The problem of coexistence of several non-Hermitian observables in $\mathcal{PT}$–symmetric quantum mechanics

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Abstract

During the recent developments of quantum theory it has been clarified that the observable quantities (like energy or position) may be represented by operators $\Lambda$ (with real spectra) which are manifestly non-Hermitian in a preselected “friendly” Hilbert space $\mathcal{H}^{(F)}$. The consistency of these models is known to require an upgrade of the inner product, i.e., mathematically speaking, a transition $\mathcal{H}^{(F)} \rightarrow \mathcal{H}^{(S)}$ to another, “standard” Hilbert space. We prove that whenever we are given more than one candidate for an observable (i.e., say, two operators $\Lambda_0$ and $\Lambda_1$) in advance, such an upgrade need not exist in general.
1 Introduction

The traditional presentation of quantum mechanics (called, by Messiah [1], “Schrödinger picture”) has recently been complemented by the formulation which will be called, for our present purposes, “$\mathcal{PT}$—symmetric quantum mechanics” (PTSQM). The distinctive feature of this innovative formulation of the theory (which has been made popular by Bender with coauthors [2] and in which $\mathcal{P}$ stands for parity and $\mathcal{T}$ for time-reversal) lies in its use of certain manifestly non-Hermitian operators of observables with real spectra (cf. also the detailed summaries of the idea in [3] or in several slightly more mathematics-oriented concise reports collected in the newest book [4] on the subject).

One of the most interesting questions connected with the applicability of the PTSQM formalism was already discussed in the earlier review by Scholtz, Geyer and Hahne [5]. This question concerns the acceptability and mutual compatibility of the two or more preselected independent non-Hermitian operators of observables with real spectra. In this perspective our present contribution to the further development of the formalism found its immediate predecessor in paper [6]. One of us proposed there a prototype quantum toy model in which the mathematical compatibility between the two non-Hermitian but $\mathcal{PT}$ symmetric observables (viz., between a non-Hermitian Hamiltonian and a non-Hermitian spin projection) has been guaranteed by their mutual commutativity.

Over-restrictive as the commutativity constraint certainly is, it found its inspiration in a few other commutativity-requiring constructions where the pairs of non-Hermitian observables were specified as the Hamiltonian plus the so called quasi-parity [7] or as the Hamiltonian plus the so called charge [8, 9]. Naturally, the situation in which one would have to deal with some two (or more) entirely independent non-Hermitian candidates for observables (say, $\Lambda_1$ and $\Lambda_2$, with real spectra) would be much more interesting.

In our present paper we intend to return to the problem and to reanalyze the operator-pair compatibility problem in the form in which the commutativity constraint $[\Lambda_1, \Lambda_2] = 0$ is replaced by a more sophisticated ad hoc condition (cf., e.g., the samples of such non-commuting pairs of observables in the series of Refs. [10, 11, 12, 13]).

We believe that up to now, a more systematic, model-independent study of the non-Hermitian compatibility problem was not published. This gap is to be filled in what follows. In particular, we shall demonstrate that there exists a subtle correspondence between the choice of the so called irreducible sets of the candidates $\Lambda_j$ for the observables and the role played by these sets in the removal of the well known ambiguity of the assignment of the Schrödinger-picture Hilbert space $\mathcal{H}^{(S)}$ to a single observable $\Lambda_0$ (cf., e.g., Ref. [14] for a rather formal but fairly exhaustive technical discussion of the latter topic).

The presentation of our results will be preceded by a concise outline of the PTSQM formalism in section 2. The formulation of the non-Hermitian compatibility problem will follow in section 3. For illustration we mention there the triviality of the case in which the
two preselected observables $H$ (or, more generally, any non-Hermitian operator $A$ alias $\Lambda_0$ with real spectrum) and $X$ (alias $B$ or $\Lambda_1$) commute (subsection 3.1). Subsequently, in subsection 3.2 we deliver the proof of the incompatibility of the entirely generic $\Lambda_0$ with the entirely generic $\Lambda_1$ (which does not commute with the former one of course), assuming only, for simplicity, that the Hilbert spaces in question are finite-dimensional.

Basically, the latter result means that the well known assignment of a proper probabilistic interpretation to a single preselected non-self-adjoint $N$ by $N$ matrix of an observable $A \neq A^\dagger$ need not necessarily admit the acceptability of another, independent $N$ by $N$ matrix of another candidate $B \neq B^\dagger$ for an observable in the same quantum system. We will be able to conclude that in a generic situation, the arbitrarily selected doublet of non-Hermitian operators $A$ and $B$ with real spectra cannot be immediately treated as representing a pair of the observable quantities. For a coexistence, the operators must be nontrivially interconnected.

The discussion of the practical applicability aspects of our present contribution is initiated in section 4. We recall there the weakly $q$–deformed version of one of the above-mentioned models (subsection 4.1). Next we show how the required compatibility conditions become simplified in the first-order perturbation approximation (subsection 4.2). Subsequently (i.e., in section 5) a few technical difficulties associated with the construction of the metric itself are discussed for the single generic input observable $\Lambda_0$ (subsection 5.1) and in the situation in which one adds another operator, $\Lambda_1$ (subsection 5.2). Section 6 is finally devoted to a few mathematical subtleties, i.e., more explicitly, to the role of the boundedness of the operators of observables (cf. subsection 6.1), to the merits of the combination of the perturbation and truncation strategies (listed in subsection 6.2) and to the explicit and exhaustive illustrative description of the compatibility criteria at $N = 2$ in subsection 6.3. The summary of our message is finally provided by section 7.

