

Twin Hamiltonians, three types of the Dyson maps, and the probabilistic interpretation problem in quasi-Hermitian quantum mechanics

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Abstract

In quasi-Hermitian quantum mechanics (QHQM) of unitary systems, an optimal, calculation-friendly form of Hamiltonian is generally non-Hermitian, $H \neq H^\dagger$. This makes its physical interpretation ambiguous. Without altering H , this ambiguity is resolved by specifying a nontrivial inner-product metric Θ in Hilbert space. Here, we focus on an alternative strategy: transforming H into a Hermitian form via the Dyson map $\Omega : H \rightarrow \mathfrak{h}$. This construction of the Hermitian isospectral twin $\mathfrak{h}$ of H does not only restore the conventional correspondence principle between quantum and classical physics, but it also provides a framework for the exhaustive classification of all admissible probabilistic interpretations of quantum systems in QHQM framework.

Keywords

non-Hermitian quantum mechanics;
isospectral pairs of a non-Hermitian and Hermitian Hamiltonian;
ambiguity of the unitary-evolution scenarios;
classification scheme;

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1 Introduction

In the majority of textbooks on quantum mechanics (see, e.g., Ref. [1]), the realistic Hamiltonians of unitary systems are usually considered in their most conventional self-adjoint form

$$\mathfrak{h} = \mathfrak{h}^\dagger = \mathfrak{h}_{(\text{free motion})} + \mathfrak{h}_{(\text{interaction})} . \quad (1)$$

In 1956, Freeman Dyson [2] found such a restriction unnecessary and, for practical purposes, possibly even counterproductive. Still, he did not leave the standard theoretical framework of textbooks. Primarily, his (implicit) criticism of the specification of quantum dynamics using Eq. (1) was technical. He fully accepted the necessity of maintaining the relationship – known as the principle of correspondence – between quantum and classical phenomenological models of experimentally accessible physical reality.

For the specific many-particle system considered in *loc. cit.*, the first component

$$\mathfrak{h}_{(\text{free motion})} = \mathfrak{h}_{(\text{kinetic energy})} \quad (2)$$

of the Hamiltonian was simply the sum of Laplacians, while the second component was also entirely conventional, consisting of local two-particle interaction potentials. What was truly revolutionary, however, was the transformation

$$\mathfrak{h} \rightarrow H = \Omega^{-1} \mathfrak{h} \Omega , \quad (3)$$

i.e., a tentative isospectral simplification of the preselected Hamiltonian, where

$$\Omega^\dagger \Omega = \Theta \neq I . \quad (4)$$

This means that the author omitted the usual requirement of unitarity of the transformation.

The price was the manifest non-Hermiticity of the upgraded Hamiltonian,

$$H \neq H^\dagger = \Theta H \Theta^{-1} . \quad (5)$$

Such a form of non-Hermiticity (called “quasi-Hermiticity” in Refs. [3, 4]) is merely an inessential consequence of the non-unitarity of the invertible mapping $\Omega : \mathfrak{h} \rightarrow H$ [cf. Eq. (4) and also Appendix A below]. Naturally, both of the isospectral twin Hamiltonians $\mathfrak{h}$ and H still carried the same information about physics, i.e., about the shared and measurable bound state energies.

A decisive advantage of the work with twins (i.e., with the Hermitian but complicated $\mathfrak{h}$ and, simultaneously, with the non-Hermitian but user-friendlier H) lied in the enhanced freedom of the description of dynamics which could vary with the changes of the nontrivial inner-product metric Θ or with its optional Dyson-map factor Ω (cf. [5, 6, 7, 8]). For an efficient evaluation of the experimentally relevant low-lying spectrum of the system characterized by a uniquely preselected self-adjoint Hamiltonian $\mathfrak{h}$, no conceptual problems arose with the ambiguity of $H = H(\Omega)$, since

both the reality of the spectrum and a consistent, unambiguous probabilistic interpretation of the system were guaranteed by ansatz (1).

The flexibility of Ω have proven extremely useful in practice – cf., e.g., its numerous subsequent applications to interacting-boson systems in nuclear physics [9], or, many years later, its role in relativistic quantum mechanics [10], in thermodynamics [11], in quantum information [12] and even beyond the realm of quantum physics [13, 14]. In the original Dyson’s calculations of Ref. [2], in particular, this flexibility led to an efficient inclusion of interaction-induced two-particle correlations, markedly accelerating convergence, and markedly enhancing the overall efficiency of otherwise routine variational approaches in many-body phenomenology (cf. [15]).

A few years later, the problem of providing a consistent probabilistic interpretation of non-Hermitian bound-state systems re-emerged, following several independent discoveries showing that certain new non-Hermitian—but computationally convenient—Hamiltonian candidates could produce real spectra even without any initial reference to Eq. (3) (cf., e.g., Refs. [4, 16, 17, 18]). It is important to notice a deep conceptual distinction of the latter approach from the Dyson’s original pragmatic strategy. Temporarily, we will denote these newly preselected non-Hermitian Hamiltonians by the tilded symbol $\tilde{H}$, therefore.

