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PSEUDO-HERMITIAN REPRESENTATION OF QUANTUM MECHANICS

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A diagonalizable non-Hermitian Hamiltonian having a real spectrum may be used to define a unitary quantum system, if one modifies the inner product of the Hilbert space properly. We give a comprehensive and essentially self-contained review of the basic ideas and techniques responsible for the recent developments in this subject. We provide a critical assessment of the role of the geometry of the Hilbert space in conventional quantum mechanics to reveal the basic physical principle motivating our study. We then offer a survey of the necessary mathematical tools, present their utility in establishing a lucid and precise formulation of a unitary quantum theory based on a non-Hermitian Hamiltonian, and elaborate on a number of relevant issues of fundamental importance. In particular, we discuss the role of the antilinear symmetries such as $\mathcal{PT}$, the true meaning and significance of the so-called charge operators $\mathcal{C}$ and the $\mathcal{CPT}$-inner products, the nature of the physical observables, the equivalent description of such models using ordinary Hermitian quantum mechanics, the pertaining duality between local-non-Hermitian versus nonlocal-Hermitian descriptions of their dynamics, the corresponding classical systems, the pseudo-Hermitian canonical quantization scheme, various methods of calculating the (pseudo-) metric operators, subtleties of dealing with time-dependent quasi-Hermitian Hamiltonians and the path-integral formulation of the theory, and the structure of the state space and its ramifications for the quantum Brachistochrone problem. We also explore some concrete physical applications and manifestations of the abstract concepts and tools that have been developed in the course of this investigation. These include applications in nuclear physics, condensed matter physics, relativistic quantum mechanics and quantum field theory, quantum cosmology, electromagnetic wave propagation, open quantum systems, magnetohydrodynamics, quantum chaos and biophysics.

Keywords: Pseudo-Hermitian; quasi-Hermitian; metric operator; unitary-equivalence; biorthonormal system; $\mathcal{PT}$-symmetry; projective space; complex potential; quantization; observable.

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Contents

1. Introduction and Overview

General Relativity (GR) and Quantum Mechanics (QM) are the most important achievements of the twentieth century theoretical physics. Their discovery has had an enormous impact on our understanding of Nature. Ironically, these two pillars of modern physics are incompatible both conceptually and practically. This has made their unification into a more general physical theory in the most fundamental problem of modern theoretical physics. The unification of Special Relativity and QM, which is by far an easier task, has been the subject of intensive research since late 1920's. It has led to the formulation of various quantum field theories. A most successful example is the Standard Model which provides a satisfactory description of all available observational data in high energy particle physics. In spite of the immensity of the amount of research activity on the subject and the fact that this is conducted by the most capable theoretical physicists of our times, the attempts at quantizing gravity have not been as successful. In fact, one can claim with confidence that these attempts have so far failed to produce a physical

theory offering concrete experimentally verifiable predictions. This state of affairs has, over the years, motivated various generalizations of GR and QM. Although none of these generalizations could be developed into a consistent physical theory capable of replacing GR or QM, the hope that they might facilitate the discovery of a unified theory of quantum gravity still motivates research in this direction.

The development of the special relativistic quantum theories has also involved attempts at generalizing QM. Among these is an idea initially put forward by Dirac in 1942 [77] and developed by Pauli [190] into what came to be known as the *indefinite-metric* quantum theories [223, 183, 185]. This is a rather conservative generalization of QM in which one considers in addition to the physical states of the system a set of hypothetical states, called *ghosts*, whose function is mainly to improve the regularity properties of the mathematical description of the physical model. The indefinite-metric quantum theories lost their interest by mid-1970's and perhaps unfortunately never found a detailed coverage in standard textbooks on relativistic quantum mechanics and quantum field theory.[a]

A more recent attempt at generalizing QM is due to Bender and his collaborators [37, 38] who adopted all its axioms except the one that restricted the Hamiltonian to be Hermitian. They replaced the latter condition with the requirement that the Hamiltonian must have an exact $\mathcal{PT}$-symmetry. Here $\mathcal{P}$ and $\mathcal{T}$ are the parity and time-reversal operators whose action on position wave functions $\psi(x)$ is given by $(\mathcal{P}\psi)(x) := \psi(-x)$ and $(\mathcal{T}\psi)(x) := \psi(x)^*$.[b] The exact $\mathcal{PT}$-symmetry of a Hamiltonian operator H means that it has a complete set of $\mathcal{PT}$-invariant eigenvectors ψ_n, i.e. $\mathcal{PT}\psi_n = a_n\psi_n$ for some complex numbers a_n. This condition assures the reality of the spectrum of H. A class of thoroughly studied examples is provided by the $\mathcal{PT}$-symmetric Hamiltonians of the form

$$H_\nu = \frac{1}{2}p^2 - (ix)^\nu, \tag{1}$$

where ν is a real number not less than 2, and the eigenvalue problem for H_ν is defined using an appropriate contour Γ in the complex plane $\mathbb{C}$ which for $\nu < 4$ may be taken as the real line $\mathbb{R}$. A correct choice for Γ assures that the spectrum of H is discrete, real, and positive [32, 33, 79, 209, 157]. Another example with identical spectral properties is the $\mathcal{PT}$-symmetric cubic anharmonic oscillator,

$$H = \frac{1}{2}p^2 + \frac{1}{2}\mu^2x^2 + i\epsilon x^3, \tag{2}$$

whose coupling constants μ and ϵ are real and its eigenvalue problem is defined along the real axis ($\Gamma = \mathbb{R}$) [40, 158].

[a] In fact, Pauli who had made fundamental contributions to the very foundations of the subject had developed strong critical views against it. For example in his Nobel Lecture of 1946, he identifies a "correct theory" with one that does not involve "a hypothetical world" [191]. For a comprehensive critical assessment of indefinite-metric quantum field theories, see [185].

[b] We use asterisk to denote complex-conjugation.

This $\mathcal{PT}$-symmetric modification of QM leads to an indefinite-metric quantum theory [116, 225, 160], if one endows the Hilbert space with the indefinite inner product,

$$\langle \cdot \,|\, \cdot \rangle_{\mathcal{P}} := \langle \cdot \,|\, \mathcal{P} \cdot \rangle, \tag{3}$$

known as the $\mathcal{PT}$-inner product [37]. The symbol $\langle \cdot \,|\, \cdot \rangle$ that appears in (3) stands for the L^2-inner product: $\langle \phi \,|\, \psi \rangle := \int_\Gamma \phi(z)^* \psi(z) dz$ that defines the Hilbert space $L^2(\Gamma)$ of square-integrable functions $\psi : \Gamma \to \mathbb{C}$, where Γ is the contour in complex plane that specifies the $\mathcal{PT}$-symmetric model [157].

The main advantage of the indefinite inner product (3) over the positive-definite inner product $\langle \cdot \,|\, \cdot \rangle$ is that the former is invariant under the time-evolution generated by the Schrödinger equation [240, 143, 155], i.e. if $\phi(t)$ and $\psi(t)$ are solutions of the Schrödinger equation for the $\mathcal{PT}$-symmetric Hamiltonian H, $\langle \phi(t) \,|\, \psi(t) \rangle_{\mathcal{P}}$ does not depend on time.

In order to employ the standard formulation of indefinite metric quantum theories [183] for a $\mathcal{PT}$-symmetric model we proceed as follows [116].

(1) We split the space $\mathcal{H}$ of state-vectors into the subspaces $\mathcal{H}_\pm := \{\psi \in \mathcal{H} \,|\, \mathrm{sgn}(\langle \psi \,|\, \psi \rangle_{\mathcal{P}}) = \pm\}$, where $\mathrm{sgn}(a) := \frac{a}{|a|}$ if a is a nonzero real number and $\mathrm{sgn}(0) := 0$. $\mathcal{H}_\pm$ are orthogonal subspaces in the sense that for all $\psi_\pm \in \mathcal{H}_\pm$, $\langle \psi_- \,|\, \psi_+ \rangle_{\mathcal{P}} = 0$.[c]

(2) We impose a superselection rule that forbids interactions mixing the elements of $\mathcal{H}_-$ and $\mathcal{H}_+$ and try to devise a solution for the difficult problem of providing a physical interpretation of the theory [183, 185]. The simplest way of dealing with this problem is to identify the elements of $\mathcal{H}_+$ with physical state-vectors [230, 110] and effectively discard the rest of state-vectors as representing unphysical or ghost states.

An alternative formulation of the theory that avoids the interpretational difficulties of indefinite-metric theories is the one based on the construction of a genuine positive-definite inner product on $\mathcal{H}$. This construction was initially obtained in [144] as a by-product of an attempt to derive a necessary and sufficient condition for the reality of the spectrum of a general Hamiltonian operator H that possesses a complete set of eigenvectors [143–145]. Under the assumption that the spectrum of H is discrete, one can show that it is real if and only if there is a positive-definite inner product $\langle \cdot \,|\, \cdot \rangle_+$ that makes it Hermitian, i.e. $\langle \cdot \,|\, H \cdot \rangle_+ = \langle H \cdot \,|\, \cdot \rangle_+$ [144, 145]. The proof of this statement involves an explicit construction of $\langle \cdot \,|\, \cdot \rangle_+$. This inner product depends on the choice of the Hamiltonian through its eigenvectors. Hence it is not unique [146, 148, 93, 162].

[c]The assumption of the existence of such an orthogonal decomposition is referred to as "decomposability" of the model in indefinite-metric theories [183]. For $\mathcal{PT}$-symmetric systems considered in the literature, this assumption is valid if there is a complete basis of common eigenvectors of the Hamiltonian and $\mathcal{PT}$.

In [37] the authors propose a different approach to the problem of identifying an appropriate inner product for the $\mathcal{PT}$-symmetric Hamiltonians such as (1). They introduce a generic symmetry of these Hamiltonians which they term as $\mathcal{C}$-symmetry and construct a class of positive-definite inner products, called the *$\mathcal{CPT}$-inner products*, that, as we show in Subsec. 3.4, turn out to coincide with the inner products $\langle\cdot\,|\,\cdot\rangle_+$ [148, 157]. The approach of [37] may be related to a much older construction originally proposed in the context of the indefinite-metric quantum theories [183, 185]. It involves the following two steps.