2 A concise outline of the theory

2.1 The Dyson’s quantum mechanics in nuce

The PTSQM formalism should be perceived as fully compatible with the traditional textbooks on quantum mechanics [1]. A more detailed explanation of this point of view may be found summarized in papers [15] or reviews [3, 5, 16]. In a way inspired also by Refs. [17, 18] we will characterize the PTSQM as a representation of quantum systems in which the use of the “standard” Hilbert space of states $\mathcal{H}^{(S)}$ (in which the observables are represented by the self-adjoint operators, $\Lambda = \Lambda^\dagger$) can be paralleled by the use of another, unphysical but mathematically friendlier Hilbert space $\mathcal{H}^{(F)}$. In the latter space the same observables appear non-Hermitian of course, $\Lambda \neq \Lambda^\dagger$, due to the underlying auxiliary intentional
simplification of the inner product.

Table 1: Non-Hermitian version of Schrödinger picture (cf. [16]).

|                  | \( \mathcal{H}^{(F)} \) | \( \mathcal{H}^{(S)} \) | \( \mathcal{H}^{(T)} \) |
|------------------|---------------------------|--------------------------|--------------------------|
|                  | = the first one,          | = the second one,        | = the third one,          |
| false space,     |                           | standard space           | of textbooks,            |
| unphysical       |                           |                          | inaccessible             |

| the purpose of their simultaneous use: |
|--------------------------------------|
| the friendlier                        | the correct space          | the friendlier            |
| mathematical representation           | \( \mathcal{H}^{(S)} \)   | probabilistic interpretation |

formally, the generic observable is, respectively,

non-Hermitian non-Hermitian self-adjoint self-adjoint self-adjoint
\( (\Lambda \neq \Lambda^\dagger) \) \( (\Lambda = \Lambda^\dagger) \) (transformed)

The structure of the resulting “three-Hilbert-space” (THS) Schrödinger-picture pattern is summarized in Table 1. The introduction of such a representation of a quantum system dates back to Dyson [17] who conjectured that one need not distinguish between the predictions made within the standard physical Hilbert space \( \mathcal{H}^{(S)} \) and within any other, unitarily equivalent alternative Hilbert space \( \mathcal{H}^{(T)} \) “of textbooks”.

In the context of applications the Dyson’s recipe was successful in nuclear physics where one always knows the self-adjoint Hamiltonian in \( \mathcal{H}^{(T)} \). Once this operator is found overcomplicated, one is well motivated to change the Hilbert space as well as to simplify the Hamiltonian. This may be achieved via certain \textit{ad hoc}, intuition-based and invertible \( \mathcal{H}^{(F)} \rightarrow \mathcal{H}^{(T)} \) mapping, to be called the Dyson’s map and to be denoted by the dedicated symbol \( \Omega \) in what follows.

2.2 The \( \mathcal{P}\mathcal{T} \)–symmetric quantum mechanics \textit{in nuce}

In the PTSQM setting the old Dyson’s recipe was inverted (cf., e.g., review paper [2] for numerous illustrations). In the first step one just picks up an auxiliary Hilbert space \( \mathcal{H}^{(F)} \) together with a sufficiently elementary (quite often, just ordinary-differential-operator) non-Hermitian but \( \mathcal{P}\mathcal{T} \)–symmetric candidate \( H \) for the Hamiltonian.

The preselected Hilbert space \( \mathcal{H}^{(F)} \) is then declared “false”. For the correct physical interpretation purposes it is to be replaced by another, “second” Hilbert space \( \mathcal{H}^{(S)} \). In the latter, non-equivalent, \( S \)–superscripted Hilbert space the initial non-Hermitian operators

\[ 4 \]
$H$ of Hamiltonians must be self-adjoint. Thus, one might write

$$H = H^\dagger. \tag{1}$$

The acceptance of such a convention could be misleading. Fortunately, its immediate use is also not necessary because via a mere redefinition of the inner product we may always postpone the study of Eq. (1) and stay working inside $\mathcal{H}^{(F)}$.

The Hermiticity property (1) does not get lost in $\mathcal{H}^{(F)}$. It remains mediated by the replacement of formula (1) valid in $\mathcal{H}^{(S)}$ by the same formula re-written (i.e., represented) in $\mathcal{H}^{(F)}$,

$$H = \Theta^{-1}H^\dagger\Theta, \quad \Theta = \Omega^\dagger\Omega. \tag{2}$$

The operator $\Theta$ is called the physical Hilbert-space metric.