We decided to use such a notation in order to emphasize more clearly that the related innovative models and studies reopened multiple methodological questions regarding the meaningful physical interpretation of the specific tilded-Hamiltonian models. Their characteristic feature is that the theory is “narrowed” and considered without any direct reference to the isospectrality mapping between the preselected non-Hermitian candidate $\tilde{H}$ for the Hamiltonian (in Schrödinger picture) and its manifestly Hermitian twin $\tilde{\mathfrak{h}}$. Indeed, such a loss of correspondence (3) has to be interpreted as a loss of a clear specification of the underlying physics, i.e., as one of the most significant weaknesses of the non-Hermitian extension of the Schrödinger picture.

In this setting it is a bit unfortunate that one of the most fundamental and obvious simplifications of the interpretation questions as provided by the transition to Heisenberg picture (cf., e.g., [19, 20]) is known to lead to certain truly serious technical complications. In the present paper, therefore, we intend to keep using the Schrödinger-picture philosophy. We will formulate, re-analyze and resolve some of the Schrödinger-picture-related interpretation issues in necessary detail.

2 A Dyson-inspired strategy: An elementary example

A few basic formal features of the replacement of an otherwise unsuitable “realistic” (Hermitian, lower-case, untilded) Hamiltonian $\mathfrak{h}$ by its “more computationally friendly” (but non-Hermitian) isospectral twin H can be most clearly illustrated using a schematic quantum system in a finite, two-dimensional Hilbert space, i.e., in an N -dimensional space $\mathcal{H}^{(N)}$ with $N = 2$.

For a simple illustration, we take the initial Hermitian reference Hamiltonian to be the following

real and symmetric 2×2 matrix

$$\mathfrak{h} = \omega \sigma_x = \begin{pmatrix} 0 & \omega \\ \omega & 0 \end{pmatrix} \quad (6)$$

with two real eigenvalues $E_{\pm} = \pm\omega$.

One must now select a methodically instructive form of the Dyson map. Within the Dyson-inspired model-building framework, it is common to choose its simplest possible form (cf., e.g., review [7]). For the purposes of the present illustration, we therefore adopt a 2×2 matrix ansatz

$$\Omega = e^{\frac{\alpha}{2}\sigma_y}, \quad \alpha \in \mathbb{R}. \quad (7)$$

Since σ_y is Hermitian and satisfies $\sigma_y^2 = I$, one has

$$\Omega^\dagger = \Omega, \quad \Omega^{-1} = e^{-\frac{\alpha}{2}\sigma_y}, \quad \Theta = e^{\frac{\alpha}{2}\sigma_y} e^{\frac{\alpha}{2}\sigma_y} = e^{\alpha\sigma_y}. \quad (8)$$

Because the eigenvalues of σ_y are ± 1 , the eigenvalues of Θ are

$$\lambda_{\pm} = e^{\pm\alpha} > 0.$$

This means that Θ is strictly positive definite and defines a new physical inner product in $\mathcal{H}^{(2)}$,

$$(\psi, \phi)_{\text{phys}} = \langle \psi | \Theta | \phi \rangle. \quad (9)$$

Next, applying the Baker–Campbell–Hausdorff formula, one can readily verify that

$$\Omega^{-1}\sigma_x\Omega = \sigma_x \cosh \alpha + i\sigma_z \sinh \alpha, \quad \Omega^{-1}\sigma_z\Omega = \sigma_z \cosh \alpha - i\sigma_x \sinh \alpha. \quad (10)$$

Should we identify

$$\kappa = \omega \cosh \alpha, \quad \gamma = \omega \sinh \alpha, \quad (11)$$

and, vice versa,

$$\omega^2 = \kappa^2 - \gamma^2, \quad \tanh \alpha = \frac{\gamma}{\kappa}, \quad (12)$$

one may recall Eq. (3) and find that

$$H = \Omega^{-1}\mathfrak{h}\Omega = \omega\Omega^{-1}\sigma_x\Omega = \omega(\sigma_x \cosh \alpha + i\sigma_z \sinh \alpha) = \kappa\sigma_x + i\gamma\sigma_z. \quad (13)$$

This defines a new Hamiltonian, which can be expressed in its final matrix form,

$$H = \begin{pmatrix} i\gamma & \kappa \\ \kappa & -i\gamma \end{pmatrix}, \quad \gamma, \kappa \in \mathbb{R}. \quad (14)$$

One immediately recognizes that the resulting matrix is non-Hermitian but $\mathcal{PT}$ -symmetric (parity-time symmetric; see, e.g., Refs. [21, 22, 23] for broader physical context). At $\gamma = \kappa$, it exhibits the so-called exceptional-point singularity (EP, see Ref. [24]), at which the system loses its observability. This phenomenon has been described as a manifestation (or as a witness) of a “quantum

catastrophe” [25] or of a “quantum phase transition” [26], arising from the characteristic [27, 28, 29] simultaneous degeneracies of both the eigenvalues and the eigenvectors.

