from equations (1) + (3) (and the like) to textbooks can be seen in the concept of cryptohermiticity (the word invented, very recently, by Smilga [13]) which, in essence, means that an operator H which appears non-Hermitian in Hilbert space $\mathcal{H}^{(\mathrm{F})}$ (where the superscript indicates the (user-)friendliness of the most current mathematical definition of the inner product – see below) may be reinterpreted, under certain circumstances, as safely Hermitian in another, Hilbert space $\mathcal{H}^{(\mathrm{S})}$ (where the superscript stands for "standard" physics). The third Hilbert space $\mathcal{H}^{(\mathrm{P})}$ emerges, quite naturally, as a space which is unitarily equivalent to $\mathcal{H}^{(\mathrm{S})}$ (i.e., it represents *strictly the same* physics so that for the purposes of physical predictions we have an entirely free choice between $\mathcal{H}^{(\mathrm{P})}$ and $\mathcal{H}^{(\mathrm{P})}$) but which is *the only* space encountered in textbooks (i.e., the metric operator in $\mathcal{H}^{(\mathrm{P})}$ remains conventional, identically equal to the unit operator).

One of the first papers presenting and reviewing such an abstract idea in a concrete application in nuclear physics appeared more than fifteen years ago [14]. The study of heavier atomic nuclei has been shown simplified by the mapping of the usual, complicated physical Hilbert space of states $\mathcal{H}^{(\mathrm{P})}$ (describing fermions and possessing, therefore, complicated antisymmetrization features) upon another, bosonic (i.e., manifestly *unphysical*) auxiliary space $\mathcal{H}^{(\mathrm{F})}$. This made the calculations perceivably facilitated. Whenever needed, the return to fermionic wave functions mediated by the not too complicated Dyson mapping Ω remained feasible via a unitary equivalence between $\mathcal{H}^{(\mathrm{P})}$ and $\mathcal{H}^{(\mathrm{S})}$ (more details may be found in [1]).

The combination of a comparatively narrow applicability in nuclear physics with a rather unusual mathematics caused that the methodical appeal of the non-unitary-mapping idea remained virtually unnoticed until its re-emergence in $\mathcal{PT}$-symmetric context. At present we witness a massive revival of interest in the parallel use of the three alternative representations $\mathcal{H}^{(\mathrm{P})}$, $\mathcal{H}^{(\mathrm{F})}$ and $\mathcal{H}^{(\mathrm{S})}$ of the *same* physical quantum system. The invertible Dyson-type mapping Ω relates the spaces $\mathcal{H}^{(\mathrm{P})}$ and $\mathcal{H}^{(\mathrm{F})}$ as well as the respective Hamiltonians or operators of other observables.

The manifest violation of the unitarity by the mapping $\Omega \neq (\Omega^\dagger)^{-1}$ requires due care in applications. For example, the physical Hamiltonian $\mathfrak{h}$ must be Hermitian (i.e., more strictly, essentially self-adjoint in the physical Hilbert space $\mathcal{H}^{(\mathrm{P})}$ exemplified by the fermionic space in the above-mentioned concrete application). It may also be perceived as a transform of another operator defined as acting in another vector space, $\mathfrak{h} = \Omega H \Omega^{-1}$. The latter "Hamiltonian" H is, by construction, defined *and* manifestly non-Hermitian in space $\mathcal{H}^{(\mathrm{F})}$ where, trivially,

$$H^\dagger = \Omega^\dagger \mathfrak{h} \left(\Omega^{-1}\right)^\dagger = \Omega^\dagger \Omega H \Omega^{-1} \left(\Omega^{-1}\right)^\dagger = \Theta H \Theta^{-1}. \tag{4}$$

We abbreviated $\Theta = \Omega^\dagger \Omega$ calling this new operator, conveniently, a metric. It is defined as acting on the kets in both Hilbert spaces $\mathcal{H}^{(\mathrm{F})}$ and $\mathcal{H}^{(\mathrm{S})}$. This mathematical ambiguity proves inessential in applications and it is also easily clarified by the following elementary graphical pattern using notation of paper I,

$$\begin{tikzcd} & \boxed{\begin{array}{c}\text{physics OK in } \mathcal{H}^{(\mathrm{P})}\\ \text{ket } |\psi\succ = \text{uncomputable}\end{array}} \arrow[dr, "\text{map } \Omega^{-1}"] & \\ \boxed{\begin{array}{c}\text{math. OK in } \mathcal{H}^{(\mathrm{F})}\\ |\psi\rangle = \text{ computable}\end{array}} \arrow[ur, "\text{map } \Omega"] \arrow[rr, "\text{map } \Omega\Omega^{-1}=I"] & & \boxed{\begin{array}{c}\text{all OK in } \mathcal{H}^{(\mathrm{S})}\\ |\psi\rangle = \text{ the same}\end{array}} \end{tikzcd}$$

This diagram reconfirms that the Hermiticity of the physical Hamiltonian $\mathfrak{h} = \Omega H \Omega^{-1} = \mathfrak{h}^\dagger = \left[\Omega^{-1}\right]^\dagger H^\dagger \Omega^\dagger$ acting in the physical Hilbert space $\mathcal{H}^{(\mathrm{P})}$ is equivalent to the cryptohermiticity constraint (4) imposed upon its partner $H = \Omega^{-1}\mathfrak{h}\Omega \neq H^\dagger$ in $\mathcal{H}^{(\mathrm{F})}$.

3.1 The ambiguity of the metric $\Theta = \Theta(H)$

Hesitations may emerge when one imagines that the Hermitian conjugation itself is not a unique operation and that it may be altered [15]. In this way equation (4) may be interpreted as assigning several alternative physical metric operators to single Hamiltonian, $\Theta \in (\Theta_1(H), \Theta_2(H), \ldots)$. The first thorough discussion and clarification of this problem of ambiguity has been published by Scholtz et al. [14]. They emphasized that besides the Hamiltonian H itself, any other operator $\mathcal{O} = \mathcal{O}_1, \mathcal{O} = \mathcal{O}_2, \ldots$ of an observable quantity must obey the same cryptohermiticity relation as $H \equiv \mathcal{O}_0$ itself. In opposite direction, for a given set of observables in $\mathcal{H}^{(\mathrm{F})}$, each eligible metric operator Θ must remain compatible with all of them,

$$\Theta\, \mathcal{O}_j = \mathcal{O}_j^\dagger \Theta, \qquad j = (0,)1, 2, \ldots, j_{\max}. \tag{5}$$

These requirements reduce the ambiguity of Θ so that at a suitable integer $j_{\max}$ the metric $\Theta = \Theta(H)$ may become, in principle, unique.

The ambiguity of Θ may acquire an enormous theoretical importance as well as phenomenological relevance. The abstract understanding of the ambiguity of Dyson maps Ω did already prove crucial not only for the above-mentioned efficient description of bound states in nuclear physics but also in a clarification of the role of the charge or ghosts in field theory [16], etc.

3.2 Classical limit in the case of cryptohermitian Hamiltonians

Persuasive demonstration of relevance of the apparently purely mathematical subtlety of the ambiguity of metric can be mediated by the popular Bessis' and Zinn-Justin's (BZJ, [17]) imaginary cubic oscillator

$$H^{(\mathrm{BZJ})}|\psi_n^{(\mathrm{F})}\rangle = E_n |\psi_n^{(\mathrm{F})}\rangle, \qquad H^{(\mathrm{BZJ})} = -\frac{d^2}{dx^2} + \mathrm{i}gx^3, \qquad n = 0, 1, \ldots \tag{6}$$

for which the quantum bound-state problem is formulated and solved in Hilbert space $\mathcal{H}^{(\mathrm{F})} \equiv L^2(\mathbb{R})$ *and* for which the spectrum is real, discrete and bounded below despite the BZJ Hamiltonian being manifestly non-Hermitian.