The preference of Eq. (2) suppresses many misunderstandings. First of all, we may keep writing the “false”, $F$—superscripted inner products in the standard Dirac’s bra-ket notation,

$$[\langle \psi_1 | \psi_2 \rangle]^{(F)} \equiv \langle \psi_1 | \psi_2 \rangle. \tag{3}$$

Secondly, the representation of the other, physical, $S$—superscripted inner products may be given virtually equally friendly form in its friendlier $F$—space representation,

$$[\langle \psi_1 | \psi_2 \rangle]^{(S)} \equiv \langle \psi_1 | \Theta | \psi_2 \rangle. \tag{4}$$

In the spirit of review [16] one can also introduce the doubled bra and the doubled ket symbols and abbreviate $\Theta | \psi \rangle \equiv | \psi \rangle$ and $\langle \psi | \Theta \equiv \langle \psi | |$. Although such a convention is fairly unusual (and it will not be used too much in the bulk text of this paper), its use can make the formalism more transparent because the set of special ketkets $| n_0 \rangle$ can be introduced as a set of eigenvectors of the conjugate Hamiltonian, $H^\dagger | n_0 \rangle = E_n | n_0 \rangle$. As a consequence one can endow the Hamiltonian operator $H$ with the menu of all of its eligible Hermitizing metrics,

$$\Theta = \sum_n | n_0 \rangle \kappa_n \langle n_0 | = \Theta(\vec{\kappa}). \tag{5}$$

The coefficients $\kappa_n$ are variable and the sequence of their values must be kept real, positive and properly bounded [14].

3 The operator-compatibility conditions

3.1 The case of commuting pairs of non-Hermitian observables

The Hilbert-space-metric operator $\Theta$ (with multiple necessary mathematical properties [5, 19, 20, 21, 22] which were not mentioned here for the sake of brevity) enables one to
pull back the $S$–space formula (1) to its explicit equivalent representation (2) in $F$–space. Naturally, the correspondence between the left eigenvectors and the general Hermitizing metric operators applies to the Hamiltonian $H = \Lambda_0$ as well as to any other non-Hermitian candidate $\Lambda_j$ for the operator of an observable. Via an analogue of formula (5), any such an operator can be assigned, *mutatis mutandis*, an exhaustive menu of eligible metrics

$$\Theta = \sum_n |n_j\rangle\langle n_j| = \Theta_j(\vec{\kappa}(j)).$$

(6)

Our present research subject can briefly be characterized, in its first nontrivial version with $j = 0$ and $j = 1$ in Eq. (6), as the analysis of the operator twin-observability constraint

$$\Theta_0(\vec{\kappa}(0)) = \Theta_1(\vec{\kappa}(1)).$$

(7)

Just the trivial versions of the solution of this relation are usually considered in the literature. Once we recall that the shared eigenvalues $E_n$ of $\Lambda_0 = H$ and of $\Lambda_0^\dagger = H^\dagger$ are, by assumption, real, we may decide to complement our knowledge of the eigenketkets $|n_0\rangle$ of the conjugate $H^\dagger$ by the standard eigenkets $|n_0\rangle$ of $H$. In this way we obtain a biorthonormalized basis [23] and a spectral-like formula

$$H = \sum_n |n_0\rangle E_n \langle\langle n_0|.$$  

(8)

If we introduce another operator $\Lambda_1 \neq \Lambda_1^\dagger$ with real spectrum and such that

$$\Lambda_1 = \sum_n |n_1\rangle b_n \langle\langle n_1|,$$

(9)

the related biorthonormal basis will be different because the new operator does not commute with the old one in general.

Once we now impose the simplifying condition of the commutativity, i.e., of the coincidence of the two eigenbases in formulae

$$\Lambda_0^{(special)} = \sum_n |n\rangle a_n \langle\langle n|, \quad \Lambda_1^{(special)} = \sum_n |n\rangle b_n \langle\langle n|$$  

(10)

we find that such an assumption immediately converts the compatibility condition (7) into an identity. In the light of Appendix of Ref. [5] the introduction of the new observable does not remove the ambiguity from the metric (5) at all. The free variability of the whole multiplet of parameters $\vec{\kappa}$ survives. In the terminology of review [5], the set of the two observables (10) remains reducible.

Let us now exclude the fully degenerate scenario of Eq. (10) as trivial and let us assume that the two biorthonormal bases entering spectral expansions (8) and (9) do not coincide. The operator-coincidence (7) will then restrict the variability of the coefficients in Eq. (5). The number of the constraints which are generated by Eq. (7) becomes *too large* for the purpose in general.

Certainly, the problem deserves a deeper, more concrete critical analysis.
3.2 The case of non-commutative non-Hermitian observables

A priori we may expect that the metric $\Theta(\Lambda_0, \Lambda_1)$ can only exist under certain constraints represented, formally, by the solvability of Eq. (7). The knowledge of these constraints will be difficult to extract in practice. This makes our present task (i.e., the search for criteria) rather nontrivial.

During the search for a guarantee of the existence of at least one acceptable metric we reveal that in contrast to the comparatively popular suppressions of the ambiguity of $\Theta$, the danger of the nonexistence of any metric is often underestimated in the literature. For example, the authors of Ref. [12] took the existence of $\Theta(\Lambda_0, \Lambda_1)$, rather naively, for granted. In an entirely general setting they considered “a definite form of the Hamiltonian $H$” (i.e., in our notation, of the first operator $\Lambda_0$) “and an additional observable” (i.e., another operator $\Lambda_1$). They claimed, expressis verbis, that “these two choices ... will fix the metric uniquely, such that there are no ambiguities left in the interpretation of the physical observables” [12].

For a technically feasible critical analysis of such a claim let us, first of all, skip certain less essential mathematical subtleties and let us restrict attention to the models living in finite-dimensional Hilbert spaces, specifying, for the sake of definiteness, $\mathcal{H}^{(F)} = \mathbb{C}^N$. In this case we may use any suitable basis and we may treat our operators $\Lambda_0, \Lambda_1, \ldots$ as the respective complex $N \times N$ matrices $A = \Lambda_0^{(N)}, B = \Lambda_1^{(N)}, \ldots$.