Further discussion of this theoretical and phenomenological peculiarity can be found, for example, in dedicated papers [30] – [38]. In this context, it is worth noting that the transition from the Hermitian toy-model Hamiltonian (6) to its non-Hermitian counterpart (14) enabled not only a consistent theoretical interpretation of the corresponding spectrum but also its experimental realization. Indeed, the non-Hermitian matrix (14) has found a widely adopted implementation in classical optics, where it describes, e.g., a $\mathcal{PT}$ -symmetric optical dimer [22].

3 Revisiting the Dyson’s model-building strategy through an inversion of the map

The simplicity of the example outlined above allows one to revisit the philosophy and, in the spirit of the early review [4], to invert the map (3). With the Hamiltonian (14) now introduced *a priori*, we would like to emphasize the distinction, so we will denote the preselected candidate for the Hamiltonian by a dedicated tilded upper-case symbol $\tilde{H}$.

Once we adopt this inverse-Dyson model-building strategy, the first task is to verify that the eigenvalues of the preselected $\tilde{H}$ are real. Fortunately, in our example, this is immediately seen to hold for $|\gamma| < \kappa$. At the same time, the condition $|\gamma| < \kappa$ ensures that α is real, so that both the non-unitary Dyson-map matrix (7) and the associated inner-product metric (8) are invertible.

One of the characteristic features of any “tilded-Hamiltonian” generalization of the theory is that the construction of models does not begin with Hamiltonian $\mathfrak{h}$ or with the map (3). Instead, one assumes that the (tilded) non-Hermitian (or, more precisely, quasi-Hermitian) upper-case candidate $\tilde{H}$ for the Hamiltonian is given directly; see, for example, the comprehensive reviews [4] or [7] for an explanation of such a quasi-Hermiticity-based approach.

The resulting updated theoretical framework may be viewed as an eligible equivalent reformulation of the standard textbook quantum mechanics. In this reformulation, typically, the physics-motivated ansatz (1) is replaced by its tilded analogue

$$\tilde{H} = \tilde{H}_{(\text{free motion})} + \tilde{H}_{(\text{non-Hermitian interaction})} \neq \tilde{H}^\dagger, \quad (15)$$

i.e., by its non-equivalent, mathematically motivated alternative.

An illustrative example of the change of paradigm can be found, for instance, in Ref. [16]. Buslaev and Grecchi (BG) studied there a truly remarkable non-Hermitian ordinary-differential “minus-quartic” anharmonic oscillator model, employing the conventional kinetic-energy term

$$\widetilde{H^{(\text{BG})}}_{(\text{free motion})} = -\frac{1}{2} \frac{d^2}{dx^2}$$

complemented by an asymptotically repulsive local interaction,

$$\widetilde{H^{(\text{BG})}}_{(\text{non-Hermitian interaction})}(g, j, \epsilon) = \frac{j^2 - 1}{8(x - i\epsilon)^2} + \frac{1}{2}(x - i\epsilon)^2 - g^2(x - i\epsilon)^4. \quad (16)$$

Regarding this truly anomalous toy model, which is constructed in the entirely conventional Hilbert space $L^2(\mathbb{R})$, the authors were the first who emphasized that their oscillator is time-reversal-parity symmetric ($\mathcal{TP}$ -symmetric; see Remark 4 in Ref. [16]), i.e., in the equivalent but more popular above-mentioned newer terminology, $\mathcal{PT}$ -symmetric.

In Ref. [16], Buslaev and Grecchi also constructed, in a closed and ϵ -independent form, one of the self-adjoint isospectral tilded twins $\widetilde{\mathfrak{h}}^{(\text{BG})}(g, j)$ of $\widetilde{H^{(\text{BG})}}(g, j, \epsilon)$ which turned out to be compatible with the conventional textbook requirement (1) (see the paper for details). Their tilded-Hamiltonian model remains exceptional, since, naturally, the simultaneous knowledge of the initial Hamiltonian and of its Hermitian isospectral twin having the conventional form of Eq. (1) resolves all questions regarding the correct physical probabilistic interpretation of the underlying quantum system.

Nontrivial and challenging interpretational questions arise only in the study of systems for which the resulting Hermitian $\widetilde{\mathfrak{h}}$ becomes complicated (i.e., typically, non-local). In the present paper, we therefore focus on such dynamical scenarios and non-exceptional, generic models in which one must work directly with $\widetilde{H}$, since its Hermitian twin $\widetilde{\mathfrak{h}}$ is far from being user-friendly [7, 39]. Accordingly, our present results can be viewed as an explicit clarification of the problem of the standard probabilistic interpretation of experiments within the framework of the general tilded-Hamiltonian theory.