Routinely, the Dyson mapping may be employed to convert the elements $|\psi^{(\mathrm{F})}\rangle \in \mathcal{H}^{(\mathrm{F})}$ of the above-mentioned space into their images $|\psi^{(\mathrm{P})}\rangle \in \mathcal{H}^{(\mathrm{P})}$ which lie in the correct representation $\mathcal{H}^{(\mathrm{P})}$ of the abstract, textbook Hilbert space of states. Superscript $^{(\mathrm{P})}$ stands for "physical" and we have $\Omega : \mathcal{H}^{(\mathrm{F})} \to \mathcal{H}^{(\mathrm{P})}$ and $|\psi^{(\mathrm{P})}\rangle = \Omega|\psi^{(\mathrm{F})}\rangle$. It is the isospectral partner $\mathfrak{h}^{(\mathrm{BZJ})} = \Omega H^{(\mathrm{BZJ})}\Omega^{-1}$ of our original Hamiltonian which becomes, by construction, safely Hermitian in physical space $\mathcal{H}^{(\mathrm{P})}$.

There is a price to be paid for the clarification of theoretical concepts. In our illustrative example (6) it was difficult to prove that the spectrum of the bound-state energies is all real [10]. In [18] one finds that even in the weak-coupling regime with a very small value of $g = \epsilon$ one arrives at an impressively complicated physical representative of Hamiltonian in $\mathcal{H}^{(\mathrm{P})}$,

$$\begin{aligned}\mathfrak{h}^{(\mathrm{BZJ})} = \Omega H^{(\mathrm{BZJ})}\Omega^{-1} = \frac{p^2}{2} + \frac{3}{16}\Bigg(\left\{x^6, \frac{1}{p^2}\right\} + 22\left\{x^4, \frac{1}{p^4}\right\} + (510 + 10\lambda_1)\left\{x^2, \frac{1}{p^6}\right\} \\ + \frac{8820 + 140\lambda_1}{p^8} - \frac{4}{3}\kappa_1\left\{x^3, \frac{1}{p^5}\right\}\mathcal{P}\Bigg)\epsilon^2 \\ + \frac{1}{4}\left(15\lambda_2\left(\left\{x^2, \frac{1}{p^{11}}\right\} + \frac{44}{p^{13}}\right) - i\kappa_2\left\{x^3, \frac{1}{p^{10}}\right\}\mathcal{P}\right)\epsilon^3 + \mathcal{O}(\epsilon^4). \qquad (7)\end{aligned}$$

This formula contains parity operator $\mathcal{P}$ and anticommutators $\{\cdot,\cdot\}$, it uses the Fourier-transformed multiplication-operator representation of the powers of p in $L^2(\mathbb{R})$ and, finally, it varies freely with four real parameters λ_j and κ_j, $j = 1, 2$. Persuasively, formula (7) demonstrates that the *explicit* form of true Hamiltonians $\mathfrak{h} = \mathfrak{h}^\dagger$ may become threateningly or even prohibitively complicated. One cannot be expected to perform practical calculations using this representation of the Hamiltonian.

The latter remark seems to imply that the explicit knowledge of maps $H \leftrightarrow \mathfrak{h}$ or, for other observables, $A \leftrightarrow \mathfrak{a}$ may be skipped as redundant. Actually, this is just a partial truth since operators $\mathfrak{h}$ or Ω may remain unavoidable, e.g., during the analysis of time-dependent systems (cf. [19] and also the recent preprint [20] in this respect). Moreover, in model (7) one could select $\lambda_2 = \kappa_2 = 0$ in order to preserve $\mathcal{PT}$-symmetry. Last but not least, the "unfriendly" Hilbert space $\mathcal{H}^{(\mathrm{P})}$ opens the way towards the classical limit of the system. From the imaginary cubic example (7) one arrives at the classical Hamiltonian function h_c defined in the classical single-particle phase space of the coordinate p_c and momentum p_c,

$$h_c^{(\mathrm{BZJ})} = \frac{p_c^2}{2m} + \epsilon^2 g(p_c)x_c^6 + \mathcal{O}(\epsilon^4), \qquad g(p_c) = \frac{3m}{8p_c^2} \qquad (8)$$

(cf. equation (62) in [18]). Thus, the limiting transition $\hbar \to 0$ reveals a hidden sextic-oscillator nature of the imaginary cubic forces in the weak-coupling regime.

3.3 Extended Dirac's bra/ket notation

The popular emphasis on the non-Hermiticity of simplified, artificial $H \neq H^\dagger$ in $\mathcal{H}^{(\mathrm{F})}$ should be perceived as attracting attention but slightly misleading. It reflects just the mathematical property (implicitly, of the only relevant, correct and physical operator $\mathfrak{h}$) with no direct connection, say, to the principle of correspondence (cf. the preceding paragraph). In contrast to the descriptions of open systems [21] where the probability is not conserved the calculations of probabilities must *all* be performed inside $\mathcal{H}^{(\mathrm{P})}$ or in one of its unitarily equivalent partner Hilbert spaces $\mathcal{H}^{(\mathrm{S})}$ where $\Theta \neq I$. We strongly recommend an explicit reference to the space in which one resides, because

- the apparent and misleading conflict between the absence of the correct physics in $\mathcal{H}^{(F)}$ and the lack of the computational feasibility in $\mathcal{H}^{(P)}$ is naturally resolved by the metric-dependent description of the system in the standardized Hilbert space $\mathcal{H}^{(S)}$;
- the Dirac notation can be used after a graphical adaptation of the bra- and ket-symbols when one speaks about the elements of the formally different Hilbert spaces $\mathcal{H}^{(F)}$, $\mathcal{H}^{(S)}$ and $\mathcal{H}^{(P)}$.

More explicitly, the *same* state ψ of a quantum system will be characterized by a spiked ket symbol in P-space, $|\psi\succ \in \mathcal{H}^{(P)}$, and by the standard ket symbol in the other two Hilbert spaces, $|\psi\rangle \in \mathcal{H}^{(F,S)}$. The two spaces $\mathcal{H}^{(F,S)}$ are chosen as identical when only their ket elements are being considered. These two spaces are identical as vector spaces which should be denoted by a dedicated symbol $\mathcal{V}^{(F)} = \mathcal{V}^{(S)}$. They only differ in the respective definition of their respective linear functionals, i.e., of the bra-vector elements of the dual vector spaces marked by the prime, $\mathcal{V}^{(F)\prime} \neq \mathcal{V}^{(S)\prime}$. The correspondence between the three dual vector spaces can be represented by the following diagram,

$$\begin{tikzcd} & \boxed{\prec\psi| \in \left(\mathcal{V}^{(P)}\right)'} \arrow[dr, "\text{map }\Omega"] & \\ \boxed{\langle\psi| \in \left(\mathcal{V}^{(F)}\right)'} \arrow[ur, "\text{map }\Omega^\dagger"] \arrow[rr, "\text{map }\Theta=\Omega^\dagger\Omega\neq I"] & & \boxed{\langle\!\langle\psi| \in \left(\mathcal{V}^{(S)}\right)'} \end{tikzcd}$$

In this notation it is easy to define $\langle\!\langle\Psi| = \langle\Psi|\Theta$ or to work with the map $\Omega : |\psi_n\rangle \to |\psi_n\succ$. It is equally easy to verify the unitarity of the map between the Hilbert spaces $\mathcal{H}^{(P)}$ and $\mathcal{H}^{(S)}$,

$$\prec\psi|\phi\succ = \langle\!\langle\psi|\phi\rangle.$$

As long as $(\mathcal{V}^{(F)})' \neq (\mathcal{V}^{(S)})'$ we must distinguish between the explicit definitions of the respective operations of Hermitian conjugation. The operation marked by single-cross superscript † in $\mathcal{H}^{(F)}$ *must be distinguished* from the one active in $\mathcal{H}^{(S)}$ and marked by double-cross ‡.