(1) Suppose that $\mathcal{H}=\mathcal{H}_+\oplus\mathcal{H}_-$ where $\mathcal{H}_\pm$ are the orthogonal subspaces we defined above, and that both $\mathcal{H}_\pm$ admit a basis consisting of the eigenvectors of H.
(2) Let $\Pi:\mathcal{H}\to\mathcal{H}$ be the projection operator onto $\mathcal{H}_+$, so that for all $\psi\in\mathcal{H}$, $\psi_+:=\Pi\psi\in\mathcal{H}_+$ and $\psi_-:=\psi-\psi_+\in\mathcal{H}_-$. Clearly $\Pi^2=\Pi$ and $\Pi\psi_-=0$.
(3) Endow $\mathcal{H}$ with the positive-definite inner product: $(\phi,\psi):=\langle\phi_+\,|\,\psi_+\rangle_{\mathcal{P}}-\langle\phi_-\,|\,\psi_-\rangle_{\mathcal{P}}$.
(4) Let $\mathcal{C}:\mathcal{H}\to\mathcal{H}$ be defined by $\mathcal{C}\psi:=\psi_+-\psi_-$. Then, in view of the orthogonality of $\mathcal{H}_\pm$,

$$(\phi,\psi)=\langle\phi\,|\,\mathcal{C}\psi\rangle_{\mathcal{P}}=\langle\mathcal{C}\phi\,|\,\psi\rangle_{\mathcal{P}}. \tag{4}$$

It is not difficult to see that $\mathcal{C}=2\Pi-I$, where I stands for the identity operator acting in $\mathcal{H}$, i.e. the operator that leaves all the elements of $\mathcal{H}$ unchanged. Obviously for all $\psi\in\mathcal{H}_\pm$, $\mathcal{C}\psi=\pm\psi$. Hence, $\mathcal{C}$ is a grading operator associated with the direct sum decomposition $\mathcal{H}=\mathcal{H}_+\oplus\mathcal{H}_-$ of $\mathcal{H}$. Furthermore, in view of the assumption (1) above, the eigenvectors of H have a definite grading. This is equivalent to the condition that $\mathcal{C}$ commutes with the Hamiltonian operator, $[\mathcal{C},H]=0$ [8]. It turns out that the $\mathcal{CPT}$-inner product introduced in [37] coincides with the inner product (4).

In [37, 38], the authors use the $\mathcal{CPT}$-inner product to formulate a unitary quantum theory based on the $\mathcal{PT}$-symmetric Hamiltonians (1). They identify the observables O of the theory with the $\mathcal{CPT}$-symmetric operators,[d] in particular

$$\mathcal{CPT}O\mathcal{CPT}=O. \tag{5}$$

This definition is motivated by the demand that the structure of the theory must not involve mathematical operations such as Hermitian conjugation and be determined only using physical conditions. The definition (5) does fulfil this demand,[e] but it

[d] To ensure that the spectrum of such a $\mathcal{CPT}$-symmetric operator O is real, one demands that O has an exact $\mathcal{CPT}$-symmetry, i.e. its eigenstates are left invariant under the action of $\mathcal{CPT}$. This does not however ensure the completeness of the eigenvectors of O.

[e] The authors of [37] emphasize this point by stating that: "In effect, we replace the mathematical condition of Hermiticity, whose physical content is somewhat remote and obscure, by the physical condition of space-time and charge-conjugation symmetry." One must note however, that in this theory, the usual coordinate operator x no longer represents a physical observable. As a result $\mathcal{P}$ does not affect a reflection in the physical space, and there is no reason why one should still refer to $\mathcal{PT}$-symmetry as the physical "space-time reflection symmetry" as done in [37, 38].

suffers from a serious dynamical inconsistency in the sense that in the Heisenberg picture an operator $O(t) := e^{itH}O(0)e^{-itH}$ that commutes with $\mathcal{CPT}$ at $t = 0$ may not commute with this operator at $t > 0$. Therefore, in general, under time-evolution an observable can become unobservable [152, 153]! This inconsistency rules out (5) as an acceptable definition of a physical observable. As noticed in [39, 42], it can be avoided, if one replaces the symmetry condition (5) with:

$$\mathcal{CPT}O\mathcal{CPT} = O^T, \tag{6}$$

where all operators are identified with their matrix representation in the coordinate-basis and O^T stands for the transpose of O. In particular, $\langle x|O^T|x'\rangle := \langle x'|O|x\rangle$.

The presence of the mathematical operation of transposition in (6) shows that apparently the theory could not be defined just using "the physical condition of space-time and charge-conjugation symmetry" as was initially envisaged [37, 38]. Note also that (6) puts an implicit and difficult-to-justify restriction on the Hamiltonian H. Being an observable commuting with $\mathcal{CPT}$, H must satisfy $H^T = H$, i.e. it is necessarily symmetric![f] Therefore (6) cannot be used to determine the observables of a theory that has a nonsymmetric Hamiltonian. The restriction to symmetric Hamiltonians may be easily lifted, if one is willing to adopt the conventional definition of the observables, namely identifying them with the operators that are Hermitian with respect to the $\mathcal{CPT}$-inner product [152, 154].

$$(\cdot, O\cdot) = (O\cdot, \cdot). \tag{7}$$

Indeed this definition is forced upon us by a well-known mathematical theorem that we present in a detailed proof of the Appendix. It states that *if a linear operator O has real expectation values computed using a given inner product, then O is necessarily Hermitian with respect to this inner product*. This shows that the requirement of the Hermiticity of observables, and in particular, the Hamiltonian has a simple "physical" justification.[g]

An important motivation for considering this so-called *$\mathcal{PT}$-symmetric Quantum Mechanics* is provided by an interesting idea that is rooted in special relativistic local quantum field theories (QFT). Among the most celebrated results of QFT is the C$\mathcal{PT}$-theorem. It states that every field theory satisfying the axioms of QFT is C$\mathcal{PT}$-invariant [98], where C is the charge-conjugation operator. Clearly replacing the axiom that the Hamiltonian is Hermitian with the statement of the C$\mathcal{PT}$-theorem might lead to a generalization of QFT. The implementation of this idea in a nonrelativistic setting corresponds to the requirement that the Hamiltonian possesses an exact $\mathcal{PT}$-symmetry. This in turn allows for the construction of a $\mathcal{C}$-operator that similarly to the charge-conjugation operator C of QFT squares to identify and generate a symmetry of the system. The idea that this establishes a nonrelativistic analog of the C$\mathcal{PT}$-theorem is quite tempting. Yet there

[f] In mathematical literature, the term "symmetric operator" is usually used for a different purpose, as discussed in footnote s below. To avoid possible confusion we will not adopt this terminology.
[g] What is however not dictated by this requirement is the choice of the inner product.

are clear indications that this is not really the case. For example, unlike the charge-conjugation operator of QFT, $\mathcal{C}$ depends on the choice of the Hamiltonian. It turns out that in fact this operator does not play the role of the relativistic charge-conjugation operator, it is merely a useful grading operator for the Hilbert space.[h] In this sense, the adopted terminology is rather unfortunate.

One of the aims of the present article is to show that $\mathcal{PT}$-symmetric QM is an example of a more general class of theories, called *pseudo-Hermitian Quantum Mechanics*, in which $\mathcal{PT}$-symmetry does not play a basic role and one does not need to introduce a $\mathcal{C}$-operator to make the theory well-defined. The analogs of $\mathcal{PT}$ and $\mathcal{C}$ operators can nevertheless be defined in general [148], but they do not play a fundamental role. All that is needed is to determine the class of non-Hermitian Hamiltonians that are capable of generating a unitary evolution and a procedure that associates to each member of this class a positive-definite inner product that renders it Hermitian. It turns out that there are always an infinite class of positive-definite inner products satisfying this condition. Each of these defines a separate physical Hilbert space with a complete set of observables. In this way one obtains a set of quantum systems that have the same Hamiltonian but different Hilbert spaces. Therefore, they are dynamically equivalent but kinematically distinct.

In order to elucidate the conceptual foundations of pseudo-Hermitian QM we will next examine some of the basic properties of the mathematical notions of the "transpose" and "Hermitian-conjugate" of a linear operator. For clarity of the presentation we will only consider the operators that act in the space of square-integrable functions $L^2(\mathbb{R})$. The discussion may be generalized to square-integrable functions defined on a complex contour [157].

In the literature on $\mathcal{PT}$-symmetric QM, notably [37, 38, 42], the transpose O^T and Hermitian-conjugate $O^\dagger$ of a linear operator O are respectively defined with respect to the coordinate-basis, $\{|x\rangle\}$, according to

$$\langle x_1|O^T|x_2\rangle := \langle x_2|O|x_1\rangle, \tag{8}$$

$$\langle x_1|O^\dagger|x_2\rangle := \langle x_2|O|x_1\rangle^*, \tag{9}$$

where x_1, x_2 are arbitrary real numbers. Therefore the terms "symmetric" and "Hermitian" respectively refer to the conditions $\langle x_1|O|x_2\rangle = \langle x_2|O|x_1\rangle$ and $\langle x_1|O|x_2\rangle^* = \langle x_2|O|x_1\rangle$. These definitions reflect the inclination to treat operators as matrices. This is certainly permissible provided that one specifies the particular basis one uses for this purpose. In this sense the following equivalent definitions are more preferable.

$$\begin{aligned} O^T &:= \int dx_1 \int dx_2 \langle x_2|O|x_1\rangle |x_1\rangle\langle x_2|, \\ O^\dagger &:= \int dx_1 \int dx_2 \langle x_2|O|x_1\rangle^* |x_1\rangle\langle x_2|. \end{aligned} \tag{10}$$

[h]One can more appropriately compare $\mathcal{C}$ with the chirality operator (γ^5) for the Dirac spinors.

A nice feature of (9) that is not shared with (8) is that it is invariant under the basis transformations that map $\{|x\rangle\}$ onto any *orthonormal basis*. For example one can easily show that if (9) holds, so do

$$\langle p_1|O^\dagger|p_2\rangle = \langle p_2|O|p_1\rangle^* \quad \text{and} \quad O^\dagger = \int dp_1 \int dp_2 \langle p_2|O|p_1\rangle^* |p_1\rangle\langle p_2|. \tag{11}$$

This invariance under orthonormal basis transformations stems from the fact that $O^\dagger$ admits a basis-independent definition: It is the linear operator satisfying

$$\langle \phi \,|\, O^\dagger \psi\rangle = \langle O\phi \,|\, \psi\rangle, \tag{12}$$

i.e. the *adjoint operator* for O.[i]

The notions of "transpose" and "symmetric operator" introduced above and employed in [37–39, 42] do not share this invariance property of "Hermitian-conjugate" and "Hermitian operator". For example, it is easy to see that $\langle x_1|(ip)|x_2\rangle = -\langle x_2|(ip)|x_1\rangle$ while $\langle p_1|(ip)|p_2\rangle = \langle p_2|(ip)|p_1\rangle$. Therefore, ip is represented by a symmetric matrix in the p-basis while it is represented by an antisymmetric matrix in the x-basis. This shows that there is no basis-independent notion of the transpose of an operator or a symmetric operator.[j]

Obviously once we specify a basis, there is no danger of using definition (8). But we must keep in mind that any theory in which one uses the notion of transposition in the sense of (8) involves the implicit assumption that the coordinate-basis is a preferred basis. The use of the notion of Hermitian-conjugation as defined by (9) does not rely on such an assumption. As we will explain in the following section, the choice of an orthonormal basis is equivalent to the choice of an inner product. This is why one can define $O^\dagger$ using its basis-independent defining relation (12) which only involves the inner product $\langle \cdot \,|\, \cdot \rangle$. In summary, while the use of the terms "transpose" and "symmetric operator" involves making a particular choice for a preferred basis, the use of the term "Hermitian-conjugate" and "Hermitian operator" involves making a particular choice for an inner product.

In conventional QM the inner product is fixed from the outset. Hence the notions of Hermitian-conjugation and Hermitian operator are well-defined. The opposite is true about the notions of transposition and symmetric operator. This does not cause any difficulty, because they never enter into quantum mechanical calculations, and in principle one does not need to introduce them at all. We will see that the same is the case in pseudo-Hermitian QM. In particular, in the discussion of $\mathcal{PT}$-symmetric systems, there is no need to identify physical observables using (6).