Several complementary remarks on tilded Hamiltonians and on the associated quasi-Hermitian quantum mechanics (QHQM) as reviewed in Refs. [4, 7] are now in order. First, it should be noted that the new form of the input information about the unitary quantum dynamics implied that the users of the tilded-Hamiltonian models had to provide a rigorous—and often nontrivial—proof that the bound-state energy eigenvalue spectra are real. For many operators $\widetilde{H}$, such proofs required the application of sophisticated mathematical techniques (cf., e.g., examples in Ref. [40]). Moreover, even the formally real spectrum can happen to be fragile or, at least, strongly sensitive to the small changes of parameters [41].

Secondly, instead of the correspondence given in Eq. (3), one should rather refer to the Buslaev-inspired [42] inverted reconstruction,

$$\widetilde{H} \rightarrow \widetilde{\mathfrak{h}} = \Omega \widetilde{H} \Omega^{-1} = \widetilde{\mathfrak{h}}(\Omega). \quad (17)$$

This brings us back to the textbook framework, with the key advantage that such a map restores the path toward the standard probabilistic interpretation of all general observability aspects, both for bound states (in the case of discrete spectrum) and/or for scattering states (cf. Refs. [43, 44]).

Thirdly, the transition from the physics-motivated ansatz (1) to its mathematics-motivated analogue (15) has narrowed the phenomenological scope of the theory, especially for a generic

initial $\tilde{H}$ chosen, typically, in the mere ordinary differential-operator form. In parallel, such a reduction of the class of models encouraged a perceivable intensification of the study of related mathematics [40, 45, 46].

4 Hiddenly Hermitian Hamiltonians: An example

For illustrative purposes, let us now recall the QHQM model of Ref. [37], in which the initial introduction of the primary, manifestly non-Hermitian (i.e., tilded, upper-case) Hamiltonian $\tilde{H}$ was perceived as a fermionic analogue of the widely studied bosonic Swanson oscillator [47]. Its Hamiltonian

$$\tilde{H} = \omega_1 c_1^\dagger c_1 + \omega_2 c_2^\dagger c_2 + \beta c_1^\dagger c_2^\dagger + \alpha c_2 c_1 \quad (18)$$

with positive $\omega_{1,2} > 0$ and with the two real parameters $\alpha \neq \beta$ (so that $H \neq H^\dagger$) involves the fermionic annihilation operators c_1 and c_2 which satisfy the canonical anti-commutation relations,

$$\{c_j, c_k^\dagger\} = \delta_{jk}, \quad \{c_j, c_k\} = 0 = \{c_j^\dagger, c_k^\dagger\}, \quad j, k = 1, 2. \quad (19)$$

This model can be viewed as a two-site truncation of the Kitaev chain [48, 49] in the absence of inter-site hopping but with superconducting-type pairing interactions made non-Hermitian by the choice of distinct real $\alpha \neq \beta$.

Denoting the vacuum state by $|0\rangle$, we have

$$c_1|0\rangle = 0, \quad c_2|0\rangle = 0. \quad (20)$$

The fermionic Fock space decomposes as

$$\mathcal{H}^{(4)} = \mathcal{H}_0^{(1)} \oplus \mathcal{H}_1^{(2)} \oplus \mathcal{H}_2^{(1)} \quad (21)$$

with

$$\mathcal{H}_0^{(1)} = \text{span}\{|0\rangle\}, \quad \mathcal{H}_1^{(2)} = \text{span}\{c_1^\dagger|0\rangle, c_2^\dagger|0\rangle\}, \quad \mathcal{H}_2^{(1)} = \text{span}\{c_1^\dagger c_2^\dagger|0\rangle\}. \quad (22)$$

Introducing the ordered basis

$$|1\rangle = |0\rangle, \quad |2\rangle = c_1^\dagger|0\rangle, \quad |3\rangle = c_2^\dagger|0\rangle, \quad |4\rangle = c_1^\dagger c_2^\dagger|0\rangle, \quad (23)$$

and choosing

$$\omega_1 = \omega, \quad \omega_2 = 1 - \omega, \quad \omega \in (0, 1), \quad (24)$$

a straightforward application of the anti-commutation relations yields

$$\tilde{H}|1\rangle = \beta|4\rangle, \quad \tilde{H}|2\rangle = \omega|2\rangle, \quad \tilde{H}|3\rangle = (1 - \omega)|3\rangle, \quad \tilde{H}|4\rangle = \alpha|1\rangle + |4\rangle. \quad (25)$$

In this basis, the 4×4 matrix representation of $\tilde{H}$ is

$$\tilde{H} = \begin{pmatrix} 0 & 0 & 0 & \alpha \\ 0 & \omega & 0 & 0 \\ 0 & 0 & (1 - \omega) & 0 \\ \beta & 0 & 0 & 1 \end{pmatrix} \quad (26)$$

which is non-Hermitian whenever $\alpha \neq \beta$, even though all parameters are real.