The acceptance of the notation recommended in this section enables us to introduce a modified bra symbol in $\mathcal{H}^{(S)}$, $(|\Psi\rangle)^\ddagger = \langle\!\langle\Psi| \in (\mathcal{V}^{(S)})'$ while keeping the traditional $(|\Psi\rangle)^\dagger = \langle\Psi| \in (\mathcal{V}^{(F)})'$ unchanged. There is no doubt that the use of three Hilbert spaces $\mathcal{H}^{(P,F,S)}$ does not contradict any principle of textbook quantum mechanics. Indeed, all the *physical* operators of observables remain Hermitian in $\mathcal{H}^{(P)}$ while the other two spaces $\mathcal{H}^{(F,S)}$ are just auxiliary.

4 Scattering and problems with long-ranged non-Hermiticities

The variability of Θs and/or Ωs could inspire optimistic expectations concerning the extension of the cryptohermitian description of physics to scattering scenario. Unfortunately, several serious obstacles were found and formulated by Jones [22]. He argued that Dyson maps Ω must be necessarily long-ranged leading to an apparent violation of causality in scattering (cf. Section 4.1 below). A return to optimism has been initiated in [23] where some of the most striking difficulties were circumvented via a replacement of the current, strictly local interactions $V(x)$ by their minimally nonlocal alternatives (cf. Section 4.2 below). The first fully satisfactory model of scattering has been found in [3] (cf. Section 4.3 below). A continuation of these developments will be reported here immediately after a brief summary of older results.

4.1 The first problem: The causality-violating waves in the scattering

In numerous recent applications of the above-mentioned three-space representation of quantum theory to bound states a conflict was encountered between the friendliness of the calculations in unphysical $\mathcal{H}^{(\mathrm{F})}$ and the unpleasant complications arising during the transition to the two alternative physical spaces $\mathcal{H}^{(\mathrm{S,P})}$. Many concrete Hamiltonians H happened to possess a particularly simple form in space $\mathcal{H}^{(\mathrm{F})}$ and vice versa.

The transition to the correct space may be perceived as a fairly unnatural operation. The more so if one tries to describe the non-Hermitian scattering [24, 25]. For these reasons, the counterintuitive character of the textbook Hermiticity of H in unfriendly $\mathcal{H}^{(\mathrm{S})}$ is reflected by the terminology in which the cryptohermitian operators are nicknamed quasi-Hermitian rather than Hermitian [14, 26].

The main difference between the two Hilbert spaces $\mathcal{H}^{(\mathrm{F,S})}$ concerns their inner products between elements $|\psi\rangle$ and $|\phi\rangle$. In the most usual coordinate representation language we have

$$\langle\psi|\phi\rangle^{(\mathrm{F})} = \int \psi^*(x)\phi(x)\,dx = \langle\psi|\phi\rangle \qquad \text{in} \quad \mathcal{H}^{(\mathrm{F})}, \tag{9}$$

and

$$\langle\psi|\phi\rangle^{(\mathrm{S})} = \iint \psi^*(x)\Theta(x,x')\phi(x')\,dxdx' = \langle\psi|\Theta|\phi\rangle \qquad \text{in} \quad \mathcal{H}^{(\mathrm{S})}, \tag{10}$$

where $\Theta(x,x') \neq \delta(x-x')$. The consequences of the transition from equation (9) to equation (10) are nontrivial. For example, according to Mostafazadeh [27] the assumption of having a short-range and strictly local $V = V(x)$ leads immediately to the necessity of using a strongly nondiagonal metric kernel $\Theta(x,x')$ in equation (10).

The latter long-range nonlocality is easily visualized in Runge–Kutta picture where the coordinates are represented by a lattice of discrete points $x = x_j$, $j = \ldots,-1,0,1,\ldots$ and where all the differences $x_{j+1} - x_j = h$ are the same. In this approximation the typical doubly infinite matrix $\Theta_{i,j} = \Theta(x_i,x_j)$ is dominated by the unperturbed unit matrix $\Theta^{(0)}_{i,j} = \delta_{i,j}$. The non-negligible correction given, e.g., by equation (16) in [22] will be strongly non-diagonal. The metric can comfortably be expanded in the sum of elementary matrices, $\sum_k e^{-\beta hk}\Theta^{(k)}_{i,j}$ where each coefficient is sparse and strongly non-diagonal,

$$\Theta^{(1)} = \left[\begin{array}{cccc|cccc}
\ddots &&&&&&& \iddots \\
& 1 &&&&& 1 & \\
&& 1 &&& 1 && \\
&&& 1 & 1 &&& \\ \hline
&&& 1 & 1 &&& \\
&& 1 &&& 1 && \\
& 1 &&&&& 1 & \\
\iddots &&&&&&& \ddots
\end{array}\right], \quad
\Theta^{(2)} = \left[\begin{array}{cccc|cccc}
& \ddots &&&&& \iddots & \\
\ddots && 1 &&& 1 && \iddots \\
& 1 && 1 & 1 && 1 & \\
&& 1 &&& 1 && \\ \hline
&& 1 &&& 1 && \\
& 1 && 1 & 1 && 1 & \\
\iddots && 1 &&& 1 && \ddots \\
& \iddots &&&&& \ddots &
\end{array}\right], \quad \ldots. \tag{11}$$

These cross-shaped matrices couple remote coordinates x_i and x_j. A conflict emerges between our use of the common Hilbert space $\mathcal{H}^{(\mathrm{F})}$ (which keeps trace of the intuitive principle of correspondence) and of its amendment $\mathcal{H}^{(\mathrm{S})}$ (only there the correct probabilistic interpretation of the observables is achieved). The core of the problem lies in the manifest loss of the concept of the asymptotically free motion. In words of [25] one has to conclude that the causality-violating nature of metric is certainly "changing the physical picture drastically".

4.2 The second problem: Spatial symmetry violations

The first steps towards the desirable return to the standard picture of scattering induced by the Hamiltonian H which proves non-Hermitian in space $\mathcal{H}^{(\mathrm{F})}$ were proposed in our comment [23]. We tried to resolve there those of the paradoxes covered by paper [25] which were available prior to publication [28]. In particular we paid attention to the apparently unavoidable presence of causality-violating waves which seemed to emerge in the right spatial infinity. In the context of the specific non-Hermitian delta-function scattering models this violation of causality seems to result from the strict locality of $V = V(x)$. We concluded that such an assumption proves too strong and that it must be weakened for the given purpose.

In a detailed discussion of the causality-violation paradox we employed the same discretization. We assumed that in Hamiltonians $H = -d^2/dx^2 + V$ the potential of any form must be combined with the tridiagonal Runge–Kutta version of the kinetic-energy operator,

$$H = -\triangle + V, \qquad -\triangle = \left[\begin{array}{cccccc} \ddots & \ddots & & & & \\ \ddots & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & -1 & 2 & -1 & \\ & & & -1 & 2 & \ddots \\ & & & & \ddots & \ddots \end{array} \right]. \tag{12}$$

This helped us to simplify some technicalities and to clarify the way in which the asymptotically non-vanishing nondiagonality in $\Theta_{i,j}$ is generated by the diagonality of potentials $V = V(x_i)$. We then decided to consider only such families of Hamiltonians for which the unpleasant non-diagonality of the metric disappears,

$$\Theta(x_j, y_k) \approx c(x_j)\delta_{j,k}, \qquad |x_j| \gg 1, \qquad |y_k| \gg 1 \tag{13}$$

(cf. equation (23) in [23]). Then we only had to recollect that the (crypto) Hermiticity of H in $\mathcal{H}^{(S)}$ is a condition which acquires the utterly elementary form (4) in $\mathcal{H}^{(F)}$. As a linear-equation constraint imposed upon the matrix elements of metric Θ this equation can serve as an independent, nonperturbative source of information about the nonlocalities in metrics (11).