[i] A rigorous definition of the adjoint operator is given in Subsec. 2.2.

[j] One can define a notion of the transpose of a linear operator O acting in a complex inner product space $\mathcal{V}$ in terms of an arbitrary antilinear involution $\tau : \mathcal{V} \to \mathcal{V}$ according to $O^T = \tau O^\dagger \tau$ [6]. A function $\tau : \mathcal{V} \to \mathcal{V}$ is called an *antilinear operator* if $\tau(a\psi + b\phi) = a^*\tau\psi + b^*\tau\phi$ for all complex numbers a, b and all elements ψ, ϕ of $\mathcal{V}$. It is called an *involution* if $\tau^2 = I$, where $I : \mathcal{V} \to \mathcal{V}$ is the identity operator. The choice of a basis to define O^T is equivalent to the choice of an antilinear involution τ. The notion of the transpose used in [37, 38, 42] corresponds to choosing the time-reversal operator $\mathcal{T}$ as τ.

The main reason for making a universal and preassigned choice for the inner product in QM is the curious fact that up to unitary-equivalence there is a unique inner product.[k] This means that using different inner products lead to physically identical theories, or more correctly to different representations of a single physical theory. In conventional QM, one eliminates the chance of employing these alternative representations by adopting the usual (L^2-) inner product as the only viable choice. The situation resembles a gauge theory in which one fixes a gauge from the outset and then forgets about the gauge symmetry. This will have no effect on the physical quantities computed using such a theory, but it is clearly not recommended. It is quite possible that an alternative choice of gauge would facilitate a particular calculation.

We wish to argue that because *no one has ever made an independent measurement of the inner product of the Hilbert space*, it must be kept as a degree of freedom of the formulation of the theory. This is the basic principle underlying pseudo-Hermitian QM.

We will see that any inner product may be defined in terms of a certain linear operator η_+. It is this so-called *metric operator* that determines the kinematics of pseudo-Hermitian quantum systems. The Hamiltonian operator H that defines the dynamics is linked to the metric operator via the pseudo-Hermiticity relation,

$$H^\dagger = \eta_+ H \eta_+^{-1}. \tag{13}$$

We will explore some of the consequences of this equation whose significance has not been fully noticed or appreciated in its earlier investigations, notably in the context of the indefinite-metric quantum theories [190].

We wish to point out that there is a very large number of publications on the subject of this article. Many of these focus on the mathematical issues related to the investigation of the spectrum of various non-Hermitian operators or formalisms developed to study such problems. Here we will not deal with these issues. The interested reader may consult the review article [80]. Another related line of research is the mathematical theory of linear spaces with an indefinite metric and its applications [53, 18]. This is also beyond the aim and the scope of the present article. There are a series of review articles by Bender and his collaborators [38, 42, 28–30] that also address the physical aspects of the subject. The approach pursued in these articles is based on the use of the $\mathcal{CPT}$-inner products and the definition of observables given by (6). This restricts the domain of validity of their results to symmetric Hamiltonians. The discussion of the classical limit of $\mathcal{PT}$-symmetric systems offered in these articles is also not satisfactory, because it does not involve a quantization scheme that would relate classical and quantum observables.

[k]This will be explained in detail in Subsec. 2.3.

It is our opinion that to gain a basic understanding of the subject demands a careful study of the underlying mathematical structures without getting trapped in the physically irrelevant mathematical details and technicalities. The need for a comprehensive and readable treatment of basic mathematical notions and their physical consequences has not been met by any of the previously published reviews. In the first part of the present article (Secs. 2 and 3), we intend to address this need. Here we only discuss the mathematical tools and results that are necessary for addressing the conceptual issues of direct relevance to the physical aspects of the subject. In Sec. 3, we use the mathematical machinery developed in Sec. 2 to present a complete formulation of pseudo-Hermitian QM and its connection with $\mathcal{PT}$- and $\mathcal{C}$-symmetries. The second part of the article (Secs. 4–9) aims to survey various recent developments. In Sec. 4 we survey different methods of computing metric operators. In Secs. 5–8 we explore systems defined on complex contours, the classical limit of pseudo-Hermitian quantum systems, the subtleties involving time-dependent Hamiltonians and the path-integral formulation of the theory, and the quantum Brachistochrone problem, respectively. In Sec. 9 we discuss some of the physical applications of pseudo-Hermitian Hamiltonians, and in Sec. 10 we present our concluding remarks.

2. Mathematical Tools and Conceptual Foundations

In this section, we survey the necessary mathematical tools and elaborate on a number of conceptual issues that are helpful in clarifying various existing misconceptions on the subject. We also offer a thorough discussion of the motivation for considering a more general formulation of QM.

One of the axioms of QM is that pure physical states of a quantum system are rays in a Hilbert space $\mathcal{H}$. Each ray may be determined in a unique manner by a nonzero element ψ of $\mathcal{H}$ which we call a *state-vector*. The physical quantities associated with a pure state are computed using a corresponding state-vector and the inner product of the Hilbert space. We begin our discussion by a precise description of Hilbert spaces, inner products, bases, Hermitian and unitary operators, biorthonormal systems, and their relevance to our investigation.

We will use the following notations and conventions: $\mathbb{R}, \mathbb{R}^+, \mathbb{C}, \mathbb{Z}, \mathbb{Z}^+, \mathbb{N}$ denote the sets of real numbers, positive real numbers, complex numbers, integers, positive integers and non-negative integers (natural numbers), respectively. The symbol ":=" means that the left-hand side is defined to be the right-hand side, "=:" means that the converse is true, and "$\in$" and "$\subseteq$" respectively stand for "is an element of" and "is a subset of". Throughout this article we will only consider time-independent Hamiltonian operators unless otherwise explicitly stated.

2.1. *Hilbert spaces and Riesz bases*

Consider a complex vector space $\mathcal{V}$ and a function $\langle\cdot\,|\,\cdot\rangle : \mathcal{V}\times\mathcal{V}\to\mathbb{C}$ that assigns to any pair ψ,ϕ of elements of $\mathcal{V}$ a complex number $\langle\psi\,|\,\phi\rangle$. Suppose that $\langle\cdot\,|\,\cdot\rangle$ has

the following properties:

(i) It is *positive-definite*, i.e. for all nonzero elements ψ of $\mathcal{V}$, $\langle\psi\,|\,\psi\rangle$ is a positive real number, and it vanishes if and only if $\psi = 0$, where we use 0 also for the zero vector.
(ii) It is Hermitian, i.e. for any pair ψ, ϕ of elements of $\mathcal{V}$, $\langle\psi\,|\,\phi\rangle^* = \langle\phi\,|\,\psi\rangle$.
(iii) It is linear in its second slot, i.e. for all $\psi, \phi, \chi \in \mathcal{V}$ and all $a, b \in \mathbb{C}$, $\langle\psi\,|\,a\phi + b\chi\rangle = a\langle\psi\,|\,\phi\rangle + b\langle\psi\,|\,\chi\rangle$.

Then $\langle\cdot\,|\,\cdot\rangle$ is called an *inner product*[l] on $\mathcal{V}$, and the pair $(\mathcal{V}, \langle\cdot\,|\,\cdot\rangle)$ is called an *inner product space.*

An inner product $\langle\cdot\,|\,\cdot\rangle$ on $\mathcal{V}$ assigns to each element ψ of $\mathcal{V}$ a non-negative real number, $\|\psi\| := \sqrt{\langle\psi\,|\,\psi\rangle}$, that is called the *norm* of ψ. We can use the norm to define a notion of distance between elements of $\mathcal{V}$, according to $\|\psi-\phi\|$, and develop analysis and geometry on the inner product space $(\mathcal{V}, \langle\cdot\,|\,\cdot\rangle)$.

A *Hilbert space* $\mathcal{H}$ is an inner product space which fulfills an additional technical condition, namely that its norm defines a *complete metric space*, i.e. for any infinite sequence $\{\psi_k\}$ of elements ψ_k of $\mathcal{H}$, the condition that $\lim_{j,k\to\infty} \|\psi_j - \psi_k\| = 0$ implies that $\{\psi_k\}$ converges to an element ψ of $\mathcal{H}$; $\lim_{k\to\infty} \|\psi - \psi_k\| = 0$. In other words, a Hilbert space is a complete inner product space.

A subset $\mathcal{S}$ of a Hilbert space $\mathcal{H}$ is said to be *dense*, if every element of $\mathcal{H}$ may be obtained as the limit of a sequence of elements of $\mathcal{S}$. A Hilbert space is said to be *separable*, if it has a countable dense subset. It turns out that $\mathcal{H}$ is separable if and only if it has a countable *basis*. The latter is a sequence $\{\chi_n\}$ of linearly independent elements of $\mathcal{H}$ such that the set of its finite linear combinations,

$$\mathcal{L}(\{\chi_n\}) = \left\{ \sum_{n=1}^{K} c_n\chi_n \,\middle|\, K \in \mathbb{Z}^+, c_n \in \mathbb{C} \right\}, \tag{14}$$

is a dense subset of $\mathcal{H}$. For an infinite-dimensional Hilbert space $\mathcal{H}$, $\{\chi_n\}$ is an infinite sequence and the assertion that $\mathcal{L}(\{\chi_n\})$ is a dense subset means that every element ψ of $\mathcal{H}$ is the limit of a convergent series of the form $\sum_{n=1}^{\infty} c_n\chi_n$ whose coefficient c_n are assumed to be uniquely determined by ψ.[m]

It is not difficult to show that any finite-dimensional inner product space is both complete and separable. In this sense infinite-dimensional separable Hilbert spaces are natural generalizations of the finite-dimensional inner product spaces. In the following we will use the label N to denote the dimension of the Hilbert space in question. $N = \infty$ will refer to an infinite-dimensional separable Hilbert space.

An important difference between finite- and infinite-dimensional Hilbert spaces is that the definition of a basis in a finite-dimensional Hilbert space does not involve the inner product while the opposite is true about the infinite-dimension Hilbert

[l]We use the terms "inner product" and "positive-definite inner product" synonymously.
[m]This notion of basis is sometimes called a *Schauder basis* [236]. It is not to be confused with the algebraic or Hamel basis, which for infinite-dimensional Hilbert spaces, is always uncountable [99].

spaces. The requirement that (14) be a dense subset makes explicit use of the norm. Therefore whether a given sequence of linearly independent vectors form a basis of an infinite-dimensional Hilbert space $\mathcal{H}$ depends in a crucial manner on the inner product of $\mathcal{H}$.