In view of Eq. (17), we now seek a Hermitian Hamiltonian $\tilde{\mathfrak{h}}$ and a Dyson map Ω such that

$$\tilde{H} = \Omega^{-1} \tilde{\mathfrak{h}} \Omega. \quad (27)$$

Assuming $\alpha\beta > 0$, one can readily verify that one of the valid isospectral twins of $\tilde{H}$ is

$$\tilde{\mathfrak{h}} = \begin{pmatrix} 0 & 0 & 0 & \sqrt{\alpha\beta} \\ 0 & \omega & 0 & 0 \\ 0 & 0 & (1 - \omega) & 0 \\ \sqrt{\alpha\beta} & 0 & 0 & 1 \end{pmatrix}. \quad (28)$$

This matrix is Hermitian and comprises a coupled two-level subsystem in the $\{|1\rangle, |4\rangle\}$ sector with real coupling $\sqrt{\alpha\beta}$, along with two decoupled eigenstates, $|2\rangle$ and $|3\rangle$, having eigenvalues ω and $1 - \omega$, respectively.

Among the available Dyson maps, one can now be particularly easily constructed in its inverse-matrix form

$$\Omega^{-1} = \begin{pmatrix} 1 & 0 & 0 & (\alpha - \sqrt{\alpha\beta}) \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ (\sqrt{\alpha\beta} - \beta) & 0 & 0 & 1 \end{pmatrix}. \quad (29)$$

The determinant of Ω^{-1} is

$$\mathcal{D} = \det(\Omega^{-1}) = 2\alpha\beta - (\alpha + \beta)\sqrt{\alpha\beta} + 1, \quad (30)$$

so that Ω exists and is invertible, provided that $\mathcal{D} \neq 0$. Noting also that this matrix is real, so that $\Omega^\dagger = \Omega^T$, a straightforward calculation yields

$$\Theta(\alpha, \beta) = \begin{pmatrix} \frac{(\beta - \sqrt{\alpha\beta})^2 + 1}{\mathcal{D}^2} & 0 & 0 & \frac{\beta - \alpha}{\mathcal{D}^2} \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \frac{\beta - \alpha}{\mathcal{D}^2} & 0 & 0 & \frac{(\alpha - \sqrt{\alpha\beta})^2 + 1}{\mathcal{D}^2} \end{pmatrix}, \quad (31)$$

i.e., the physical inner-product metric is given in a closed, compact, and sparse-matrix form.

5 Towards a classification of the Dyson-map operators

Given any “input-information” operator $\tilde{H}$ within the QHQM framework, we will henceforth drop the tildes. We will also refrain from distinguishing between the directions of the isospectrality-mapping arrows in the Dyson-inspired Eq. (3) and its inverse (17) (cf. Table 1). It should be kept in mind that what is assumed to be known in advance is solely the quasi-Hermitian operator H representing the observable energy Hamiltonian.

Table 1: Two alternative choices of the Hamiltonian

symbol	definition	self-adjoint	interpretation	example
$\mathfrak{h}$	Eq. (1)	yes	conventional	Dyson [2]
H	Eq. (15)	no	via twin $\mathfrak{h}$	Buslaev [42]

5.1 The search for special, diagonal $\mathfrak{h} = \mathfrak{h}_I$

If we restrict our attention to the relationship between theory and measurement in closed quantum systems that support N -plets of non-degenerate, stable bound states (with N finite or infinite, $N \leq \infty$), it becomes sufficient to consider Schrödinger equation

$$H |\psi_n\rangle = E_n |\psi_n\rangle, \quad n = 1, 2, \dots, N \quad (32)$$

and, due to the non-Hermiticity $H \neq H^\dagger$, also its conjugate version

$$H^\dagger |\psi_n\rangle\rangle = E_n |\psi_n\rangle\rangle, \quad n = 1, 2, \dots, N \quad (33)$$

in which we used the notation convention of Ref. [6], i.e., the double-ket symbol for the right eigenvectors of $H^\dagger$ (and, if needed, also its double-bra alternative $\langle\langle\psi_n|$ for their conjugates).

In both of these equations, the normalization of the eigenvectors may be chosen arbitrarily but kept fixed. Once fixed, the set of all column vectors $|\psi_n\rangle\rangle$ can be concatenated and interpreted as an $N \times N$ matrix [50],

$$\{|\psi_1\rangle\rangle, |\psi_2\rangle\rangle, \dots, |\psi_N\rangle\rangle\} := \Omega_I^\dagger. \quad (34)$$

Subsequently, a comparison of Eq. (33) with Eq. (3)—or with Eq. (17), keeping in mind that we now ignore the tildes—reveals a remarkable conclusion: the matrix $\Omega_I^\dagger$ of Eq. (34) is precisely the Hermitian conjugate of the Dyson map that renders the Hermitian avatar of H diagonal.