Once we abbreviate, in parallel, $\kappa^{(0)} = \overrightarrow{\alpha}$ and $\kappa^{(10)} = \overrightarrow{\beta}$, the respective metrics in Eq. (7) may be perceived as the well defined Hermitian-matrix functions of the real and positive variables. This enables us to rewrite Eq. (7) as the algebraic set

$$\Theta^{(A)}_{mn}(\overrightarrow{\alpha}) = \Theta^{(B)}_{mn}(\overrightarrow{\beta}), \quad m, n = 1, 2, \ldots, N$$

of $N^2$ linear equations. The left-hand-side matrix with eigenvalues $\theta^{(A)}_{n}(\overrightarrow{\alpha})$ may be diagonalized by a suitable unitary matrix $U(\overrightarrow{\alpha})$. This yields an equivalent set of relations

$$\theta^{(A)}_{n}(\overrightarrow{\alpha})\delta_{mn} = \left[U(\overrightarrow{\alpha}) \Theta^{(B)}(\overrightarrow{\beta}) U^\dagger(\overrightarrow{\alpha})\right]_{mn}, \quad m, n = 1, 2, \ldots, N.$$  \hspace{1cm} (12)

For an arbitrary “input” choice of the $N-$plet of variable parameters $\alpha_n$ this certainly provides the $N-$plet of constraints

$$\theta^{(A)}_{n}(\overrightarrow{\alpha}) = \left[U(\overrightarrow{\alpha}) \Theta^{(B)}(\overrightarrow{\beta}) U^\dagger(\overrightarrow{\alpha})\right]_{mn}, \quad n = 1, 2, \ldots, N$$

which may be read as an implicit-function definition of the “output” $N-$plet of quantities $\beta_n = \beta_n(\overrightarrow{\alpha})$.

We are now left with the remaining independent $N(N-1)/2$ conditions forming the upper triangular matrix in (12) and reflecting the presence of the left-hand-side zeros,

$$\left[U(\overrightarrow{\alpha}) \Theta^{(B)}(\overrightarrow{\beta}(\overrightarrow{\alpha})) U^\dagger(\overrightarrow{\alpha})\right]_{mn} = 0, \quad m = n+1, n+2, \ldots, N, \quad n = 1, 2, \ldots, N-1$$  \hspace{1cm} (14)
Our remaining available $N$–plet of the real and positive variables $\alpha^\ell$ is constrained by the overdetermined set of the $N(N-1)/2$ complex (i.e., of the $N(N-1)$ real) nonlinear algebraic equations. In the generic case one can use the roughmost estimate of the number of solutions and conclude that at $N > 2$ the nontrivial real and positive roots $\alpha_n$ need not exist at all. Indeed, the number of equations (14) will not exceed the number of unknowns only when $N(N-1) \leq N$, i.e., at $N \leq 2$.

In the opposite direction the requirement of the existence of at least one real and positive $N$–plet of parameters $\alpha_n$ necessarily imposes certain nontrivial restrictions upon our freedom of the choice of the “dynamical input” operators $A$ and $B$. Naturally, the latter set of restrictions becomes perceivably more stringent when one decides to accommodate more than two “dynamical input” operators $\Lambda_j$ with $j \leq j_{\text{max}} > 1$. At the same time, our theoretical ambitions should not be exaggerated. Thus, for $j_{\text{max}} \gg 1$ at least, it seems to make good sense to follow the common practice of the traditional textbooks where, typically, a trivial unit-matrix metric $\Theta = I$ is chosen and fixed in advance.

In the present generalized setting the acceptance of the same philosophy will merely mean that one simplifies the strategy and picks up and fixes a suitable nontrivial initial matrix $\Theta^{(A)} \neq I$. In this framework one then admits only those additional observables which obey the Dieudonné’s quasi-Hermiticity condition

$$\Lambda_j \Theta^{(A)} = \Theta^{(A)} \Lambda_j^\dagger$$

in $\mathcal{H}^{(F)}$ (cf. Eq. (2)), i.e., the hidden-Hermiticity requirement $\Lambda_j = \Lambda_j^\dagger$ in the fixed physical Hilbert space $\mathcal{H}^{(S)}$.

4 Applications of the theory

The sufficient relations as sampled by Eq. (10) might prove insufficiently general. The less restrictive and more general $N \leq \infty$ formula (14) is too implicit for being useful in practice. Only the study of specific toy models can lead to some more definite conclusions.

4.1 Working with weakly deformed oscillator algebras

The uncertainty relations for positions and momenta acquire rather unusual forms after a tentative replacement of the solvable harmonic oscillator by its suitable $q$–deformed analogues [24]. In a way related to the Connes’ phenomenology-oriented conjecture of making the geometry non-commutative [25], these developments had a perceivable impact also upon quantum physics [12, 26].