Given a basis $\{\chi_n\}$ of a separable Hilbert space $\mathcal{H}$, one can apply the Gram–Schmidt process [198, 66] to construct an *orthonormal basis*, i.e. a basis $\{\xi_n\}$ satisfying

$$\langle \xi_m \,|\, \xi_n \rangle = \delta_{mn} \quad \text{for all } m, n \in \{1, 2, 3, \ldots, N\}, \tag{15}$$

where δ_{mn} denotes the Kronecker delta symbol: $\delta_{mn} := 0$ if $m \neq n$ and $\delta_{nn} := 1$ for all n. For an orthonormal basis $\{\xi_n\}$, the coefficients c_n of the basis expansion,

$$\psi = \sum_{n=1}^{N} c_n \xi_n, \tag{16}$$

of the elements ψ of $\mathcal{H}$ are given by

$$c_n = \langle \xi_n \,|\, \psi \rangle. \tag{17}$$

Furthermore, in view of (15)–(17),

$$\langle \phi \,|\, \psi \rangle = \sum_{n=1}^{N} \langle \phi \,|\, \xi_n \rangle \langle \xi_n \,|\, \psi \rangle \quad \text{for all } \phi, \psi \in \mathcal{H}. \tag{18}$$

In particular,

$$\|\psi\|^2 = \sum_{n=1}^{N} |\langle \xi_n \,|\, \psi \rangle|^2 \quad \text{for all } \psi \in \mathcal{H}. \tag{19}$$

Equation (18) implies that the operator $\mathcal{I}$ defined by $\mathcal{I}\psi := \sum_{n=1}^{N} \langle \xi_n \,|\, \psi \rangle \xi_n$ equals the identity operator I acting in $\mathcal{H}$; $\mathcal{I} = I$.[n] This is called the *completeness relation* which in Dirac's bracket notation takes the familiar form: $\sum_{n=1}^{N} |\xi_n\rangle\langle\xi_n| = I$.

Next, we wish to examine if *given a basis* $\{\zeta_n\}$ *of a separable Hilbert space* $\mathcal{H}$, *there is an inner product* $(\cdot \,|\, \cdot)$ *on* $\mathcal{H}$ *with respect to which* $\{\zeta_n\}$ *is orthonormal*. Because $\{\zeta_n\}$ is a basis, for all $\psi, \phi \in \mathcal{H}$ there are unique complex numbers c_n, d_n such that $\psi = \sum_{n=1}^{N} c_n \zeta_n$ and $\phi = \sum_{n=1}^{N} d_n \zeta_n$. We will attempt to determine $(\psi \,|\, \phi)$ in terms of c_n and d_n.

First, consider the finite-dimensional case, $N < \infty$. Then, in view of Eq. (18), the condition that $\{\zeta_n\}$ is orthonormal with respect to $(\cdot \,|\, \cdot)$ defines the latter according to

$$(\psi \,|\, \phi) := \sum_{n=1}^{N} c_n^* d_n. \tag{20}$$

[n]Let $\psi_1, \psi_2 \in \mathcal{H}$ be such that for all $\phi \in \mathcal{H}, \langle \phi \,|\, \psi_1 \rangle = \langle \phi \,|\, \psi_2 \rangle$. Then $\langle \phi \,|\, \psi_1 - \psi_2 \rangle = 0$ for all $\phi \in \mathcal{H}$. Setting $\phi = \psi_1 - \psi_2$, one then finds $\|\psi_1 - \psi_2\|^2 = 0$ which implies $\psi_1 = \psi_2$. In view of this argument, $\langle \phi \,|\, \mathcal{I}\psi \rangle = \langle \phi \,|\, \psi \rangle$ for all $\psi, \phi \in \mathcal{H}$ implies $\mathcal{I}\psi = \psi$ for all $\psi \in \mathcal{H}$. Hence $\mathcal{I} = I$.

We can easily check that $(\cdot\,|\,\cdot)$ possesses the defining properties (i)–(iii) of an inner product and satisfies $(\zeta_m\,|\,\zeta_n)=\delta_{mn}$. It is also clear from Eq. (18) that any other inner product with this property must satisfy (20). This shows that $(\cdot\,|\,\cdot)$ is the unique inner product that renders $\{\zeta_n\}$ orthonormal.

The case $N=\infty$ may be similarly treated, but in general there is no guarantee that the right-hand side of (20) is a convergent series. In fact, it is not difficult to construct examples for which it is divergent. Therefore, an inner product that makes an arbitrary basis $\{\zeta_n\}$ orthonormal may not exist. The necessary and sufficient condition for the existence of such an inner product $(\cdot\,|\,\cdot)$ is that $\psi=\sum_{n=1}^{\infty}c_n\zeta_n$ implies $\sum_{n=1}^{\infty}|c_n|^2<\infty$ for all $\psi\in\mathcal{H}$.[o] Furthermore, we shall demand that the inner product space $\mathcal{H}'$ obtained by endowing the underlying vector space of $\mathcal{H}$ with the inner product $(\cdot\,|\,\cdot)$ is a Hilbert space. As we will discuss in Subsec. 2.3, any two infinite-dimensional separable Hilbert spaces, in particular $\mathcal{H}$ and $\mathcal{H}'$, have the same topological properties, i.e. the set of open subsets of $\mathcal{H}$ coincides with that of $\mathcal{H}'$. This restricts $(\cdot\,|\,\cdot)$ to be *topologically equivalent* to $\langle\cdot\,|\,\cdot\rangle$, i.e. there are positive real numbers c_1 and c_2 satisfying $c_1\langle\psi\,|\,\psi\rangle\leq(\psi\,|\,\psi)\leq c_2\langle\psi\,|\,\psi\rangle$ for all $\psi\in\mathcal{H}$. It turns out that the inner product (20) that renders the basis $\{\zeta_n\}$ orthonormal and is topologically equivalent to $\langle\cdot\,|\,\cdot\rangle$ exists and is unique if and only if it is obtained from an orthonormal basis $\{\xi_n\}$ through the action of an everywhere-defined bounded invertible linear operator $A:\mathcal{H}\to\mathcal{H}$, i.e. $\zeta_n=A\xi_n$. A basis $\{\zeta_n\}$ having this property is called a *Riesz basis* [94, 236]. In summary, we can construct a new separable Hilbert space $\mathcal{H}'$ in which $\{\zeta_n\}$ is orthonormal if and only if it is a Riesz basis. We will give a derivation of a more explicit form of the inner product of $\mathcal{H}'$ in Subsec. 2.4.

2.2. *Bounded, invertible, and Hermitian operators*

Consider two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ with inner products $\langle\cdot\,|\,\cdot\rangle_1$ and $\langle\cdot\,|\,\cdot\rangle_2$, respectively, and a linear operator A that maps $\mathcal{H}_1$ to $\mathcal{H}_2$. The *domain* $\mathcal{D}(A)$ of A is the subset of $\mathcal{H}_1$ such that the action of A on any element of $\mathcal{D}(A)$ yields a unique element of $\mathcal{H}_2$. The range $\mathcal{R}(A)$ of A is the subset of $\mathcal{H}_2$ consisting of elements of the form $A\psi_1$ where ψ_1 belongs to $\mathcal{D}(A)$. If $\mathcal{D}(A)=\mathcal{H}_1$, one says that A has *full domain*, or that it is *everywhere-defined*. If $\mathcal{R}(A)=\mathcal{H}_2$, one says that A has *full range*, i.e. it is an *onto* function. As an example, consider the momentum operator p acting in $\mathcal{H}_1=\mathcal{H}_2=L^2(\mathbb{R})$, $(p\psi)(x):=-i\hbar\frac{d}{dx}\psi(x)$. Then $\mathcal{D}(p)$ consists of the square-integrable functions that have a square-integrable derivative, and $\mathcal{R}(p)$, is the set of square-integrable functions ψ_2 such that $\psi_1(x)=\int_{-\infty}^{x}\psi_2(u)du$ is also square-integrable. In particular, p is not everywhere-defined, but its domain is a dense

[o]If $(\cdot\,|\,\cdot)$ exists, (20) must hold because $\{\zeta_n\}$ is orthonormal with respect to $(\cdot\,|\,\cdot)$. Hence the left-hand side of (20) is well-defined and its right-hand must be convergent. In particular, for $\phi=\psi$ we find that $(\psi\,|\,\psi)=\sum_{n=1}^{\infty}|c_n|^2$ must be finite. This establishes the necessity of the above condition. Its sufficiency follows from the inequality: For all $K\in\mathbb{Z}^+$, $|\sum_{n=1}^{K}c_n^*d_n|^2\leq\sum_{n=1}^{\infty}|c_n|^2\sum_{m=1}^{\infty}|d_m|^2<\infty$.

subset of $L^2(\mathbb{R})$. Such an operator is said to be *densely-defined*. All the operators we encounter in this article and more generally in QM are densely-defined.

A linear operator $A : \mathcal{H}_1 \to \mathcal{H}_2$ is said to be *bounded* if there is a positive real number M such that for all $\psi \in \mathcal{D}(A)$, $\|A\psi\|_2 \leq M\|\psi\|_1$, where $\|\cdot\|_1$ and $\|\cdot\|_2$ are respectively the norms defined by the inner products $\langle\cdot\,|\,\cdot\rangle_1$ and $\langle\cdot\,|\,\cdot\rangle_2$. The smallest M satisfying this inequality is called the norm of A and denoted by $\|A\|$. A characteristic feature of a bounded operator is that all its eigenvalues a are bounded by its norm, $|a| \leq \|A\|$. Furthermore, a linear operator is bounded if and only if it is continuous [195].[p] Linear operators relating finite-dimensional Hilbert spaces are necessarily bounded. Therefore, the concept of boundedness is only important for infinite-dimensional Hilbert spaces.

$A : \mathcal{H}_1 \to \mathcal{H}_2$ is called an *invertible operator* if it satisfies both of the following conditions [105].[q]

(1) A is one-to-one and onto, so $A^{-1} : \mathcal{H}_2 \to \mathcal{H}_1$ exists and has a full domain;
(2) A^{-1} is a bounded operator.

If A is bounded, one-to-one and onto, then according to a theorem due to Banach its inverse is also bounded; it is invertible [127].[r] An important class of bounded invertible operators that play a fundamental role in QM is the unitary operators. We will examine them in Subsec. 2.3.

Next, consider a linear operator $A : \mathcal{H}_1 \to \mathcal{H}_2$ that has a dense domain $\mathcal{D}(A)$. Let $\mathcal{D}'$ be the subset of $\mathcal{H}_2$ whose elements ψ_2 satisfy the following condition: For all $\psi_1 \in \mathcal{D}(A)$, there is an element ϕ_1 of $\mathcal{H}_1$ such that $\langle\psi_2\,|\,A\psi_1\rangle_2 = \langle\phi_1\,|\,\psi_1\rangle_1$. Then there is a unique linear operator $A^\dagger : \mathcal{H}_2 \to \mathcal{H}_1$ fulfilling [195]

$$\langle\psi_1\,|\,A^\dagger\psi_2\rangle_1 = \langle A\psi_1\,|\,\psi_2\rangle_2 \quad \text{for all } \psi_1 \in \mathcal{D}(A) \quad \text{and } \psi_2 \in \mathcal{D}'. \tag{21}$$

This operator is called the *adjoint* or *Hermitian-conjugate* of A. By construction, $\mathcal{D}'$ is the domain of $A^\dagger$; $\mathcal{D}(A^\dagger) = \mathcal{D}'$.