The latter map as well as the Hermitian avatar of H may be I -subscripted, so we have

$$(\mathfrak{h}_I)_{nn} = E_n, \quad n = 1, 2, \dots, N, \quad N \leq \infty. \quad (35)$$

In this matrix, all of the eigenvalues of H , or equivalently of $H^\dagger$, appearing on its diagonal are real.

5.2 A broader class of Dyson maps

The above construction makes it clear that the resulting operator Ω_I is not unique. Many other Dyson maps may exist. The reason is that, at every index n , Eq. (33) remains unchanged under multiplication by any real or complex constant $\kappa_n \neq 0$. So, a different concatenation (34) would result. Consequently, we may introduce a diagonal and invertible matrix K (whose diagonal entries are precisely these constants) and define the product

$$\Omega_K = K^\dagger \Omega_I, \quad (36)$$

i.e., the equally admissible Dyson-map operator, which is parametrized by the K matrix (and, correspondingly, carrying the K -matrix subscript). Thus, the Dyson map Ω_I of the preceding paragraph (carrying the I subscript corresponding to the identity matrix) can be viewed as the mere special $K = I$ case of a more general N -parametric family (36).

Two immediate conclusions can be drawn. First, a change in K implies a change in the inner product metric in general [cf. Eq. (4)],

$$\Theta = \Theta_K = \Omega_K^\dagger \Omega_K = \Omega_I^\dagger K K^\dagger \Omega_I \neq \Theta_I = \Omega_I^\dagger \Omega_I. \quad (37)$$

Second, as long as

$$\mathfrak{h}_K = K^\dagger \mathfrak{h}_I (K^\dagger)^{-1} = \mathfrak{h}_I, \quad (38)$$

none of the different K -subscripted metrics leads to a violation of diagonality of the Hermitian-matrix twin $\mathfrak{h}_I$ of our preselected non-Hermitian Hamiltonian H .

5.3 The most general form of the Dyson map

In the light of the illustrative example of Buslaev and Grecchi [16], given by Eq. (16), it becomes clear that even the most elementary diagonal matrix $\mathfrak{h}_K = \mathfrak{h}_I$ need not, in fact, be the preferred choice for the Hermitian isospectral twin of H . Indeed, if any (not necessarily diagonal) matrix $\mathfrak{h}$ is to serve as the background for a meaningful probabilistic interpretation of the quantum system in question, its optimal form may, in general, be merely a suitable unitary transformation of $\mathfrak{h}_I$,

$$\mathfrak{h} = \mathcal{U} \mathfrak{h}_I \mathcal{U}^\dagger := \mathfrak{h}[\mathcal{U}], \quad \mathcal{U}^{-1} = \mathcal{U}^\dagger. \quad (39)$$

The authors of Ref. [16] provided a clear and explicit example

$$\mathfrak{h}^{(\text{BG})} = -\frac{d^2}{dy^2} + y^2 (gy - 1)^2 - j (gy - 1/2) \quad (40)$$

of such an optimal, albeit non-diagonal, operator $\mathfrak{h}[\mathcal{U}]$ which depends on a nontrivial $\mathcal{U} \neq I$.

For our illustrative example in Eq. (40), both the probabilistic interpretation and the stable bound-state nature of the eigenstates of this self-adjoint double-well Hamiltonian are standard.

Consequently, for conceptual and interpretational purposes alone, diagonalizing operator (40) would be, from the correct interpretation point of view, entirely superfluous.

In similar cases, it may easily happen that the diagonalization $\mathcal{U} : \mathfrak{h} \rightarrow \mathfrak{h}_I$ is only approximate. Again, for a physically meaningful interpretation of the system, reconstructing $\mathcal{U}$ (which might be purely numerical) is entirely redundant. Thus, we may conclude that in addition to the constructions of the Dyson map $\Omega = \Omega_I$ [cf. Eqs. (34) and (33)] and of its K -reparametrized descendants $\Omega = \Omega_K$ [cf. Eq. (36)], it remains for us to consider the third class of the Dyson maps

$$\Omega_{K\mathcal{U}} = \mathcal{U} K^\dagger \Omega_I \quad (41)$$

characterizing the physics behind models with nontrivial $\mathcal{U} \neq I$, i.e., with both the K - and $\mathcal{U}$ -parametrized family of the fully general Dyson maps (cf. the ultimate classification scheme in Table 2).

Table 2: Three alternative choices of variable parameters.

parameters	Dyson map Ω	Hermitization of H	metric Θ
-	Ω_I	$\mathfrak{h}_I$	Θ_I
K	$K^\dagger \Omega_I = \Omega_K$	$\mathfrak{h}_I$	Θ_K
$K, \mathcal{U}$	$\mathcal{U} K^\dagger \Omega_I = \Omega_{K\mathcal{U}}$	$\mathcal{U} \mathfrak{h}_I \mathcal{U}^\dagger = \mathfrak{h}[\mathcal{U}]$	Θ_K

6 Discussion

6.1 Complete sets of independent quasi-Hermitian observables

A generic quantum model is usually characterized not only by its Hamiltonian but also by a number of additional observables. For example, in Ref. [39], the authors considered a QHQM model with a non-Hermitian Hamiltonian $H \neq H^\dagger$ and with a non-Hermitian particle-position operator $X \neq X^\dagger$. Although the necessity and feasibility of similar extensions of the theory were already discussed by Scholtz et al. [4], only a few implementations of such an idea appear in the literature.