In [23] we decided to shorten the range of the influence of the non-Hermiticity. After the insertion of ansatz (13) in equation (4) a series of our algebraic trial and error experiments revealed that in order to achieve a certain internal consistency of our requirements we might replace the usual complex and diagonal non-Hermitian matrix $V(x_i)$ in $H = -\triangle + V(x)$ by its two-diagonal real and non-Hermitian analogue of the form

$$V^{(a,b,c,\ldots)} = \left[\begin{array}{cccc|cccc} & \ddots & & & & & & \\ \ddots & & -c & & & & & \\ & c & & -b & & & & \\ & & b & & -a & & & \\ \hline & & & a & & -b & & \\ & & & & b & & -c & \\ & & & & & c & & \ddots \\ & & & & & & \ddots & \end{array} \right]. \tag{14}$$

A multiparametric Schrödinger Hamiltonian $H = -\triangle + V^{(a,b,c,\ldots)}$ has been found which is Hermitian in the Hilbert space $\mathcal{H}^{(S)}$ where the exact metric operator has the following nontrivial but still fully diagonal form,

$$
\Theta^{(a,b,c,\dots)} = \left[\begin{array}{cccc|cccc}
\ddots & & & & & & & \\
 & \theta_{-5} & & & & & & \\
 & & \theta_{-3} & & & & & \\
 & & & \theta_{-1} & & & & \\
\hline
 & & & & \theta_1 & & & \\
 & & & & & \theta_3 & & \\
 & & & & & & \theta_5 & \\
 & & & & & & & \ddots
\end{array} \right]. \tag{15}
$$

Matrix elements are explicitly known,

$$
\begin{aligned}
\theta_{\pm 1} &= (1 \pm a)(1 - b^2)(1 - c^2)(1 - d^2) \cdots , \\
\theta_{\pm 3} &= (1 \pm a)(1 \pm b)^2(1 - c^2)(1 - d^2) \cdots , \\
\theta_{\pm 5} &= (1 \pm a)(1 \pm b)^2(1 \pm c)^2(1 - d^2) \cdots .
\end{aligned}
$$

We separated the "in" and "out" solutions not only in $\mathcal{H}^{(\mathrm{F})}$ but also in $\mathcal{H}^{(\mathrm{S})}$. A causality-observing physical picture of scattering was demonstrated to exist. Unfortunately, the amendment of the potentials proved incomplete. We did not manage to remove another shortcoming of equation (15) where, for a generic set of parameters $a, b, \dots$, the asymptotic measure $c(x_j) - 1$ of the anomaly of the flux in equation (13) remains long-ranged (cf. a footnote in [25]).

4.3 Problems resolved: $\mathcal{PT}$-symmetric models of scattering of [3]

Having accepted the above-cited words of critique we sought for a removal of the long-range anomalies. In letter [3] we made another step towards a fundamental theory of scattering based on the Hamiltonians which appear non-Hermitian in space $\mathcal{H}^{(\mathrm{F})}$. Another, amended family of Runge–Kutta Hamiltonians has been found there preserving the kinetic + potential-energy structure, $H = T + V$. We restricted our attention to the following two-diagonal matrix interaction proportional to real coupling parameter g and mimicking the existence of two interaction centers at a distance $\sim 2M$,

$$
V^{(g)} = \left[\begin{array}{cc|cc|cc|cc|cc}
 & \ddots & & & & & & & & \\
\ddots & & 0 & & & & & & & \\
\hline
 & 0 & & -g & & & & & & \\
 & & g & & 0 & & & & & \\
\hline
 & & & 0 & & \ddots & & & & \\
 & & & & \ddots & & 0 & & & \\
\hline
 & & & & & 0 & & g & & \\
 & & & & \multicolumn{2}{c|}{\underbrace{\qquad\qquad}} & -g & & 0 & \\
\hline
 & & & & \multicolumn{2}{c|}{2M-3} & & 0 & & \ddots \\
 & & & & \multicolumn{2}{c|}{\text{columns}} & & & \ddots &
\end{array} \right]. \tag{16}
$$

The key point was that we achieved an asymptotic spatial symmetry of the metric operator,

$$
c(x_j) = c(-x_j) = 1, \qquad |x_j| \gg 1. \tag{17}
$$

The overall picture offered by equation (17) looks satisfactory, in the discrete-coordinate approximation at least. The metric assigned to our Hamiltonian H remains diagonal, even though it is still different from the unit matrix. We can reasonably expect that for the majority of interactions the diagonality of this matrix may easily happen to lead just to a smooth change of the measure in equation (9) giving just the replacement $dx \to d\mu(x)$ in the limit $h \to 0$. In spite of having a nontrivial Hilbert space, the changes due to $\Theta \neq I$ may remain inessential and the limiting metric Θ may be called "local".

In contrast, whenever we relax the constraint of diagonality and admit a $(2R-1)$-diagonal metric Θ with $R \geq 2$, the decrease of the discretization length $h \to 0$ may lead, in general, to a matrix Θ which can be, say, a polynomial function of the kinetic energy operator $\triangle$ of equation (12). The $h \to 0$ limit of the discrete inner product would not lead to the mere double-integration formula (10) but rather to a very complicated (e.g., integro-differential) recipe.

In our present text we intend to omit the discussion of all the similar mathematical subtleties, emphasizing only that they might play an important role even in the present class of illustrative examples. This is also the reason why we call our band-matrix metrics quasilocal. In the limit $h \to 0$, their range will certainly shrink to zero but the same feature characterizes also the kinetic-energy operator $\triangle$.

5 Band-matrix metrics: their meaning and construction

The fact that we can only reconstruct the reality from our discretized scattering models via the limiting transition $h \to 0$ has an important constructive aspect. Let us recollect that the core of the consistence of the theory at $h = 0$ lies in a reconciliation of the non-Hermiticity of differential equation (1) in $\mathcal{H}^{(\mathrm{F})}$ with the asymptotic locality of boundary conditions (2). We saw that at $h > 0$ both these problems found their resolution in [3] where H was simply re-interpreted as Hermitian in $\mathcal{H}^{(\mathrm{S})}$ and where the diagonality of the metric at $h > 0$ offered an easy guarantee of its locality in the limit $h = 0$.

Now we have to add that the classification of possibilities as presented in [3] is incomplete because we required there the strict locality of the metric. On this background we may briefly characterize our present new results as a broadening of the picture of unitary scattering as offered in [3].

Our present key idea is that the standard form of the asymptotic boundary conditions for scattering (defined, naturally, in terms of plane waves) would not be lost even if we assume that our metric Θ becomes weakly non-diagonal. For example, certain constant tridiagonal matrices Θ constructed at a given lattice constant $h > 0$ may appear as proportional to the Laplace operator (i.e., to the kinetic-energy operator) in the continuous coordinate limit $h \to 0$.

This point of view can be generalized to all of the $(2R-1)$-diagonal matrices of the metric Θ where the integer R remains fixed during the decrease of $h \to 0$. The resulting limits Θ may often prove expressible in terms of the powers of the Laplace operator so that we may call all of these $h = 0$ metrics quasilocal.

As a consequence, a broad family of new metrics Θ could be obtained in the limit $h = 0$. They would still, by construction, leave the scattering unitary. The resulting picture of physics will vary with the choice of their structure at $h > 0$. In order to be able to understand this situation we would need to be able to construct the $(2R-1)$-diagonal matrices Θ in closed form at any $h > 0$.

This possibility has been ignored before. Let us now fill this gap via our solvable non-Hermitian example.