For the case $\mathcal{H}_2 = \mathcal{H}_1 =: \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space with inner product $\langle\cdot\,|\,\cdot\rangle$, a linear operator $A : \mathcal{H} \to \mathcal{H}$ having a dense domain $\mathcal{D}(A)$ is called a *self-adjoint* or *Hermitian* operator[s] if $A^\dagger = A$. In particular, $\mathcal{D}(A^\dagger) = \mathcal{D}(A)$ and

$$\langle\psi_1\,|\,A\psi_2\rangle = \langle A\psi_1\,|\,\psi_2\rangle \quad \text{for all } \psi_1, \psi_2 \in \mathcal{D}(A). \tag{22}$$

[p] A function $f : \mathcal{H}_1 \to \mathcal{H}_2$ is said to be continuous if for all $\psi \in \mathcal{D}(f)$ and every sequence $\{\psi_n\}$ in $\mathcal{D}(f)$ that converges to ψ, the sequence $\{f(\psi_n)\}$ converges to $f(\psi)$.
[q] Some authors do not require the second condition. The above definition is the most convenient for our purposes.
[r] A continuous one-to-one onto function with a continuous inverse is called a *homeomorphism*. The domain and range of a homeomorphism have the same topological properties. If $f : \mathcal{H}_1 \to \mathcal{H}_2$ is a homeomorphism relating two Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_1$, a sequence $\{x_n\}$ of elements x_n of $\mathcal{H}$ converges to an element $x \in \mathcal{H}$ if and only if the $\{f(x_n)\}$ converges to $f(x)$ in $\mathcal{H}_2$.
[s] In some mathematics texts, e.g. [195], the term "Hermitian" is used for a more general class of operators which satisfy (22) but have $\mathcal{D}(A) \subseteq \mathcal{D}(A^\dagger)$. A more commonly used term for such an operator is "symmetric operator". We will avoid using this terminology which conflicts with the terminology used in the literature on $\mathcal{PT}$-symmetric QM [37, 38, 42].

An occasionally useful property of Hermitian operators is that *every Hermitian operator having a full domain is necessarily bounded*. This is known as the *Hellinger–Toeplitz theorem* [195].

Hermitian operators play an essential role in QM mainly because of their spectral properties [229]. In particular, their spectrum[t] is real, their eigenvectors with distinct eigenvalues are orthogonal, and they yield a *spectral resolution of the identity operator* I. For a Hermitian operator A with a discrete spectrum the latter takes the following familiar form, if we use the Dirac bracket notation.

$$I = \sum_{n=1}^{N} |\alpha_n\rangle\langle\alpha_n|, \tag{23}$$

where $\{\alpha_n\}$ is an orthonormal basis consisting of the eigenvectors α_n of A whose eigenvalues a_n are not necessarily distinct,

$$A\alpha_n = a_n\alpha_n, \quad \text{for all } n \in \{1, 2, 3, \ldots, N\}. \tag{24}$$

Equations (23) and (24) imply that A is *diagonalizable* and admits the following *spectral representation*

$$A = \sum_{n=1}^{N} a_n|\alpha_n\rangle\langle\alpha_n|. \tag{25}$$

Well-known analogs of (23) and (25) exist for the cases that the spectrum is not discrete [123].

An important property that makes Hermitian operators indispensable in QM is the fact that for a given densely-defined[u] linear operator A with $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$, the expectation value $\langle\psi \,|\, A\psi\rangle$ is real-valued for all unit state-vectors $\psi \in \mathcal{D}(A)$ if and only if the Hermiticity condition (22) holds [123].[v] This shows that in a quantum theory that respects von Neumann's measurement (projection) axiom, the observables cannot be chosen from among non-Hermitian operators even if they have a real spectrum. The same conclusion may be reached by realizing that the measurement axiom also requires the eigenvectors of an observable with distinct eigenvalues to be orthogonal, for otherwise the reading of a measuring device that is to be identified with an eigenvalue of the observable will not be sufficient to determine the state of the system immediately after the measurement [175]. This is because an eigenvector that is the output of the measurement may have a nonzero component along an eigenvector with a different eigenvalue. This yields nonzero probabilities for the system to be in two different physical states, though one measures the eigenvalue of one of them only!

[t]For a precise definition of the spectrum of a linear operator, see Subsec. 3.3.
[u]Observables must have dense domains, for otherwise one can construct a state in which an observable cannot be measured!
[v]A simple proof of this statement is given in the Appendix.

Let $\{\xi_n\}$ be an orthonormal basis of $\mathcal{H}$ and A be a Hermitian operator acting in $\mathcal{H}$, then according to property (ii) of the inner product and the Hermiticity condition (22) we have

$$A_{mn} := \langle \xi_m \,|\, A\xi_n\rangle = \langle \xi_n \,|\, A\xi_m\rangle^* = A^*_{nm}. \tag{26}$$

This shows that A is represented in the basis $\{\xi_n\}$, according to

$$A = \sum_{n=1}^{N} A_{mn}|\xi_m\rangle\langle\xi_n|, \tag{27}$$

using the $N \times N$ *Hermitian matrix*[w] $\underline{A} := (A_{mn})$.

It is essential to realize that a Hermitian operator can be represented by a non-Hermitian matrix in a non-orthonormal basis. This implies that having the expression for the matrix representation of an operator and knowing the basis used for this representation are not sufficient to decide if the operator is Hermitian. One must in addition know the inner product and be able to determine if the basis is orthonormal. *Referring to an operator as being Hermitian or non-Hermitian* (*using its matrix representation*) *without paying attention to the inner product of the space it acts in is a dangerous practice.*

For example, it is not difficult to check that the Hermitian matrix $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ represents the operator $L : \mathbb{C}^2 \to \mathbb{C}^2$ defined by $L\left(\begin{smallmatrix} z_1 \\ z_2 \end{smallmatrix}\right) := \left(\begin{smallmatrix} z_1 \\ z_1 - z_2 \end{smallmatrix}\right)$ in the basis $\mathcal{B} := \left\{\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right), \left(\begin{smallmatrix} 1 \\ 1 \end{smallmatrix}\right)\right\}$. The same operator is represented in the standard basis $\mathcal{B}_0 := \left\{\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right), \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)\right\}$ using the non-Hermitian matrix $\left(\begin{smallmatrix} 1 & 0 \\ 1 & -1 \end{smallmatrix}\right)$. We wish to stress that this information is, in fact, not sufficient to ascertain if L is a Hermitian operator, unless we fix the inner product on the Hilbert space $\mathbb{C}^2$. For instance, if we choose the standard Euclidean inner product which is equivalent to requiring $\mathcal{B}_0$ to be orthonormal, then L is a non-Hermitian operator. If we choose the inner product that makes the basis $\mathcal{B}$ orthonormal, then L is a Hermitian operator. We can use (20) to construct the latter inner product. It has the form $(\vec{z}\,|\,\vec{w}) := z_1^*(w_1 - w_2) + z_2^*(-w_1 + 2w_2)$, where $\vec{z} = \left(\begin{smallmatrix} z_1 \\ z_2 \end{smallmatrix}\right)$, and $\vec{w} = \left(\begin{smallmatrix} w_1 \\ w_2 \end{smallmatrix}\right)$.

The above example raises the following natural question. Given a linear operator H that is not represented by a Hermitian matrix in an orthonormal basis, is there another (non-orthonormal) basis in which it is represented by a Hermitian matrix? This is equivalent to asking if one can modify the inner product so that H becomes Hermitian. The answer to this question is: No, in general. As we will see in the sequel, there is a simple necessary and sufficient condition on H that ensures the existence of such an inner product.

2.3. *Unitary operators and unitary-equivalence*

Equations (17) and (18) may be employed to derive one of the essential structural properties of separable Hilbert spaces, namely that up to unitary-equivalence they

[w]A square matrix M is called Hermitian if its entries M_{mn} satisfy $M_{mn} = M^*_{nm}$ for all m and n.

are uniquely determined by their dimension. To achieve this we first explain how one compares inner product spaces. Two inner product spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ with inner products $\langle\cdot\,|\,\cdot\rangle_1$ and $\langle\cdot\,|\,\cdot\rangle_2$ are said to be *unitary-equivalent*, if there is an everywhere-defined onto linear operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that for every ϕ_1, ψ_1 in $\mathcal{H}_1$ we have

$$\langle U\phi_1\,|\,U\psi_1\rangle_2 = \langle\phi_1\,|\,\psi_1\rangle_1. \tag{28}$$

Such an operator is called a *unitary operator*. In view of (12) and (28), we have

$$U^\dagger U = I_1, \tag{29}$$

where I_1 denotes the identity operator acting on $\mathcal{H}_1$. One can use (28) and the ontoness property of U to show that U is an invertible operator and its inverse U^{-1}, that equals $U^\dagger$, is also unitary.

Unitary-equivalence is an equivalence relation.[x] Therefore to establish the unitary-equivalence of all N-dimensional separable Hilbert spaces, it suffices to show that all of them are unitary-equivalent to a chosen one. The most convenient choice for the latter is the Hilbert space

$$\mathcal{H}_0^N = \begin{cases} \mathbb{C}^N & \text{for } N \neq \infty \\ \ell^2 & \text{for } N = \infty, \end{cases}$$

where $\mathbb{C}^N$ is the set of N-dimensional complex column vectors endowed with the standard Euclidean inner product $\langle\vec{w}\,|\,\vec{z}\rangle := \vec{w}^* \cdot \vec{z}$, a dot denotes the usual dot product, ℓ^2 is the set of square-summable sequences, $\ell^2 := \{\{c_n\}\,|\,c_n \in \mathbb{C}, \sum_{n=1}^\infty |c_n|^2 < \infty\}$, equipped with the inner product: $\langle\{\tilde{c}_n\}|\{c_n\}\rangle := \sum_{n=1}^\infty \tilde{c}_n^* c_n$, and $\{\tilde{c}_n\}, \{c_n\} \in \ell^2$. Now, let $\mathcal{H}$ be any N-dimensional separable Hilbert space with inner product $(\cdot\,|\,\cdot)$, $\{\xi_n\}$ be an orthonormal basis of $\mathcal{H}$, and $U : \mathcal{H} \to \mathcal{H}_0^N$ be defined by $U(\psi) := \{(\xi_n\,|\,\psi)\}$ for all ψ in $\mathcal{H}$. It is not difficult to see that U is an everywhere-defined and onto linear map. Furthermore in view of (18) it satisfies, $\langle U\phi\,|\,U\psi\rangle = \sum_{n=1}^N (\xi_n\,|\,\phi)^*(\xi_n\,|\,\psi) = (\phi\,|\,\psi)$, for all $\phi, \psi \in \mathcal{H}$. Hence, (28) holds, U is a unitary operator, and $\mathcal{H}$ is unitary-equivalence to $\mathcal{H}_0^N$.