The reasons are far from obvious, and not too many authors have noticed that under the quasi-Hermiticity constraint (5), the simultaneous H - and K -dependence of the inner-product metric Θ [cf. Eqs. (33), (34), and (37)] strongly limits its compatibility with any other, independently chosen (preselected) non-Hermitian operator $A \neq A^\dagger$ having real spectrum [51]. Even the guarantee of compatibility of two preselected non-Hermitian observables H and A (with real spectra) is a nontrivial task requiring, in general, the full freedom and generality of the K - and $\mathcal{U}$ -dependent Dyson map as represented by Eq. (41) (cf. also the last line of Table 2).

By construction, the unitary-matrix factor $\mathcal{U}$ mediates only the diagonalization of the Hamiltonian $\mathfrak{h}$, but generally not that of the A -associated twin $\mathfrak{a}$. Consequently, for a fixed $\mathcal{U}$, any other linearly independent and admissible non-Hermitian (more precisely, Θ_K -quasi-Hermitian) candidate A for an independent observable must belong to a rather restricted family of eligible (i.e., probabilistically interpretable) Hermitian avatars

$$\mathfrak{a} = \mathcal{U} K^\dagger \Omega_I A \Omega_I^{-1} (K^\dagger)^{-1} \mathcal{U}^{-1}. \quad (42)$$

They are, in general, manifestly K - and $\mathcal{U}$ -dependent,

$$\mathfrak{a} = \mathfrak{a}_K[\mathcal{U}].$$

All of this holds unless the central matrix factor $\Omega_I A \Omega_I^{-1}$ in (42) is diagonal; that is, unless all of the eigenstates of $A^\dagger$ coincide with the eigenstates $|\psi_n\rangle\rangle$ of $H^\dagger$ as determined by the conjugate Schrödinger equation (33).

One can conclude that the general Hermitian Hamiltonian (39) remains independent of K [cf. Eq. (38)], while the general metric operator, due to Eq. (41), remains independent of the unitary matrix $\mathcal{U}$. Nevertheless, the two-matrix dependence (41) of the general Dyson map remains crucial, as it enlarges the class of admissible pairs of independent observables H and A .

6.2 Models in which the Dyson map is required Hermitian

The guarantee of compatibility between H and an independent A becomes trivial if we first choose H , construct a suitable metric $\Theta = \Theta(H)$, and then define the class of admissible A operators via the relation

$$A^\dagger \Theta = \Theta A = \mathcal{M} = \mathcal{M}^\dagger \quad (43)$$

in which the $N \times N$ Hermitian matrix $\mathcal{M}$ (with $N \leq \infty$) is treated as an input choice. This allows one to define all of the eligible observable $A = A(\mathcal{M})$ by the following explicit matrix-multiplication formula

$$A(\mathcal{M}) = \Theta^{-1} \mathcal{M} \quad (44)$$

in which the Hermitian matrix of parameters $\mathcal{M}$ is arbitrary.

In many applications, the theory is often complemented by an additional (and, in fact, entirely formal) requirement of having the Dyson map defined in the specific form of a Hermitian square root of the metric, i.e., such that $\Omega = \Omega^\dagger$: for a sample of such a purely mathematically motivated auxiliary postulate see Eq. (8) above. Within the context of our exhaustive classification of H -compatible Dyson maps $\Omega = \Omega(H)$ (cf. Table 2), such an optional Hermiticity condition imposes, in effect, a fairly nontrivial constraint upon the parameters, i.e., upon all of the matrix elements of $\mathcal{U}$ and, as a consequence, upon the class of the other, complementary eligible observables

$A = A(\mathcal{M})$. At the same time, the Hermiticity condition $\Omega = \Omega^\dagger$ remains tractable and can be satisfied when re-expressed in its $N \times N$ -matrix quadratic-equation form

$$\mathcal{U} \Omega_K \mathcal{U} = \Omega_K^\dagger. \quad (45)$$

The number of the unknown (real) parameters equals the number of the independent scalar constraints, so that the equation can generally be solved and specify the unitary matrix $\mathcal{U}$, in principle at least. Even in practice the recipe still seems to lead to a feasible construction, especially when the Hilbert-space dimension N remains finite and is not too large. Again, an elementary example of the result can be found here in section 2 above.