5.1 The choice of the model

Let us select the class of interaction models (16) of [3] and, for illustration purposes, let us pick up the special case where, formally, $2M-3=-1$,

$$H = \left[\begin{array}{cccccccc} \ddots & & & & & & & \\ \ddots & 2 & -1 & & & & & \\ & -1 & 2 & -1-g & & & & \\ & & -1+g & 2 & -1+g & & & \\ & & & -1-g & 2 & -1 & & \\ & & & & -1 & 2 & \ddots & \\ & & & & & \ddots & \ddots & \end{array}\right]. \quad (18)$$

This is a tridiagonal, doubly infinite Hamiltonian matrix which can be complemented by a discrete version of asymptotic boundary conditions (2) for scattering wave functions. The details including the explicit formulae for the reflection coefficient $R(E)$ and for the transmission coefficient $T(E)$ may be found in [3] showing that $|T(E)|^2 + |R(E)|^2 = 1$. This means that the standard probability flow is conserved (i.e., the process is unitary) even when the scattering is controlled by our non-Hermitian Hamiltonian (18).

The unitarity of the model is related to the existence of a metric which is asymptotically diagonal. At any nonvanishing $h > 0$ we may easily find the fully diagonal metric containing just a single anomalous matrix element,

$$\Theta = \Theta_1 = \left[\begin{array}{ccccc} \ddots & & & & \\ & 1 & & & \\ & & (1+g)/(1-g) & & \\ & & & 1 & \\ & & & & \ddots \end{array}\right]. \quad (19)$$

Having worked in discrete coordinate representation we may conclude that our matrix Θ_1 commutes with the usual diagonal operator of the coordinate. The anomalous matrix element $z_1 = (1+g)/(1-g) = 1+2g/(1-g)$ degenerates to 1 in the no-interaction limit (i.e., Hermitian limit) $g \to 0$. One should notice that the spectral singularity [29] emerges at $g = \pm 1$.

5.2 The existence of band-matrix metrics with $2R-1 \leq 9$ diagonals

Our choice of the elementary toy-model Hamiltonian (18) facilitates the constructive search for the alternatives to the diagonal metric (19). Indeed, whenever we perceive the class of admissible metrics $\Theta = \Theta(H)$ as composed of *all* the possible Hermitian, positive and invertible matrices which are compatible with the Hamiltonian-dependent quasi-Hermiticity constraint (4) we may (and shall) take this equation simply as a linear algebraic system of (infinitely many) equations which are to be satisfied by our pair of matrices H (which is given in advance) and Θ (which is to be specified as one of solutions of equation (4)).

There exist several technical obstacles which make such a project not entirely trivial. Firstly, we have to employ some "manual" linear algebra in order to reduce the infinite-dimensional equation (4) to its finite-dimensional subsystem. By the trial and error techniques we succeeded in revealing that such a reduction may even preserve many parallels with diagonal Θ_1. In this spirit we decided to search for certain doubly-infinite-matrix solutions Θ_R which exhibit a very specific band-matrix property $(\Theta_R)_{k,m} = 0$ whenever $|k - m| > R$. Empirically we revealed that each such sparse, $(2R-1)$-diagonal matrix solution Θ_R may, furthermore, be required to contain solely R nonvanishing diagonals. This possibility is supported by the tridiagonal matrix ansatz for Θ_R at $R = 2$ giving

$$\Theta_2 = \left[\begin{array}{ccccccc}
 & \ddots & & & & & \\
\ddots & \ddots & 1 & & & & \\
 & 1 & 0 & 1+g & & & \\
 & & 1+g & 0 & 1+g & & \\
 & & & 1+g & 0 & 1 & \\
 & & & & 1 & \ddots & \ddots \\
 & & & & & \ddots &
\end{array}\right].$$

A reconfirmation is found at $R = 3$, with

$$\Theta_3 = \left[\begin{array}{ccccccccc}
\ddots & \ddots & \ddots & & & & & & \\
\ddots & 1 & 0 & 1 & & & & & \\
\ddots & 0 & 1 & 0 & 1+g & & & & \\
 & 1 & 0 & 1-g^2 & 0 & 1-g^2 & & & \\
 & & 1+g & 0 & \dfrac{(1+g)\left(1-2\,g^2\right)}{1-g} & 0 & 1+g & & \\
 & & & 1-g^2 & 0 & 1-g^2 & 0 & 1 & \\
 & & & & 1+g & 0 & 1 & 0 & \ddots \\
 & & & & & 1 & 0 & 1 & \ddots \\
 & & & & & & \ddots & \ddots & \ddots
\end{array}\right],$$

and at $R = 4$, with

$$\Theta_4 = \left[\begin{array}{ccccccccccc}
 & \ddots & & \ddots & & & & & & & \\
\ddots & \ddots & 1 & \ddots & 1 & & & & & & \\
 & 1 & 0 & 1 & 0 & a & & & & & \\
\ddots & \ddots & 1 & \ddots & b & \ddots & b & & & & \\
 & 1 & 0 & b & & c & & b & & & \\
 & & a & \ddots & c & & c & \ddots & a & & \\
 & & & b & & c & & b & 0 & 1 & \\
 & & & & b & \ddots & b & \ddots & 1 & \ddots & \ddots \\
 & & & & & a & 0 & 1 & 0 & 1 & \\
 & & & & & & 1 & \ddots & 1 & \ddots & \ddots \\
 & & & & & & & \ddots & & \ddots &
\end{array}\right],$$

where we abbreviated $a = 1 + g$, $b = 1 - g^2$ and $c = (1 + g)(1 - 2g^2)$. Finally, we also solved equation (4) with the similar $R = 5$ ansatz

$$
\Theta_5 = \left[\begin{array}{ccccccccccccc}
\ddots & & \ddots & & \ddots & & & & & & & & \\
& 1 & & 1 & & 1 & & & & & & & \\
\ddots & & 1 & & 1 & & a & & & & & & \\
& 1 & & 1 & & b & & b & & & & & \\
\ddots & & 1 & & b & & c & & b & & & & \\
& 1 & & b & & d & & d & & b & & & \\
& & a & & c & & z_5 & & c & & a & & \\
& & & b & & d & & d & & b & & 1 & \\
& & & & b & & c & & b & & 1 & & \ddots \\
& & & & & b & & b & & 1 & & 1 & \\
& & & & & & a & & 1 & & 1 & & \ddots \\
& & & & & & & 1 & & 1 & & 1 & \\
& & & & & & & & \ddots & & \ddots & & \ddots
\end{array} \right]
$$

and we obtained, again, $a = 1 + g$, $b = 1 - g^2$, $c = (1 + g)(1 - 2\,g^2)$, $d = (1 - g^2)(1 - 2g^2)$ and

$$
z_5 = \frac{(1 + g)\left(1 - 2\,g^2\right)^2}{1 - g}.
$$

5.3 The extrapolation and construction of all the metrics $\boldsymbol{\Theta_R}$

As a result of our computer-assisted exact and systematic reconstruction of the metrics $\Theta = \Theta_k$ compatible with Hamiltonian H via quasi-Hermiticity condition (4) we arrive at the following extrapolation of our $k \le 5$ rigorous symbolic-manipulation results to any integer $k > 5$.