For a quantum system having $\mathbb{R}$ as its configuration space, one usually uses the coordinate wave functions $\psi(x)$ to represent the state-vectors. The latter are elements of the Hilbert space $L^2(\mathbb{R})$ of square-integrable complex-valued functions $\psi : \mathbb{R} \to \mathbb{C}$. The inner product of $L^2(\mathbb{R})$ has the form

$$\langle\phi\,|\,\psi\rangle = \int_{-\infty}^{\infty} dx\ \phi(x)^*\psi(x). \tag{30}$$

A concrete example for an orthonormal basis $\{\xi_n\}$ for $L^2(\mathbb{R})$ is the basis consisting of the standard normalized eigenfunctions $\xi_n = \psi_{n-1}$ of the unit simple harmonic oscillator Hamiltonian [139], or equivalently that of the operator $-\frac{d^2}{dx^2} + x^2$,

[x]This means that every inner product space is unitary-equivalent to itself; if $\mathcal{H}_1$ is unitary-equivalent to $\mathcal{H}_2$, so is $\mathcal{H}_2$ to $\mathcal{H}_1$; if $\mathcal{H}_1$ is unitary-equivalent to $\mathcal{H}_2$ and $\mathcal{H}_2$ is unitary-equivalent to $\mathcal{H}_3$, then $\mathcal{H}_1$ is unitary-equivalent to $\mathcal{H}_3$.

i.e. $\psi_m(x) = \pi^{-\frac{1}{4}}(m!2^m)^{-\frac{1}{2}}e^{-\frac{x^2}{2}}H_m(x)$, where $H_m(x) = e^{\frac{x^2}{2}}(x - \frac{d}{dx})^m e^{-\frac{x^2}{2}}$ are Hermite polynomials and $m \in \mathbb{N}$. For this example, switching from the coordinate-representation of the state-vectors to their representation in terms of the energy eigenbasis of the above harmonic oscillator corresponds to affecting the unitary operator U.

Unitary operators have a number of important properties that follow from (28). For example if $U : \mathcal{H}_1 \to \mathcal{H}_2$ is a unitary operator relating two separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$, then

(1) U is an everywhere-defined, bounded, and invertible operator.
(2) If $\{\xi_n\}$ is an orthonormal basis of $\mathcal{H}_1$, then $\{U\xi_n\}$ is an orthonormal basis of $\mathcal{H}_2$.[y]
(3) Let $A_1 : \mathcal{H}_1 \to \mathcal{H}_1$ be a Hermitian operator with domain $\mathcal{D}(A_1)$. Then $UA_1U^\dagger : \mathcal{H}_2 \to \mathcal{H}_2$ is a Hermitian operator with domain $U(\mathcal{D}(A_1)) = \{U\psi_1 \in \mathcal{H}_2 \,|\, \psi_1 \in \mathcal{D}(A_1)\}$.

A direct consequence of statement 1 above and the fact that the inverse of a unitary operator is unitary is that unitary operators are homeomorphisms.[z] As a result, all N-dimensional separable Hilbert spaces have identical topological properties. In particular, if two separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ share an underlying vector space, a sequence $\{x_n\}$ converges to x in $\mathcal{H}_1$ if and only if it converges to x in $\mathcal{H}_2$.

Next, we recall that every quantum system s is uniquely determined by a separable Hilbert space $\mathcal{H}$ that determines the kinematic structure of s and a Hamiltonian operator $H : \mathcal{H} \to \mathcal{H}$ that gives its dynamical structure via the Schrödinger equation. Let s_1 and s_2 be quantum systems corresponding to the Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$ and the Hamiltonians $H_1 : \mathcal{H}_1 \to \mathcal{H}_1, H_2 : \mathcal{H}_2 \to \mathcal{H}_2$. By definition the observables of the system s_i, with $i \in \{1, 2\}$, are Hermitian operators $O_i : \mathcal{H}_i \to \mathcal{H}_i$. s_1 and s_2 are physically equivalent, if there is a one-to-one correspondence between their states and observables in such a way that the physical quantities associated with the corresponding states and observables are identical. Such a one-to-one correspondence is mediated by a unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ according to

$$\psi_1 \to \psi_2 := U\psi_1 \qquad O_1 \to O_2 := UO_1U^\dagger. \tag{31}$$

In particular, if $\psi_i(t)$ is an evolving state-vector of the system s_i, i.e. it is a solution of the Schrödinger equation $i\hbar\frac{d}{dt}\psi_i(t) = H_i\psi_i(t)$, we have $\psi_2(t) = U\psi_1(t)$. The necessary and sufficient condition for the latter is $H_2 = UH_1U^\dagger$. This observation motivates the following theorem.

Theorem 1. *As physical systems $s_1 = s_2$, if there is a unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ satisfying $H_2 = UH_1U^\dagger$.*

[y] The converse is also true in the sense that given an orthonormal basis $\{\xi'_n\}$ of $\mathcal{H}_2$ there is a unique unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ such that $\xi'_n = U\xi_n$ for all $n \in \{1, 2, \ldots, N\}$.
[z] See footnote r for the definition.

To prove this assertion we recall that all physical quantities in QM may be expressed as expectation values of observables. Suppose that such a unitary operator exists, and let us prepare a state of s_1 that is represented by $\psi_1 \in \mathcal{H}_1$ and measure the observable O_1. The expectation value of this measurement is given by

$$\frac{\langle \psi_1 \,|\, O_1 \psi_1 \rangle_1}{\langle \psi_1 \,|\, \psi_1 \rangle_1} = \frac{\langle U^\dagger \psi_2 \,|\, U^\dagger O_2 U \psi_1 \rangle_1}{\langle U^\dagger \psi_2 \,|\, U^\dagger \psi_2 \rangle_1} = \frac{\langle \psi_2 \,|\, O_2 \psi_2 \rangle_2}{\langle \psi_2 \,|\, \psi_2 \rangle_2}, \tag{32}$$

where $\langle \cdot \,|\, \cdot \rangle_i$ is the inner product of $\mathcal{H}_i$, and we have used (31) and the fact that $U^\dagger$ is also a unitary operator. Equations (32) show that the above measurement is identical with measuring O_2 in a state of s_2 represented by the state-vector ψ_2. This argument is also valid for the case that ψ_1 is an evolving state-vector. It shows that the existence of U implies the physical equivalence of s_1 and s_2.[aa]

If the hypothesis of Theorem 1 holds, i.e. there is a unitary operator $U : \mathcal{H}_1 \to \mathcal{H}_2$ satisfying $H_2 = UH_1U^\dagger$, we say that the pairs $(\mathcal{H}_1, H_1)$ and $(\mathcal{H}_2, H_2)$ and the quantum systems they define are *unitary-equivalent*.

In conventional QM one mostly considers unitary operators that act in a single Hilbert space $\mathcal{H}$. These generate linear transformations that leave the inner product of the state-vectors invariant. They form the unitary group $\mathcal{U}(\mathcal{H})$ of the Hilbert space which includes the time-evolution operator $e^{-itH/\hbar}$ as a one-parameter subgroup.[bb] Given a quantum system s with Hamiltonian H, one may use the unitary operators $U \in \mathcal{U}(\mathcal{H})$ to generate unconventional unitary-equivalent systems $s_{_U}$ having the same Hilbert space. If x and p are the standard position and momentum operators of s, the position, momentum, and Hamiltonian operators for $s_{_U}$ are respectively given by $x_{_U} := UxU^\dagger, p_{_U} := UpU^\dagger$, and $H_{_U} := UHU^\dagger$. The transformation $x \to x_{_U}$, $p \to p_{_U}$ and $H \to H_{_U}$ is the quantum analog of a classical time-independent canonical transformation. Therefore, unitary transformations generated by the elements of $\mathcal{U}(\mathcal{H})$ play the role of canonical transformations.

2.4. *Biorthonormal systems*

Let $\{\psi_n\}$ be a basis of an N-dimensional separable Hilbert space $\mathcal{H}$, with $N \leq \infty$, and $\{\xi_n\}$ be the orthonormal basis obtained by performing the Gram–Schmidt process on $\{\psi_n\}$. Because $\{\psi_n\}$ is a basis, there are unique complex numbers $B_{mn} \in \mathbb{C}$ such that for all $m \in \{1, 2, 3, \ldots, N\}$

$$\xi_m = \sum_{n=1}^{N} B_{nm} \psi_n, \tag{33}$$

[aa]The converse of Theorem 1 can be formulated similarly to the Wigner's symmetry theorem [231, p. 91].
[bb]All possible symmetry, dynamical, and kinematic groups are also subgroups of $\mathcal{U}(\mathcal{H})$ [142].

and because $\{\xi_n\}$ is an orthonormal basis,

$$\psi_n = \sum_{k=1}^{N} \langle \xi_k \,|\, \psi_n \rangle \xi_k, \tag{34}$$

for all $n \in \{1, 2, 3, \ldots, N\}$. If we substitute (34) in (33) and use the orthonormality of ξ_n, we find $\sum_{n=1}^{N} B_{nm} \langle \xi_j \,|\, \psi_n \rangle = \delta_{mj}$ for all $m, j \in \{1, 2, 3, \ldots, N\}$. This shows that the $N \times N$ matrix $\underline{\mathrm{B}} = (B_{mn})$ is invertible and the entries of $\underline{\mathrm{B}}^{-1}$ are given by $B^{-1}_{mn} = \langle \xi_m \,|\, \psi_n \rangle$. We can use this relation to express (34) in the form

$$\psi_n = \sum_{k=1}^{N} B^{-1}_{kn} \xi_k. \tag{35}$$

This equation suggests that the vectors ϕ_m defined by

$$\phi_m := \sum_{j=1}^{N} B^{*}_{mj} \xi_j \quad \text{for all } m \in \{1, 2, 3, \ldots, N\}, \tag{36}$$

fulfil

$$\langle \phi_m \,|\, \psi_n \rangle = \delta_{mn} \quad \text{for all } m, n \in \{1, 2, 3, \ldots, N\}. \tag{37}$$

Furthermore, employing (16), (35), and (36), we can show that for all $\psi \in \mathcal{H}$, $\sum_{n=1}^{N} \langle \phi \,|\, \psi \rangle \psi_n = \psi$. We can use Dirac's bracket notation to express this identity as

$$\sum_{n=1}^{N} |\psi_n\rangle\langle\phi_n| = I. \tag{38}$$

This is a generalization of the more familiar completeness relation (23).

A sequence $\{(\psi_n, \phi_n)\}$ of ordered pairs of elements of $\mathcal{H}$ that satisfy (37) is called a *biorthonormal system* [201, 205, 236]. A biorthonormal system satisfying (38) is said to be *complete*.

Let $\{\psi_n\}$ be a basis of a separable Hilbert space $\mathcal{H}$, and $\{\phi_n\}$ be a sequence in $\mathcal{H}$ such that $\{(\psi_n, \phi_n)\}$ is a complete biorthonormal system. Then, one can show that $\{\phi_n\}$ is the unique sequence with this property and that it is necessarily a basis of $\mathcal{H}$ [236]. $\{\phi_n\}$ is called the *biorthonormal basis* associated with $\{\psi_n\}$, and the biorthonormal system $\{(\psi_n, \phi_n)\}$ is called a *biorthonormal extension* of $\{\psi_n\}$.