A typical build up of quantum models of this type starts from Heisenberg algebra. A coordinate $x$ and momentum $p$ or, alternatively, an annihilation operator $a$ and a creation
operator $a^+$ may be deformed, typically, in such a way that $(a, a^+) \to (\hat{a}, \hat{a}^+)$ and

$$\hat{a}\hat{a}^+ - q\hat{a}^+\hat{a} \equiv [\hat{a}, \hat{a}^+]_q = 1.$$  \hspace{1cm} (16)

Some of the complications become simplified in a vicinity of the zero-deformation limit $q = 1$, i.e., at small $\varepsilon = q - 1 \neq 0$. One may recall Eq. (16), ignore the higher-order corrections and construct, in a simplified leading-order approximation,

$$\hat{a} = \frac{1}{\sqrt{2}} (\hat{X}_q + i\hat{P}_q) = a + \frac{1}{4} \varepsilon a^+ a^2 + \mathcal{O}(\varepsilon^2),$$ \hspace{1cm} (17)

$$\hat{a}^+ = \frac{1}{\sqrt{2}} (\hat{X}_q - i\hat{P}_q) = a^+ + \frac{1}{4} \varepsilon a^{+2} a + \mathcal{O}(\varepsilon^2).$$ \hspace{1cm} (18)

One may then rewrite the Hamiltonian of the deformed harmonic oscillator in its perturbation-approximation form

$$A = \hat{H}_q = \hat{P}_q^2 + \hat{X}_q^2 = H_0 + \frac{1}{8} \varepsilon H_1 + \mathcal{O}(\varepsilon^2).$$ \hspace{1cm} (19)

The standard textbook harmonic oscillator Hamiltonian $H_0 = p^2 + x^2 = H_0^\dagger$ is, in the leading-order approximation, complemented by a manifestly non-selfadjoint alias non-Hermitian interaction operator

$$H_1 = 2x^4 - x^2 + 3p^2 - 3 + 2ix^3 p + 2ixp^3 + 2x^2 p^2 - 8ixp \neq H_1^\dagger.$$ \hspace{1cm} (20)

Such a model was studied in [27] and its spectrum was found, in the leading-order approximation, real. This opened the question of the possible coexistence of the observability, say, of the Hamiltonian (i.e., operator $A = \hat{H}_q$) and of the coordinate (operator $B = \hat{X}_q$—cf. also Refs. [12] and [28] in a slightly different context).

### 4.2 The perturbative Hermitizability of $A \neq A^\dagger$ and $B \neq B^\dagger$

The study of the $q$–deformed Hamiltonian $A = \hat{H}_q \neq A^\dagger$ originated from its interesting spatial geometry features [26, 29]. The Hermitization of the Hamiltonian must be accompanied by the equally relevant Hermitization of the operator of the coordinate

$$B = \hat{X}_q = x + \frac{1}{8} \varepsilon (x^3 - xp^2 + ix^2 p - x + ip^3 + pxp + p^2 x) + \mathcal{O}(\varepsilon^2).$$ \hspace{1cm} (21)

We may even try to work with a multiplet of observables $\hat{\Lambda}_j$ where $\hat{\Lambda}_0 = A = H$, $\hat{\Lambda}_1 = B$, etc. All of these operators of observables must satisfy the observability constraint,

$$\hat{\Lambda}_j = \hat{\Lambda}_j^\dagger \equiv \Theta^{-1}\hat{\Lambda}_j^\dagger \Theta, \quad j = 0, 1, \ldots, j_{\text{max}}.$$ \hspace{1cm} (22)

These relations must all contain the same physical metric operator $\Theta$. 


In the limit of infinitesimally small non-Hermiticities it is nontrivial to guarantee the existence of at least one formal set of quantities $\beta_n$, $\alpha_n$, $\Theta$, $A$ and $B$ which would be compatible with the twin-observability condition (11). In the leading-order approximation one can consider, in the spirit of Eqs. (19) and (21), the $N$ by $N$ matrices

$$A = A_0 + \varepsilon A_1 + \ldots, \quad A_0 = A_0^\dagger$$

and

$$B = B_0 + \varepsilon B_1 + \ldots, \quad B_0 = B_0^\dagger$$

of the relevant observables. The latter ansatz could be generalized to a higher-order precision and/or to a larger number of operators $j_{\text{max}} > 1$. For its current $j_{\text{max}} = 1$ form, our task may be now formulated as the construction of the leading-order metric

$$\Theta = I + \varepsilon F + \ldots, \quad F = F^\dagger.$$ 

The latter operator must make both of the input operators $A$ and $B$ of observables compatible, within given precision, with the respective hidden-Hermiticity constraints (22). Thus, the following two commutator-containing equations

$$A_0 F - F A_0 = A_1 - A_1^\dagger \equiv i R, \quad R = R^\dagger,$$ 

$$B_0 F - F B_0 = B_1 - B_1^\dagger \equiv i S, \quad S = S^\dagger$$

are to be solved for the unknown complex first-order metric-operator component $F = F^\dagger$. Due to the use of the perturbation theory, their form is perceptibly simpler than that of their non-perturbative predecessors (7) and (11).