- By construction, each metric Θ_k possesses the form of a doubly infinite and symmetric $(2k - 1)$-diagonal real matrix with k nonvanishing diagonals interlaced by $k - 1$ zero diagonals.
- Up to their central k-plets, all the matrix elements of Θ_k along each non-vanishing diagonal are equal to one.
- If we assume $k \ge 2$ and abbreviate $a = 1 + g$ and $b = 1 - g^2$ the leftmost non-trivial k-plet $(a, b, b, \ldots, b, b, a)$ of non-unit matrix elements of our metric Θ_k contains two boundary a's complemented by the $(k - 2)$-plet of b's.
- After we abbreviate $c = (1+g)\,(1-2\,g^2)$ and $d = (1-g^2)(1-2g^2)$ and assume that $k \ge 4$, we obtain the subsequent k-plet in the explicit form $(b, c, d, d, \ldots, d, d, c, b)$ filled by $k - 4$ d's.
- With $e = (1 + g)(1 - 2g^2)^2$ and $f = (1 - g^2)(1 - 2g^2)^2$ and $k \ge 6$ we get the next k-plet $(b, d, e, f, f, \ldots, f, f, e, d, b)$ containing $k - 6$ f's. Etc.

The general pattern is obvious: the quadruplets of matrix elements sitting in the four (viz., "North", "East", "South" and "West") corners may be ordered in an inwards-running sequence of vertices $a = A_1$, $c = A_2$, $e = A_3$, $\ldots$ (cf. Table 1). These values are complemented by the related multiplets of the wedge-filling elements $b = B_1$, $d = B_2$, $f = B_3$, $\ldots$. At the odd subscripts there emerges an anomalous, non-polynomial central matrix element z_k equal to fractions $a/(1 - g)$, $c/(1 - g)$, $e/(1 - g)$, $\ldots$ at $k = 1, 3, 5, \ldots$, respectively.

Table 1. Matrix elements of the metrics Θ_R.

R	central element	corner element	wedge element
1	$z_1 = A_1/(1-g)$	—	—
3	$z_3 = A_2/(1-g)$	$a = A_1 = (1+g)$	$b = B_1 = (1-g^2)$
5	$z_5 = A_3/(1-g)$	$c = A_2 = (1+g)(1-2g^2)$	$d = B_2 = (1-g^2)(1-2g^2)$
7	$z_7 = A_4/(1-g)$	$e = A_3 = (1+g)(1-2g^2)^2$	$f = B_3 = (1-g^2)(1-2g^2)^2$
9	$z_9 = A_5/(1-g)$	$A_4 = (1+g)(1-2g^2)^3$	$B_4 = (1-g^2)(1-2g^2)^3$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$2k+1$	$z_{2k+1} = A_{k+1}/(1-g)$	$A_k = (1+g)(1-2g^2)^{k-1}$	$B_k = (1-g^2)(1-2g^2)^{k-1}$

The existence of the above extrapolation rules enables us to formulate a simplified ansatz for the next matrix Θ_R at $R = 6$,

$$\Theta_6 = \left[\begin{array}{ccccccccccccccc}
 & \ddots & & \ddots & & \ddots & & & & & & & & & \\
\ddots & & 1 & & 1 & & 1 & & & & & & & & \\
 & 1 & & 1 & & 1 & & a & & & & & & & \\
\ddots & & 1 & & 1 & & b & & b & & & & & & \\
 & 1 & & 1 & & b & & c & & b & & & & & \\
\ddots & & 1 & & b & & d & & d & & b & & & & \\
 & 1 & & b & & d & & e & & d & & b & & & \\
 & & a & & c & & e & & e & & c & & a & & \\
 & & & b & & d & & e & & d & & b & & 1 & \\
 & & & & b & & d & & d & & b & & 1 & & \ddots \\
 & & & & & b & & c & & b & & 1 & & 1 & \\
 & & & & & & b & & b & & 1 & & 1 & & \ddots \\
 & & & & & & & a & & 1 & & 1 & & 1 & \\
 & & & & & & & & 1 & & 1 & & 1 & & \ddots \\
 & & & & & & & & & \ddots & & \ddots & & \ddots &
\end{array} \right] .$$

It passes the test after insertion in equation (4). The tedious computer-assisted direct solution becomes replaced by an elementary verification of the choice of $e = (1+g)\left(1-2g^2\right)^2$.

In a climax of our analysis let us now complement our algorithmic set of extrapolation rules by their rigorous proof. For this purpose we may select an odd integer $R = 2k+1$ and reinterpret Table 1 as a recurrent pattern (i.e., the proof proceeds by mathematical induction). The corner element A_k is most easily deduced from the previous line since $A_k = (1-g)z_{2k-1}$ and only the values of B_k and z_{2k+1} must be deduced from the quasi-Hermiticity condition (4) rewritten as a doubly infinite matrix set of linear equations using the input Hamiltonian (18),

$$\left[H^\dagger \Theta_{2k+1} - \Theta_{2k+1} H\right]_{mn} = 0, \qquad m, n = 0, \pm 1, \ldots . \tag{20}$$

This task is facilitated by the tridiagonality of H and it may be also guided by our last illustrative sparse-matrix ansatz for Θ_R at the next odd $R = 7$,

$$\Theta_7 = \left[\begin{array}{ccccccccccccccccc}
 & & & & \ddots & & \ddots & & & & & & & & & & \\
 & & & \ddots & & 1 & & 1 & & & & & & & & & \\
 & & \ddots & & 1 & & 1 & & a & & & & & & & & \\
 & \ddots & & 1 & & 1 & & b & & b & & & & & & & \\
\ddots & & 1 & & 1 & & b & & c & & b & & & & & & \\
 & 1 & & 1 & & b & & d & & d & & b & & & & & \\
\ddots & & 1 & & b & & d & & e & & d & & b & & & & \\
 & 1 & & b & & d & & f & & f & & d & & b & & & \\
 & & a & & c & & e & & z_7 & & e & & c & & a & & \\
 & & & b & & d & & f & & f & & d & & b & & 1 & \\
 & & & & b & & d & & e & & d & & b & & 1 & & \ddots \\
 & & & & & b & & d & & d & & b & & 1 & & 1 & \\
 & & & & & & b & & c & & b & & 1 & & 1 & & \ddots \\
 & & & & & & & b & & b & & 1 & & 1 & & \ddots & \\
 & & & & & & & & a & & 1 & & 1 & & \ddots & & \\
 & & & & & & & & & 1 & & 1 & & \ddots & & & \\
 & & & & & & & & & & \ddots & & \ddots & & & &
\end{array} \right].$$

Having the latter structure and illustration in mind we can contemplate any $R = 2k + 1$ and verify, by direct calculation, that the rightmost unknown in the last line of Table 1 (i.e., the value of the wedge element B_k) emerges from equation (20) as defined, recurrently, at any one of the eight pairs of the subscripts $(m, n) = (-2, \pm 1)$, $(m, n) = (-1, \pm 2)$, $(m, n) = (1, \pm 2)$ or $(m, n) = (2, \pm 1)$. Similarly, the leftmost and last unknown of Table 1 (i.e., the value of the central matrix element z_{2k+1}) becomes determined, in terms of the freshly pre-determined B_k, by the $(m, n) = (-1, 0)$ item of equation (20). Due to the symmetry of our ansatz for Θ we could have also used $(m, n) = (0, \pm 1)$ or $(m, n) = (0, -1)$, with the same result of course.

6 Nonequivalent isospectral Hermitian Hamiltonians $\mathfrak{h}$

In principle, there exist many non-equivalent factorizations of a given quasilocal metric with $(2R-1) \geq 3$ diagonals. In our illustrative example we may consider, in general, the superposition

$$\Theta = \Theta(\alpha_1, \alpha_2, \ldots, \alpha_R) = \alpha_1 \Theta_1 + \alpha_2 \Theta_2 + \cdots + \alpha_R \Theta_R \tag{21}$$

and factorize $\Theta = \Omega^\dagger \Omega$.