If $N < \infty$, the right-hand side of (36) is well-defined and the above construction yields the biorthonormal basis $\{\phi_n\}$ associated with every basis $\{\psi_n\}$ of $\mathcal{H}$. If $N = \infty$, $\{\phi_m\}$ can be constructed provided that the right-hand side of (36) converges. This is the case if and only if

$$\sum_{j=1}^{\infty} |B_{mj}|^2 < \infty \quad \text{for all } m \in \mathbb{Z}^{+}. \tag{39}$$

A theorem due to Bari [94] states that given a basis $\{\psi_n\}$, the biorthonormal system $\{(\psi_n, \phi_n)\}$ exists and $\sum_{n=1}^{\infty} |\langle \psi_n | \psi \rangle|^2$ and $\sum_{n=1}^{\infty} |\langle \phi_n | \psi \rangle|^2$ both converge

for all $\psi \in \mathcal{H}$, if and only if $\{\psi_n\}$ is a Riesz basis, i.e. there are an orthonormal basis $\{\chi_n\}$ and an everywhere-defined bounded invertible operator $A : \mathcal{H} \to \mathcal{H}$ such that $\psi_n = A\chi_n$.[cc] In this case $\{\phi_n\}$ is also a Riesz basis, and $\{(\psi_n, \phi_n)\}$ is the unique biorthonormal extension of $\{\psi_n\}$ [94, 201, 236].

The coefficients of the expansion of a vector $\psi \in \mathcal{H}$ in a Riesz basis $\{\psi_n\}$ can be expressed in terms of its biorthonormal basis $\{\phi_n\}$. Given $\psi = \sum_{n=1}^{N} c_n\psi_n$ we have, in light of (37), $c_n = \langle\phi_n \,|\, \psi\rangle$. Hence, for all $\psi \in \mathcal{H}$,

$$\psi = \sum_{n=1}^{N} \langle\phi_n \,|\, \psi\rangle\psi_n. \tag{40}$$

Clearly the roles of $\{\phi_n\}$ and $\{\psi_n\}$ are interchangeable. In particular, $\sum_{n=1}^{N} |\phi_n\rangle\langle\psi_n| = I$ and $\psi = \sum_{n=1}^{N} \langle\psi_n \,|\, \psi\rangle\phi_n$ for all $\psi \in \mathcal{H}$.

Let $\{\psi_n\}$ be a Riesz basis and $\{(\psi_n, \phi_n)\}$ be its biorthonormal extension. As we explained in Subsec. 2.1, we can construct a unique inner product $(\cdot \,|\, \cdot)$ on $\mathcal{H}$ that makes a Riesz basis orthonormal. We can use (20) and (40) to obtain the following simplified expression for this inner product.

$$(\psi \,|\, \phi) := \sum_{n=1}^{N} \langle\psi \,|\, \phi_n\rangle\langle\phi_n \,|\, \phi\rangle = \langle\psi \,|\, \eta_+\phi\rangle, \quad \text{for all } \psi, \phi \in \mathcal{H}, \tag{41}$$

where we have introduced the operator $\eta_+ : \mathcal{H} \to \mathcal{H}$ according to

$$\eta_+\psi := \sum_{n=1}^{N} \langle\phi_n \,|\, \psi\rangle\phi_n. \tag{42}$$

Using Dirac's bracket notation we can write it in the form

$$\eta_+ = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n|. \tag{43}$$

Because $\{\psi_n\}$ is a Riesz basis, the inner product (41) is defined for all $\psi, \phi \in \mathcal{H}$. This shows that η_+ is everywhere-defined. Furthermore, it is not difficult to see, by virtue of (37), that it has an everywhere-defined inverse given by

$$\eta_+^{-1} := \sum_{n=1}^{N} |\psi_n\rangle\langle\psi_n|. \tag{44}$$

This shows that η_+ is a one-to-one onto linear operator. As suggested by (43) it is also Hermitian, which in particular implies that both η_+ and η_+^{-1} are bounded. Moreover, in view of (43), $\langle\psi \,|\, \eta_+\psi\rangle = \sum_{n=1}^{N} |\langle\phi_n \,|\, \psi\rangle|^2$, for all $\psi \in \mathcal{H}$. Therefore η_+ is a positive operator. Finally because it is an invertible operator, its spectrum is

[cc] As any pair of orthonormal bases are related by a unitary operator $U : \mathcal{H} \to \mathcal{H}$ which is an everywhere-defined bounded invertible operator, one can take $\chi_n = \xi_n$ without loss of generality. This allows for the identification of the infinite matrix $\underline{B}$ with the matrix representation of A^{-1} in the basis $\{\xi_n\}$, for we have $B_{mn} = \langle\xi_m \,|\, A^{-1}\xi_n\rangle$.

strictly positive. A Hermitian operator with this property is called a *positive-definite operator*. The operator η_+ constructed above is an everywhere-defined, bounded, positive-definite and invertible operator. A linear operator with these properties is called a *metric operator*.

2.5. *Metric operators and conventional QM*

Consider a pair of separable Hilbert spaces $\mathcal{H}_1$ and $\mathcal{H}_2$ that are identical as vector spaces but have different inner products. We will denote the inner products of $\mathcal{H}_1$ and $\mathcal{H}_2$ by $\langle\cdot\,|\,\cdot\rangle_1$ and $\langle\cdot\,|\,\cdot\rangle_2$, respectively, and view $\langle\cdot\,|\,\cdot\rangle_2$ as an alternative inner product on $\mathcal{H}_1$. Our aim is to find a way to express $\langle\cdot\,|\,\cdot\rangle_2$ in terms of $\langle\cdot\,|\,\cdot\rangle_1$. We will first consider the case that the underlying vector space $\mathcal{V}$ of both $\mathcal{H}_1$ and $\mathcal{H}_2$ is finite-dimensional, i.e. $N<\infty$.

Let $\{\xi_n\}$ be an orthonormal basis of $\mathcal{H}_1$. As we argued above, it satisfies the completeness relation: $\sum_{n=1}^N |\xi_n\rangle_{1\,1}\langle\xi_n| = I$, where I is the identity operator of $\mathcal{V}$. In general, $\{\xi_n\}$ is not an orthonormal basis of $\mathcal{H}_2$ and the operator

$$\eta_+ := \sum_{n=1}^N |\xi_n\rangle_{2\,2}\langle\xi_n|, \tag{45}$$

does not coincide with I. Equation (45), which we can express in the more conventional form:

$$\eta_+\psi := \sum_{n=1}^N \langle\xi_n\,|\,\psi\rangle_2\,\xi_n, \quad \text{for all } \psi\in\mathcal{V}, \tag{46}$$

defines η_+ as a linear operator $\eta_+ : \mathcal{V}\to\mathcal{V}$ having a full domain.

Now, let ϕ be an arbitrary element of $\mathcal{V}$. In view of (16), we can express it as

$$\phi = \sum_{m=1}^N \langle\xi_m\,|\,\phi\rangle_1\,\xi_m. \tag{47}$$

Using Eqs. (46), (47) and the properties (ii) and (iii) shared by both the inner products, we can easily show that η_+ fulfils

$$\langle\phi\,|\,\psi\rangle_2 = \langle\phi\,|\,\eta_+\psi\rangle_1 \quad \text{for all } \psi,\phi\in\mathcal{V}. \tag{48}$$

Employing properties (i) and (ii) of $\langle\cdot\,|\,\cdot\rangle_2$, we can also verify that

$$\langle\phi\,|\,\eta_+\psi\rangle_1^* = \langle\psi\,|\,\eta_+\phi\rangle_1 \quad \text{for all } \psi,\phi\in\mathcal{V}, \tag{49}$$

$$\langle\psi\,|\,\eta_+\psi\rangle_1 > 0 \qquad \text{for all nonzero } \psi\in\mathcal{V}. \tag{50}$$

Equation (49) shows that η_+ is a Hermitian operator acting in $\mathcal{H}_1$, in particular it has a real spectrum. Equation (50) implies that indeed the spectrum of η_+ is strictly positive; η_+ is a positive-definite operator.

If $\mathcal{H}_1$ and $\mathcal{H}_2$ are infinite-dimensional, the sum appearing in (46) stands for an infinite series and we must address the issue of its convergence. The convergence of

this series is equivalent to the requirement that $\sum_{n=}^{\infty} |\langle \xi_n \,|\, \psi\rangle_2|^2 < \infty$ for all $\psi \in \mathcal{V}$. According to the above-mentioned theorem of Bari this requirement is fulfilled provided that $\{\xi_n\}$ is a Riesz basis of $\mathcal{H}_2$. Under this assumption (46) defines a linear operator η_+ acting in $\mathcal{H}_1$ and satisfying (48). It is a positive-definite (in particular Hermitian) operator with a full domain. Being Hermitian and everywhere-defined it is also necessarily bounded.

Next, we exchange the roles of $\mathcal{H}_1$ and $\mathcal{H}_2$. This gives rise to an everywhere-defined bounded positive-definite operator η'_+ acting in $\mathcal{H}_2$ such that $\langle \phi \,|\, \psi\rangle_1 = \langle \phi \,|\, \eta'_+\psi\rangle_2$ for all ψ, ϕ in $\mathcal{V}$. Combining this equation and (48) yields $\langle \phi \,|\, \psi\rangle_1 = \langle \phi \,|\, \eta_+\eta'_+\psi\rangle_1$ for all ψ, ϕ in $\mathcal{V}$. This in turn implies that $\eta'_+\eta_+ = I$.[dd] Because η'_+ is a bounded operator with a full domain, η_+ is an invertible operator with inverse $\eta_+^{-1} = \eta'_+$.[ee] Therefore η_+ is a metric operator.

The above construction of the metric operator η_+ is based on the choice of an orthonormal basis $\{\xi_n\}$ of $\mathcal{H}_1$. We will next show that indeed η_+ is independent of this choice. Let $\eta'_+ : \mathcal{V} \to \mathcal{V}$ be an everywhere-defined linear operator satisfying

$$\langle \phi \,|\, \psi\rangle_2 = \langle \phi \,|\, \eta'_+\psi\rangle_1 \quad \text{for all } \psi, \phi \in \mathcal{V}. \tag{51}$$

Equations (48) and (51) show that $\langle \phi \,|\, (\eta'_+ - \eta_+)\psi\rangle_1 = 0$ for all $\psi, \phi \in \mathcal{V}$. In view of the argument presented in footnote n, this implies $\eta'_+\psi = \eta_+\psi$ for all $\psi \in \mathcal{V}$, i.e. $\eta'_+ = \eta_+$. This establishes the uniqueness of the metric operator η_+ which in turn means that *the inner products that make a complex vector space $\mathcal{V}$ into a separable Hilbert space are in one-to-one correspondence with the metric operators η_+ acting in one of these Hilbert spaces.*

To employ the characterization of the inner products in terms of metric operators we need to select a Hilbert space $\mathcal{H}$. We will call this Hilbert space a *reference Hilbert space*. We will always fix a reference Hilbert space and use its inner product $\langle \cdot \,|\, \cdot \rangle$ to determine if a given linear operator acting in $\mathcal{V}$ is Hermitian or not. The following are some typical examples.

- For systems having a finite number (N) of linearly independent state-vectors, i.e. when $\mathcal{V} = \mathbb{C}^N$, $\mathcal{H}$ is defined by the Euclidean inner product, $\langle \vec{\phi} \,|\, \vec{\psi}\rangle := \vec{\phi}^* \cdot \vec{\psi}$, for all $\vec{\phi}, \vec{\psi} \in \mathbb{C}^N$.
- For systems whose configuration space is a differentiable manifold M with an integral measure $d\mu(x)$, $\mathcal{V}$ is the space $L^2(M)$ of all square-integrable functions $\psi : M \to \mathbb{C}$ and $\mathcal{H}$ is defined by the L^2-inner product: $\langle \phi \,|\, \psi\rangle := \int_M \phi(x)^*\psi(x)d\mu(x)$, for all $\phi, \psi \in L^2(M)$. The systems whose configuration space is a Euclidean space ($M = \mathbb{R}^d$) or a complex contour ($M = \Gamma$) belong to this class. We will discuss the latter systems in Sec. 5.