5 The perturbative construction of the metric

5.1 The single-observable problem

Without a pre-selected $\Theta$ the constructive treatment of the observability constraints (22) is difficult [30]. Fortunately, people are often interested only in the observability of the Hamiltonian,

$$\widehat{H}_q = \Theta^{-1} \widehat{H}_q^\dagger \Theta.$$ 

The analysis of this equation may be facilitated by additional assumptions. The restriction to bounded operators is the most important one. Another postulate, remarkably efficient in applications, introduces the auxiliary $\mathcal{PT}$–symmetry property which is equivalent to the relation $\widehat{H}_q^\dagger \mathcal{P} = \mathcal{P} \widehat{H}_q$ where $\mathcal{P}$ denotes the operator of parity.
Once we turn attention from the Hamiltonian of Eq. (28), say, to the coordinate of Eq. (21) with property
\[ \hat{X}_q^+ = \hat{X}_q + \frac{\varepsilon}{8} (2xp^2 - ixp^3 - 2ip^3 - 2p^2x - ipx^2) + \mathcal{O}(\varepsilon^2) \] (29)
we may recall constraint (22), i.e.,
\[ X_q^+ = \Theta X_q \Theta^{-1} \] (30)
and we may search for such a form of the metric which would be positive, invertible and factorizable,
\[ \Theta = \Omega^+ \Omega . \] (31)
One of such formal solutions can be found and expressed as an exponential,
\[ \Theta_0 = e^{\varepsilon f(x,p)+\mathcal{O}(\varepsilon^2)} = 1 + \varepsilon f(x,p) + \mathcal{O}(\varepsilon^2) \] (32)
with
\[ f(x,p) = \frac{1}{4} \left[ \frac{1}{4} (x^2p^2 + p^4 + p^2x^2) + \frac{i}{3} (xp^3 - p^3x) \right] . \] (33)
Such a solution signals several warnings at once. It is not acceptable, first of all, because of its unboundedness. In the next paragraph we will pay more attention to the consistency between Eqs. (30) and (32). We shall show that nontrivial as it is, this solution cannot render the Hamiltonian selfadjoint.

5.2 Tentative Hermitizations and their failures

According to the expectations as expressed in Refs. [10, 11, 12, 13, 27] the single-observable construction of preceding paragraph should suffice for the necessary Hermitization of the Hamiltonian. According to the same sources the use of the most common special mapping
\[ \hat{H}_q \rightarrow h_0 = \Omega_0 \hat{H}_q \Omega_0^{-1} \] (34)
with the widely recommended choice of the square-root form of \( \Omega_0 = \sqrt{\Theta_0} \) might yield a manifestly Hermitian partner Hamiltonian \( h_0 = h_0^\dagger \) acting in \( \mathcal{H}^{(T)} \).

Although the analysis of this hypothesis is far from easy, the straightforward evaluation of the difference \( \Delta = h_0 - h_0^\dagger \) falsifies the hypothesis, \( \Delta \neq 0 \). The validity of such a proof was also reconfirmed via its computer-assisted re-verification [31]. One can conclude that the coordinate-Hermitizing Dyson-mapping operator
\[ \Omega_0 = e^{\varepsilon g(x,p)+\mathcal{O}(\varepsilon^2)} = 1 + \varepsilon g(x,p) + \mathcal{O}(\varepsilon^2) \] (35)
with
\[ g(x,p) = \frac{1}{8} \left[ \frac{1}{4} (x^2p^2 + p^4 + p^2x^2) + \frac{i}{3} (xp^3 - p^3x) \right] \] (36)
does not Hermitize the Hamiltonian. This disproves the hypothesis and reopens the methodical question of the possibility of formulation of the criteria of the non-existence, existence and/or uniqueness of a shared metric $\Theta$, for some two pre-selected candidates for physical quantum observables $A$ and $B$ at least.

6 Merits of perturbative considerations

Using a toy model we re-confirmed, in subsection 5.1, the well known fact that even in the case of the single given observable $A \neq A^\dagger$ with real spectrum and even in the not too complicated models with an infinitesimally small non-Hermiticity the construction of a correct Hermitizing physical metric $\Theta$ may be a formidable task.

6.1 Models with bounded-operator observables $A, B, \ldots$

The existence, number and construction of the solutions $\Theta$ specified by Eqs. (14) or (26) + (27) will all vary with the dynamical input $A, B, \ldots$. One of the best analyses of these possibilities was presented in [5], i.e., paradoxically, in one of the oldest papers published on the subject. The assumptions made in loc. cit. (and, in particular, the restriction of the scope of the paper to the bounded operators of observables) may be greeted (it renders the mathematics entirely reliable and rigorous) as well as damned (because the assumption excludes many models due to the unbounded nature of their observables).

6.2 $N$ by $N$ complex-matrix observables $A, B, \ldots$

The analysis of the generic $A - B$ compatibility conditions (14) or (26) + (27) remains far from easy even in the Hilbert spaces of a finite dimension $N < \infty$. This analysis may be assisted by the computers. Various finite-dimensional complex-matrix special cases of Eqs. (26) and (27) may be considered as approximating realistic scenarios. In the most common (and suitably truncated) harmonic-oscillator basis, both of our respective toy-model exemplifications (20) and (21) of $A_0$ and $B_0$ will be sparse matrices.

The truncation of bases could clarify the questions of the existence of the metric in the limit $N \rightarrow \infty$. In the hypothetical case of an affirmative answer, the recipe could render the construction of $F$ feasible. The analysis could be also performed in an opposite direction, i.e., the existence of the metric may be required in advance. Then one can deduce the necessary conditions and constraints imposed upon the pair of perturbations $A_1$ and $B_1$.