6.1 $R = 1$ and the diagonal Dyson mappings Ω

By far the most popular reconstruction of the Dyson operator Ω from a given metric $\Theta = \Omega^\dagger \Omega$ is based on an *ad hoc* assumption of Hermiticity $\Omega = \Omega^\dagger = \sqrt{\Theta}$ (cf., e.g., [22]). For our present class of band-matrix models Θ_R such an assumption does not lead to any problems when the metric is diagonal, $R = 1$. For illustration let us select Θ_1 of equation (19). Postulating the diagonality and positivity of the related Dyson map Ω_1 in its factorization $\Theta_1 = \Omega_1^\dagger \Omega_1$ we arrive at the following unique result,

$$\Omega_1 = \left[\begin{array}{cccc}
\ddots & & & \\
 & 1 & & \\
 & & \sqrt{(1+g)/(1-g)} & \\
 & & & 1 \\
 & & & & \ddots
\end{array} \right]$$

knowledge of which enables us to evaluate the related matrix of the Hamiltonian in the physical Hilbert space $\mathcal{H}^{(\rm P)}$,

$$
\mathfrak{h} = \left [\begin{array}{cccccc}
\ddots & & & & & \\
\ddots & 2 & -1 & & & \\
 & -1 & 2 & -\sqrt{1-g^2} & & \\
 & & -\sqrt{1-g^2} & 2 & -\sqrt{1-g^2} & \\
 & & & -\sqrt{1-g^2} & 2 & -1 \\
 & & & & -1 & 2 & \ddots \\
 & & & & & \ddots & \ddots
\end{array}\right]\,. \qquad (22)
$$

The off-diagonal elements $-\sqrt{1-g^2} = -1 + (1 - \sqrt{1-g^2}) = -1 + g^2/(1 + \sqrt{1-g^2})$ are composed of the kinetic-energy term (-1) and a positive function of the coupling.

6.2 $R = 2$ and a tridiagonal Dyson mapping Ω

We should issue a warning that the usual assumption of Hermiticity of factors $\Omega = \Omega^\dagger$ would be rather counterproductive because the Hermitian square root of our sparse matrices Θ would be a non-sparse matrix. The quasilocality property (i.e., a convergence to locality during the limiting transition $h \to 0$) would be lost for the Dyson map. In opposite direction, when we preserve the quasilocality (i.e., the band-matrix structure) of Dyson matrices, we achieve, at any nonzero $h > 0$, a significant simplification of the physical representation of our operators of observables in $\mathcal{H}^{(\rm P)}$.

Without any significant loss of generality the merits of such a strategy may be illustrated via the most general tridiagonal metric $\Theta(\gamma) = 2\Theta_1 + \gamma\,\Theta_2$. First of all we have to guarantee its positivity and invertibility but both these properties are easily shown to be guaranteed inside the open interval of $\gamma \in (-1, 1)$.

Secondly, we have to demonstrate the *practical* feasibility of the rather difficult extraction of a quasilocal factor Ω from a given quasilocal $\Theta = \Omega^\dagger\Omega$. For this purpose, let us slightly simplify the presentation of the argument and choose $\gamma \to -1$ lying on the boundary of the open domain of existence of the metric operator (21). In this limiting case our doubly infinite metric acquires a rather elementary matrix form,

$$
\Theta = \left [\begin{array}{cccccccc}
\ddots & \ddots & & & & & & \\
\ddots & 2 & -1 & & & & & \\
 & -1 & 2 & -1 & & & & \\
 & & -1 & 2 & -1-g & & & \\
 & & & -1-g & 2\,\frac{1+g}{1-g} & -1-g & & \\
 & & & & -1-g & 2 & -1 & \\
 & & & & & -1 & 2 & -1 \\
 & & & & & & -1 & 2 & \ddots \\
 & & & & & & & \ddots & \ddots
\end{array}\right]\,.
$$

This matrix is most easily factorized into band-matrix Dyson-mapping factors, $\Theta = \Omega^\dagger\Omega$ when we postulate the following special form of the Dyson-mapping matrix which is asymmetric and tridiagonal,

$$\Omega=\left[\begin{array}{cccc|c|cccc}
\ddots & \ddots & & & & & & & \\
 & 1 & -1 & & & & & & \\
 & & 1 & -1 & & & & & \\
 & & & 1 & -1-g & & & & \\
\hline
 & & & & \sqrt{\frac{2g^2(1+g)}{1-g}} & & & & \\
\hline
 & & & & -1-g & 1 & & & \\
 & & & & & -1 & 1 & & \\
 & & & & & & -1 & 1 & \\
 & & & & & & & \ddots & \ddots
\end{array}\right]. \tag{23}$$

During the transition to a measurable coordinate y_m appearing as the argument in the physical wave function $\psi^{(\mathrm{P})}(y_m) \in \mathcal{H}^{(\mathrm{P})}$, the similar quasilocal Dyson mappings enter the scene via finite sums

$$\psi^{(\mathrm{P})}(y_m) := \sum_n \Omega(y_m, x_n)\psi^{(\mathrm{F})}(x_n). \tag{24}$$

In an effective theory as advocated in [25], both the arguments x_m and y_m may be considered, in some sense, observable. Then, equation (24) introduces just a certain "smearing" of coordinates, at the non-vanishing lattice sizes $h > 0$ at least. The extent of this smearing is proportional to the number of diagonals in Ω.

We have to remember that we choose the parameter $\gamma = 1$ which lies, strictly speaking, *out of* the open interval of its admissible values. Due care is needed when working with this option. Nevertheless, a part of its undeniable methodical appeal still recurs with the easiness of the evaluation of the inverse

$$\Omega^{-1}=\left[\begin{array}{cccc|c|cccc}
\ddots & \ddots & \ddots & \vdots & \vdots & & & & \\
 & 1 & 1 & 1 & \sqrt{\frac{1-g^2}{2g^2}} & & & & \\
 & & 1 & 1 & -\sqrt{\frac{1-g^2}{2g^2}} & & & & \\
 & & & 1 & \sqrt{\frac{1-g^2}{2g^2}} & & & & \\
\hline
 & & & & \sqrt{\frac{1-g}{2g^2(1+g)}} & & & & \\
\hline
 & & & & \sqrt{\frac{1-g^2}{2g^2}} & 1 & & & \\
 & & & & -\sqrt{\frac{1-g^2}{2g^2}} & 1 & 1 & & \\
 & & & & \sqrt{\frac{1-g^2}{2g^2}} & 1 & 1 & 1 & \\
 & & & & \vdots & \vdots & \ddots & \ddots & \ddots
\end{array}\right].$$

The extreme $\gamma = 1$ example also offers a very useful guide for transition to the generic $|\gamma| < 1$ where an ansatz for $\Omega(\gamma)$ may be made with the same sparse-matrix structure. This would lead to an efficient factorization recipe based on the use of continued fractions in the definition of inverse matrix (at $R = 2$, cf. its sample in [30]). A generalization of this algorithm to $R > 2$ using the so called extended continued fractions also exists (cf. [31]).

Let us now return to our $R = 2$ schematic example with the initial Hamiltonian H of equation (18) and with the tridiagonal metric $\Theta(\gamma)$ where $\gamma = 1$. Easily we may show, by direct computation, that the related isospectral Hermitian Hamiltonian $\mathfrak{h}$ reads

$$\mathfrak{h}=\left[\begin{array}{ccc|ccc|ccc}
\ddots & \ddots & & & & & & & \\
\ddots & 2 & -1 & & & & & & \\
 & -1 & 2 & -1 & & & & & \\
\hline
 & & -1 & 2-g^2 & -\sqrt{2g^2(1-g^2)} & 1-g^2 & & & \\
 & & & -\sqrt{2g^2(1-g^2)} & 2\,g^2 & -\sqrt{2g^2(1-g^2)} & & & \\
 & & & 1-g^2 & -\sqrt{2g^2(1-g^2)} & 2-g^2 & -1 & & \\
\hline
 & & & & & -1 & 2 & -1 & \\
 & & & & & & -1 & 2 & \ddots \\
 & & & & & & & \ddots & \ddots
\end{array}\right].$$

We see that it remains sparse but different from its diagonal-metric predecessor (22).