7 Summary

The Dyson-inspired non-Hermiticity-admitting simplification $\mathfrak{h} \rightarrow H \neq H^\dagger$ of a preselected Hermitian Hamiltonian [cf. Eq. (3)] is, from a purely physical and phenomenological point of view, trivial. In contrast, a truly nontrivial physical interpretation problem arises when one starts from a non-Hermitian H with a real spectrum. Indeed, the entirely formal decomposition of Eq. (17) can hardly be given a sound observable meaning without a clear reconstruction of its isospectral Hermitian twin.

In the present paper, we formulated and addressed this problem. We proposed that, in general, the reconstruction of $\mathfrak{h}$ can be classified as summarized in Table 2. In this scheme, increasing the flexibility of the process—that is, increasing the number of available free parameters that determine the complexity of the Dyson map and of the Hermitian avatar $\mathfrak{h}$ of H —naturally leads to a corresponding increase in the complexity of the correct physical probabilistic interpretations of the quantum system in question.

Our systematic analysis of the underlying mathematical structures was complemented by several illustrative examples, in which we emphasized the balance between the complexity of the model and its constructive tractability. On this basis, we conclude that once the parameters (i.e., the two finite or infinite matrices K and $\mathcal{U}$) are explicitly controlled, as ensured by our triple Dyson-map classification, the QHQM formalism is well suited to accommodate a wide range of current and future realistic applications.

A Introduction to Dyson-map theory ‘for pedestrians’: Definition, fundamental properties, and terminology

For the sake of clarity—especially for non-expert readers—we briefly recall the core definition and essential properties of the operators and terminology used throughout the present paper. Such an addendum provides an alternative summary of the QHQM theory presented from a slightly different, complementary point of view. For the sake of definiteness, the non-expert readers might assume that the Hilbert-space dimension is finite, $N < \infty$. Still, the word of warning is that only some of the related observations can readily be extended to hold at $N = \infty$ as well. In the latter case, indeed, the use of a more subtle mathematics may prove unavoidable (see, e.g., [40]).

In a finite- N reformulation of the theory, the *Dyson map* is *any* linear and invertible operator that “Hermitizes” a non-Hermitian Hamiltonian. Concretely, under certain purely technical assumptions concerning the given non-Hermitian Hamiltonian H with a real spectrum, a Dyson map Ω satisfies Eq. (3) as well as its inversion

$$\mathfrak{h} = \Omega H \Omega^{-1} \tag{A1}$$

with this operator required to be Hermitian, $\mathfrak{h} = \mathfrak{h}^\dagger$. The Dyson map defines the physical inner product (metric) in the original Hilbert space $\mathcal{H}^{(N)}$ by formula (4), i.e.,

$$\Theta = \Omega^\dagger \Omega. \tag{A2}$$

This corresponds to the fact that H is Θ -quasi-Hermitian (cf. Eq. (5)):

$$H^\dagger \Theta = \Theta H. \tag{A3}$$

Thus, the essential properties of the QHQM theory may be summarized as follows.

- Hermitization: Ω establishes an isospectral equivalence between the non-Hermitian H and the Hermitian twin $\mathfrak{h}$, hence both share the same energy spectrum.
- Unitary evolution: Time evolution generated by H is unitary with respect to the inner product defined by Θ .
- Observables: An operator A is a physical observable in the same representation iff it is Θ -quasi-Hermitian: $A^\dagger \Theta = \Theta A$. Equivalently, its Hermitian avatar is $\mathfrak{a} = \Omega A \Omega^{-1}$.
- Non-uniqueness: The Dyson map is not unique; different choices of Ω may yield different inner-product metrics $\Theta = \Theta_K$ and therefore different physical interpretations of the unitary quantum system in question.

As we have emphasized in the main text, different constructions of Ω lead to non-equivalent probabilistic interpretations of the observables H and A , etc. More explicitly, this is an observation which has been discussed in section 6 and summarized in Table 2. It also underlies the classification of admissible Dyson maps and metrics. Naturally, this is a formal ambiguity with many immediate consequences in applications. *Pars pro toto*, let us mention that recently, the concept of the Dyson map was also proposed to play the role of a (generalized) vielbein [52], highlighting the connection between the QHQM formalism and the standard vielbein approach widely used in many areas of physics, including general relativity, supergravity, and superstring theory.

Remark on terminology: In this paper we use the terms Hermitian avatar and isospectral twin of a non-Hermitian Hamiltonian H . Specifically, a *Hermitian avatar* of H is the Hermitian operator $\mathfrak{h}$ defined by Eq. (A1) with a Dyson map Ω . It represents the same quantum system as H , but expressed in the standard Hilbert-space inner product. Moreover, an *isospectral twin* emphasizes that H and $\mathfrak{h}$ share the same spectrum, $\text{spec}(H) = \text{spec}(\mathfrak{h})$, and are related by a (typically, non-unitary) similarity transformation. Thus the Hermitian avatar $\mathfrak{h}$ is simultaneously the *isospectral twin* of the non-Hermitian Hamiltonian H .

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