It makes sense to split the complex $N$ by $N$ matrices in the real and imaginary parts. Once we use subscripts $s$ and $a$ marking, respectively, the symmetric and antisymmetric
real matrices, the input information encoded in the Hermitian, complex \( N \) by \( N \) matrices
\[
A_0 = A_s + iA_a, \quad B_0 = B_s + iB_a, \quad R = R_s + iR_a, \quad S_0 = S_s + iS_a
\]  
(37)
will generate the desirable ultimate Hermitian matrix solution \( F = F_s + iF_a \) via Eqs. (26) + (27), i.e., with commutators in the real-matrix relations
\[
[A_s, F_s] - [A_a, F_a] = -R_a \quad [A_s, F_s] + [A_a, F_a] = R_s
\]  
(38)
and
\[
[B_s, F_s] - [B_a, F_a] = -S_a \quad [B_s, F_s] + [B_a, F_a] = S_s.
\]  
(39)
We may recall the symmetries/antisymmetries of matrices and omit the diagonal (i.e., trivially satisfied) part of the first items in both Eqs. (38) and (39). Using an arbitrary ordering of all of the independent and nontrivial matrix elements this enables us to re-arrange the upper triangular part of all of the \( a \)-subscripted upper-case real and antisymmetric \( N \) by \( N \) matrices into the respective \( M \)-dimensional lower-case column vectors with \( M = N(N - 1)/2 \) (i.e., we replace \( R_a \) by, say, \( \tilde{r}^{(M)} \), etc). Similarly, with \( V = N(N + 1)/2 \) we compress the information carried by the real and symmetric upper-case \( N \) by \( N \) matrix \( R_s \) to a lower-case vector \( \tilde{s}^{(V)} \). We take the upper triangular part of any \( s \)-subscripted matrix and we replace it by its real \( V \)-dimensional column-vector representation.

The procedure eliminates the redundancy and preserves the linearity of Eqs. (38) and (39). Using the self-explanatory abbreviation for commutators we may finally convert the equations into their respective compact final versions
\[
L^{(VV)}(A) \tilde{f}^{(V)}(A) + L^{(VM)}(A) \tilde{f}^{(M)}(A) = \tilde{r}^{(V)}, \quad L^{(MV)}(A) \tilde{f}^{(V)}(A) - L^{(MM)}(A) \tilde{f}^{(M)}(A) = -\tilde{r}^{(M)}
\]  
(40)
and
\[
L^{(VV)}(B) \tilde{f}^{(V)}(B) + L^{(VM)}(B) \tilde{f}^{(M)}(B) = \tilde{s}^{(V)}, \quad L^{(MV)}(B) \tilde{f}^{(V)}(B) - L^{(MM)}(B) \tilde{f}^{(M)}(B) = -\tilde{s}^{(M)},
\]  
(41)
i.e., in the partitioned block-matrix notation,
\[
\begin{pmatrix}
L^{(VV)}(A) & L^{(VM)}(A) \\
-L^{(MV)}(A) & L^{(MM)}(A)
\end{pmatrix}
\begin{pmatrix}
\tilde{f}^{(V)}(A) \\
\tilde{f}^{(M)}(A)
\end{pmatrix}
= \begin{pmatrix}
\tilde{r}^{(V)} \\
\tilde{r}^{(M)}
\end{pmatrix}
\]  
(42)
and
\[
\begin{pmatrix}
L^{(VV)}(B) & L^{(VM)}(B) \\
-L^{(MV)}(B) & L^{(MM)}(B)
\end{pmatrix}
\begin{pmatrix}
\tilde{f}^{(V)}(B) \\
\tilde{f}^{(M)}(B)
\end{pmatrix}
= \begin{pmatrix}
\tilde{s}^{(V)} \\
\tilde{s}^{(M)}
\end{pmatrix}.
\]  
(43)
Equations (26) and (27) alias (42) and (43) may be finally re-read as a pair (or as a multiplet) of the real and linear matrix relations
\[
\mathcal{A} \tilde{f} = i \tilde{r}, \quad \tilde{\mathcal{A}} \tilde{f} = i \tilde{s}, \quad \ldots
\]  
(44)
containing the same vector \( \tilde{f} \). By construction, the \( N^2 \) by \( N^2 \) matrices \( \mathcal{A} \) and \( \tilde{\mathcal{A}} \) (etc) are all real.
Both the existence and non-existence of the real solution vector $\vec{f}$ (with $N^2$ components) remains admitted by the first-order perturbation approach. No qualitative change in the conclusions is detected when one simplifies the mathematics and when one moves from the general case to the scenario with infinitesimally small non-Hermiticites. The transition from existence to non-existence of the metric depends on the dynamical input encoded into matrices $A$ and $B$ as well as into vectors $\vec{r}$ and $\vec{s}$.

The former, large-matrix part of the encoded dynamical input is determined by the self-adjoint zero-order components of the observables in Eqs. (23) and (24). The second, vectorial part of the input carrying the information about the non-Hermiticites seems more compact. This feature of Eqs. (44) should be attributed to the neglect of the higher-order $O(\varepsilon^2)$ terms in Eqs. (23) and (24).