7 Discussion

Beyond the horizons given by our present sample of $\mathcal{PT}$-symmetric H we may expect that many other models would also profit from the $h > 0$ approximation treating the coordinate x as a discretized quantity $x_k = hk$. This approach enabled us to construct the $(2R-1)$-diagonal metrics at all R and it also allowed us to postpone the study of the continuous coordinate limit $h \to 0$ to the very end of all the calculations. Let us note now that this limiting transition need not necessarily be easy. Sometimes, it may be necessary to replace the simple-minded function $\Theta(x, x')$ of two real variables in formula (10) by a suitable (e.g., momentum-dependent) operator generalization.

At a fixed level of approximation $h > 0$ one can usually skip the difficult discussions of the continuous coordinate limit. Even then, due care must be paid to the (approximate) discrete theory where the values x_n of the individual coordinates play the role of arguments in wave functions $\psi^{(\mathrm{F})}(x_n) \in \mathcal{H}^{(\mathrm{F})}$ *without* probabilistic interpretation. The same discretized coordinates also enter the correspondence-principle-reflecting definitions of the potential and of the kinetic-energy operator $\triangle$ of equation (12). All of these operators certainly carry the decisive information about the dynamics of the quantum system, provided only that the wave functions $\psi^{(\mathrm{F})}(x_n)$ are mapped, into the physical space $\mathcal{H}^{(\mathrm{P})}$, according to the following diagram,

$$\begin{array}{ccc}
 & \boxed{\begin{array}{c}\psi \text{ transferred in } \mathcal{H}^{(\mathrm{P})}:\\ \textbf{physics} \;=\; \text{transparent}\\ \text{calculations} \;=\; \text{prohibitively difficult}\end{array}} & \\
\textbf{simplification} \ \swarrow & & \searrow\nwarrow \ \textbf{unitary equivalence} \\
\boxed{\begin{array}{c}\psi \text{ calculated in } \mathcal{H}^{(\mathrm{F})}:\\ \text{calculations} \;=\; \textbf{feasible}\\ \text{physical meaning} \;=\; \text{lost}\end{array}} & \xrightarrow{\textbf{hermitization}} & \boxed{\begin{array}{c}\psi \text{ reinterpreted in } \mathcal{H}^{(\mathrm{S})}:\\ \text{metric } \Theta \neq I \;=\; \textbf{strange}\\ \text{inner product} \;=\; \text{unusual}\end{array}}
\end{array}$$

Physical predictions necessitate a transfer of wave functions from the computation-facilitating Hilbert space $\mathcal{H}^{(\mathrm{F})}$ to the correct physical Hilbert space $\mathcal{H}^{(\mathrm{P})}$. The *ambiguity* of this transfer is well illustrated by equation (7) containing the set of free parameters λ_j and κ_j which reflects their presence also in the related Dyson map $\Omega = \Omega(\lambda_j, \kappa_j)$.

The main consequence of such a departure from the dictum of textbooks is that for a quantized point particle our construction and knowledge of wave functions must be complemented by a suitable upgrade of Hilbert space, i.e., usually, of the unphysical $\mathbb{L}^2(\mathbb{R}) := \mathcal{H}^{(\mathrm{F})}$. In our present models it has to be accompanied by the limiting transition $h \to 0$. In this way the unphysical version of the discrete normalization condition

$$\sum_{k=0}^{\infty} \psi^*(x_k)\psi(x_k) = 1 \qquad \text{in} \quad \mathcal{H}^{(\mathrm{F})}, \tag{25}$$

will be replaced by its continuous limit (cf. equation (9)) while, similarly, its physical, "standardized" counterpart

$$\sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \psi^*(x_j)\Theta(x_j, x_k)\psi(x_k) = 1 \qquad \text{in} \quad \mathcal{H}^{(\mathrm{S})} \tag{26}$$

will be assumed convergent to a double integral formula with $h \to 0$ (cf. equation (10)).

In this setting the main message of our present paper can be read as a proposal of transition from the diagonal Runge–Kutta metrics (say, of [3, 23]) to their non-diagonal, $(2R-1)$-diagonal sparse-matrix generalizations with $R \geq 2$. Under this generalization the latter assumption of convergence $\Theta(x_j, x_k') \to \Theta(x, x')$ need not always be satisfied since, in general, we have to expect the emergence of a more complicated structure in the quasilocal metric $\Theta = \lim_{h\to 0} \Theta(x_j, x_k')$. Typically, in a way inspired by the inspection of equation (7) we might expect the emergence of a complicated dependence of our quasilocal metrics on momenta, etc.

The study of the criteria distinguishing the metrics with a smooth x-dependence (i.e., with operators represented by the mere functions of two variables $\Theta(x, x')$) from the other operators of metrics without such an elementary representation lies far beyond the scope of our present paper. Only a few comments may be added.

In the first one we repeat that the physical probabilistic interpretation of the system requires the introduction of the "standard" Hilbert space $\mathcal{H}^{(\mathrm{S})} \neq \mathbb{L}^2(\mathbb{R})$ where the time-evolution becomes unitary. Although this space may be defined as spanned by the same functions of x, their norm must be defined differently. This postulate degenerates back to the standard textbook scenario when one returns to the Dirac's local metric, $\Theta(x, x') \to \delta(x - x')$. *Vice versa*, for non-Hermitian $H \neq H^\dagger$ with real spectra one may, sometimes, succeed in constructing the corresponding *ad hoc* metric kernel $\Theta(x, x') \neq \delta(x - x')$.

Our second comment will emphasize that our work with difference-equation approximants has been motivated by the tedious nature of some alternative perturbation-expansion techniques to Schrödinger equations, say, of [22, 25]. In the conclusion let us mention a particularly interesting possibility of a change of perspective. It emerged with the publication of paper [32] where the first-quantized Klein–Gordon equation has been considered. In this case, the three-Hilbert space formulation of quantum mechanics offers certain interesting new possibilities of the interpretation of the role of individual spaces. The point is that the initial Hamiltonian $H \neq H^\dagger$ acquired the physical meaning (i.e., relativistic covariance) in $\mathcal{H}^{(\mathrm{F})}$ rather than in $\mathcal{H}^{(\mathrm{P})}$. In our present language this would lead to the modified theoretical arrangement of our three Hilbert spaces,

$$\begin{array}{ccc}
 & & \boxed{\begin{array}{c}\text{in the third space } \mathcal{H}^{(\mathrm{P})}: \\ \text{textbook } \textbf{physics},\ \mathfrak{h} = \mathfrak{h}^\dagger \\ (\text{ambiguity of } \mathfrak{h} = \Omega H \Omega^{-1})\end{array}} \\
 & & \nwarrow \ \textbf{equivalence} \\
\boxed{\begin{array}{c}\text{in the } \textbf{first} \text{ space } \mathcal{H}^{(\mathrm{F})}: \\ \text{kinematics} \implies H \neq H^\dagger \\ (\text{relativistic covariance})\end{array}} & \overset{\textbf{quasi-hermitization}}{\longrightarrow} & \boxed{\begin{array}{c}\text{in the } \textbf{second} \text{ space } \mathcal{H}^{(\mathrm{S})}: \\ H = H^\ddagger = \Theta^{-1} H^\dagger \Theta \\ (\text{ambiguous } \ \Theta = \Omega^\dagger \Omega\,)\end{array}}
\end{array}$$

New ways towards old problems could be sought/found in this direction. For example, in the light of some recently obtained new results on the first quantization of relativistic particles with spin [33], an extension of these studies to a scattering arrangement (e.g., along the lines indicated in our present paper) would be a particularly challenging task.

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