### 6.3 Illustration: $N = 2$

Let us employ the row-wise vectorial compactification of matrices at the first nontrivial dimension $N = 2$ with $V = 3$, $M = 1$ and with the replacements

$$F_s = \begin{pmatrix} x & z \\ z & y \end{pmatrix} \rightarrow \vec{f}^{(3)} = \begin{pmatrix} x \\ z \\ y \end{pmatrix}, \quad F_a = \begin{pmatrix} 0 & p \\ -p & 0 \end{pmatrix} \rightarrow \vec{f}^{(1)} = \begin{pmatrix} p \end{pmatrix}$$

etc. Then, the most general choice of the Hermitian part of the dynamical input

$$A_s = \begin{pmatrix} a & c \\ c & b \end{pmatrix}, \quad A_a = \begin{pmatrix} 0 & d \\ -d & 0 \end{pmatrix}$$

leads to the following explicit $N^2$ by $N^2$ matrix form of Eq. (40),

$$\begin{pmatrix} 0 & 2d & 0 & -2c \\ -d & 0 & d & a - b \\ 0 & -2d & 0 & 2c \\ -c & a - b & c & 0 \end{pmatrix} \begin{pmatrix} x \\ z \\ y \\ p \end{pmatrix} = \begin{pmatrix} r_1^{(3)} \\ r_2^{(3)} \\ r_3^{(3)} \\ r_1^{(1)} \end{pmatrix}.$$  

(47)

Once we compare the first and third line we may conclude that there exist no nontrivial components $z$ and $p$ (i.e., the metric remains trivial, diagonal) unless the non-Hermiticity $A_1$ in ansatz (23) and in relation (26) satisfies the non-diagonality constraint

$$r_1^{(3)} (= (R_s)_{11}) = -r_3^{(3)} (= -(R_s)_{22}).$$  

(48)

Under the latter assumption we have just three linearly independent equations for the four real unknowns $x, z, y$ and $p$ so that, in accord with the expectations [32], the admissible two-by-two metrics will form a one-parametric family.
An analogous elementary analysis has to be applied in the situation with $j_{\text{max}} = 1$ in which, under the non-triviality assumption (48) (plus under its $B-$related analogue), the three independent lines of Eq. (47) become complemented by their three independent $B-$related analogues marked, for the sake of simplicity, by tildas. With the latter additional dynamical information at our disposal we arrive at the set of six equations

$$\begin{pmatrix} 0 & 2d & 0 & -2c \\ -d & 0 & d & a-b \\ -c & a-b & c & 0 \\ 0 & 2 \tilde{d} & c & -2 \tilde{c} \\ -\tilde{d} & 0 & \tilde{d} & \tilde{a}-\tilde{b} \\ -\tilde{c} & \tilde{a}-\tilde{b} & \tilde{c} & 0 \end{pmatrix} \begin{pmatrix} x \\ z \\ y \\ p \end{pmatrix} = \begin{pmatrix} r_{1}^{(3)} \\ r_{2}^{(3)} \\ r_{1}^{(1)} \\ s_{1}^{(3)} \\ s_{2}^{(3)} \\ s_{1}^{(1)} \end{pmatrix}. \quad (49)$$

The values of $z$ and $p$ get evaluated most easily. After their re-insertion (reflected by our adding a hat to the right-hand side vector elements) we are left with the following four linear equations for the last two unknowns,

$$\begin{pmatrix} -d & d \\ -c & c \\ -\tilde{d} & \tilde{d} \\ -\tilde{c} & \tilde{c} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} r_{2}^{(3)} \\ r_{1}^{(1)} \\ s_{2}^{(3)} \\ s_{1}^{(1)} \end{pmatrix}. \quad (50)$$

We have to avoid the non-existence of the metric, i.e., we have to impose the triple restriction

$$\frac{r_{2}^{(3)}}{d} = \frac{r_{1}^{(1)}}{c} = \frac{s_{2}^{(3)}}{\tilde{d}} = \frac{s_{1}^{(1)}}{\tilde{c}} \quad (51)$$

upon the dynamical input information. The nontrivial solvability is then guaranteed while the one-parametric ambiguity of the shared physical metric will survive. Its suppression would require either the choice of $j_{\text{max}} > 1$ or an inclusion of the second-order perturbation corrections in $\varepsilon$.

7 Summary

After one requires that a given pair of operators $A$ and $B$ with real and non-degenerate spectra represents two quantum observables, the specification of the $S-$superscripted physical Hilbert space via the definition of the metric $\Theta$ may be impossible, unique or ambiguous. An optimal scenario will be only realized in the case of uniqueness of the metric. Still, even in the presence of an ambiguity the authors of review [5] argued that our knowledge of any formally correct metric will be welcome, e.g., for variational-calculations purposes.

Such a pragmatic approach was accepted in virtually all of the related literature. Some of the authors insisted on the optimality (i.e., uniqueness) of the metric [32]. Often, they
believed that such a goal is rather easy to achieve. In our present paper we demonstrated that it is not always so.

The reasons and consequences have been explained in detail. In particular, we came to the conclusion that the straightforward, best known and successful suppression of the ambiguity of the metric via the identification of the second observable with a “charge” ($B = C$ such that $C^2 = 1$, cf. [2] for all details) was exceptional, having been only rendered possible due to a number of additional, *ad hoc* assumptions.

One can characterize the popular choice of the charge $C$ as a special implementation of the general recipe given in Ref. [5] and requiring the irreducibility of the set $A, B, \ldots$ of the quasi-Hermitian representations of the physical quantum observables. Using a number of toy models we explained why the consistent coexistence of more than one preselected non-Hermitian candidate for the observable $\Lambda_j$ should be considered exceptional.

In other words, whenever one tries to work with the two or more independent and manifestly non-Hermitian candidates for quantum observables, the absence of the reliable (and, in general, difficult!) proof of the existence of the shared metric $\Theta$ should not be tolerated because it might really very easily result in the loss of the applicability of the entire sophisticated PTSQM formalism.

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