[dd] The proof uses the argument given in footnote n.

[ee] If we use the prescription of Subsec. 2.1 to obtain the inner product $(\cdot \,|\, \cdot)$ on $\mathcal{H}_2$ that renders the Riesz basis $\{\xi_1\}$ orthonormal, we find by its uniqueness that $(\cdot \,|\, \cdot) = \langle \cdot \,|\, \cdot\rangle_1$. According to (41), there is an everywhere-defined bounded invertible operator $\tilde{\eta}_+$ such that $\langle \cdot \,|\, \cdot\rangle_1 = \langle \cdot \,|\, \tilde{\eta}_+\cdot\rangle_2$. It is given by $\tilde{\eta}_+ = \eta_+^{-1}$.

In summary, given a separable Hilbert space $\mathcal{H}$ with inner product $\langle\cdot\,|\,\cdot\rangle$, we can characterize every other inner product on $\mathcal{H}$ by a metric operator $\eta_+ : \mathcal{H} \to \mathcal{H}$ according to

$$\langle\cdot\,|\,\cdot\rangle_{\eta_+} := \langle\cdot\,|\,\eta_+\cdot\rangle. \tag{52}$$

Each choice of η_+ defines a unique separable Hilbert space $\mathcal{H}_{\eta_+}$. Because η_+ is a positive-definite operator, we can use its spectral representation to construct its positive square root $\rho := \sqrt{\eta}_+$. As a linear operator acting in $\mathcal{H}$, ρ is a Hermitian operator satisfying $\rho^2 = \eta_+$. We can use this observation to establish

$$\langle\phi\,|\,\psi\rangle_{\eta_+} = \langle\phi\,|\,\eta_+\psi\rangle = \langle\rho^\dagger\phi\,|\,\rho\psi\rangle = \langle\rho\,\phi\,|\,\rho\,\psi\rangle, \quad \text{for all } \phi,\psi\in\mathcal{H}. \tag{53}$$

This relation shows that as a linear operator mapping $\mathcal{H}_{\eta_+}$ onto $\mathcal{H}$, ρ is a unitary operator.[ff] It provides a realization of the unitary-equivalence of the Hilbert spaces $\mathcal{H}_{\eta_+}$ and $\mathcal{H}$.

In ordinary QM one fixes the physical Hilbert space of the system to be one of the reference Hilbert spaces listed above and develops a theory based on this preassigned Hilbert space. The argument that the unitary-equivalence of all separable Hilbert spaces justifies this convention is not quite acceptable. For example, although for all $d \in \mathbb{Z}^+$, $L^2(\mathbb{R}^d)$ is unitary-equivalent to $L^2(\mathbb{R})$, we never use $L^2(\mathbb{R})$ to describe a system having more than one real degree of freedom. *The choice of the particular Hilbert space should in principle be determined by physical considerations or left as a freedom of the formulation of the theory.* In view of lack of a direct measurement of the inner product or the associated metric operator, we propose to adopt the second option. We will see that this does not lead to a genuine generalization of QM, but reveals a set of alternative and equally useful representations of QM which could not be utilized within its conventional formulation. Furthermore, the introduction of the freedom in choosing the metric operator may be used as an interesting method of extending QM by relaxing some of the restrictions put on the metric operator. Indeed the indefinite-metric quantum theories are examples of such a generalization.

3. Pseudo-Hermitian QM: Ingredients and Formalism

3.1. *Quasi-Hermitian versus pseudo-Hermitian QM*

To the best of our knowledge, the first publication investigating the consequences of the freedom in the choice of the metric operator is the article by Scholtz, Geyer and Hahne [207] in which the choice of the metric operator is linked to that of an *irreducible* set of linear operators. The latter is any (minimal) set $\mathcal{S}$ of operators O_α acting in a vector space $\mathcal{V}$ that do not leave any proper subspace of

[ff] Strictly speaking (53) shows that ρ is an isometry. However, in view of the fact that η_+ is invertible, so does ρ. This implies that $\rho : \mathcal{H}_{\eta_+} \to \mathcal{H}$ is a genuine unitary operator.

$\mathcal{V}$-invariant, i.e. the only subspace $\mathcal{V}'$ of $\mathcal{V}$ that satisfies: "$O_\alpha \in \mathcal{S}$ and $\psi \in \mathcal{V}'$ imply $O_\alpha\psi \in \mathcal{V}'$," is $\mathcal{V}$.

The approach pursued in [207] involves using the physical characteristics of a given system to determine an irreducible set of operators (that are to be identified with the observables of the theory) and employing the latter to fix a metric operator and the associated inner product of the Hilbert space. We will call this formalism *quasi-Hermitian Quantum Mechanics*. The main problem with this formalism is that it is generally very difficult to implement. This stems from the fact that the operators belonging to an irreducible set must in addition be compatible, i.e. there must exist an inner product with respect to which all the members of the set are Hermitian. In order to use this formalism to determine the inner product, one must in general employ a complicated iterative scheme.

- Select a linear operator O_1 with a complete set of eigenvectors and a real spectrum;
- Find the set $\mathfrak{U}_1$ of all possible metric operators that make O_1 Hermitian, and select a linear operator O_2, linearly independent of O_1, from among the linear operators that are Hermitian with respect to the inner product defined by some $\eta_+ \in \mathfrak{U}_1$;
- Find the set $\mathfrak{U}_2$ of all possible metric operators that make O_2 Hermitian, and select a linear operator O_3, linearly independent of O_1 and O_2, from among the linear operators that are Hermitian with respect to the inner product defined by some $\eta_+ \in \mathfrak{U}_1 \cap \mathfrak{U}_2$, where $\cap$ stands for the intersection of sets;
- Repeat this procedure until the inner product (respectively, metric operator η_+) is fixed up to a constant coefficient.

As we see, in trying to employ quasi-Hermitian QM, one needs a procedure to compute the most general metric operator associated with a given diagonalizable linear operator with a real spectrum. This is the main technical tool developed within the framework of pseudo-Hermitian QM.

Pseudo-Hermitian QM differs from quasi-Hermitian QM in that, in the former, one chooses O_1 to be the Hamiltonian, finds $\mathfrak{U}_1$ and leaves the choice of O_2 arbitrary, i.e. identifies all the operators O that are Hermitian with respect to the inner product associated with some unspecified metric operator η_+ belonging to $\mathfrak{U}_1$. The metric operator η_+ fixes a particular inner product and defines the "*physical Hilbert space*" $\mathcal{H}_{\rm phys}$ of the system. The "*physical observables*" are the Hermitian operators O acting in $\mathcal{H}_{\rm phys}$. We can use the unitary-equivalence of $\mathcal{H}_{\rm phys}$ and $\mathcal{H}$ realized by $\rho := \sqrt{\eta}_+$ to construct the physical observables O using those of the conventional QM, i.e. Hermitian operators o acting in the reference Hilbert space $\mathcal{H}$. This is done according to [152, 175]

$$O = \rho^{-1} o \rho. \tag{54}$$

Note that as an operator mapping $\mathcal{H}_{\rm phys}$ onto $\mathcal{H}$, ρ is a unitary operator. Hence O is a Hermitian operator acting in $\mathcal{H}_{\rm phys}$ if and only if o is a Hermitian operator acting in $\mathcal{H}$.

For instance, let $\mathcal{H} = L^2(\mathbb{R}^d)$ for some $d \in \mathbb{Z}^+$. Then we can select the usual position x_i and momentum p_i operators to substitute for o in (54). This defines a set of basic physical observables,

$$X_i := \rho^{-1} x_i \rho, \quad P_i := \rho^{-1} p_i \rho, \tag{55}$$

which we respectively call the *η_+-pseudo-Hermitian position and momentum operators*. They furnish an irreducible unitary representation of the Weyl–Heisenberg algebra,

$$[X_i, X_j] = [P_i, P_j] = 0, \quad [X_i, P_j] = \hbar \delta_{ij} I, \quad \text{for all } i, j \in \{1, 2, \ldots, d\}. \tag{56}$$

In principle, we can express the Hamiltonian H as a function of X_i and P_i and attempt to associate a physical meaning to it by devising a quantum-to-classical *correspondence principle*. One way of doing this is to define the underlying classical Hamiltonian H_c for the system as

$$H_c(\vec{x}_c, \vec{p}_c) := \lim_{\hbar \to 0} H(\vec{X}, \vec{P})\Big|_{\substack{\vec{X} \to \vec{x}_c \\ \vec{P} \to \vec{p}_c}}, \tag{57}$$

where $\vec{w} := (w_1, w_2, \ldots, w_d)^T$ for $\vec{w} = \vec{X}, \vec{P}, \vec{x}_c, \vec{p}_c$; and $\vec{x}_c$ and $\vec{p}_c$ stand for classical position and momentum variables. Supposing that the right-hand side of (57) exists, one may reproduce the quantum system described by the Hilbert space $\mathcal{H}_{\rm phys}$ and Hamiltonian H by quantizing the classical system corresponding to H_c according to

$$\vec{x}_c \to \vec{X}, \quad \vec{p}_c \to \vec{P}, \quad \{\cdot, \cdot\}_c \to -i\hbar^{-1}[\cdot, \cdot], \tag{58}$$

where $\{\cdot, \cdot\}_c$ and $[\cdot, \cdot]$ stand for the Poisson bracket and the commutator, respectively. This is called the *η_+-pseudo-Hermitian canonical quantization* scheme [175, 158].

The quantum system described by $\mathcal{H}_{\rm phys}$ and H admits a representation in conventional QM in which the Hilbert space is $\mathcal{H} = L^2(\mathbb{R}^d)$, the observables are Hermitian operators acting in $\mathcal{H}$, and the Hamiltonian is given by

$$h := \rho H \rho^{-1}. \tag{59}$$

Because $\rho : \mathcal{H}_{\rm phys} \to \mathcal{H}$ is unitary, so is its inverse $\rho^{-1} : \mathcal{H} \to \mathcal{H}_{\rm phys}$. This in turn implies that h is a Hermitian operator acting in $\mathcal{H}$. We will call the representation of the quantum system that is based on the Hermitian Hamiltonian h the *Hermitian representation*. In this representation, we can proceed employing the usual prescription for identifying the underlying classical Hamiltonian, namely as

$$H_c(\vec{x}_c, \vec{p}_c) := \lim_{\hbar \to 0} h(\vec{x}, \vec{p})\Big|_{\substack{\vec{x} \to \vec{x}_c \\ \vec{p} \to \vec{p}_c}}. \tag{60}$$

Note that this relation is consistent with (57), because in view of (55) and (59), $h = f(\vec{x}, \vec{p})$ if and only if $H = f(\vec{X}, \vec{P})$, where we suppose that $f : \mathbb{R}^{2d} \to \mathbb{C}$ is a piecewise real-analytic function.

Each choice of a metric operator $\eta_+ \in \mathfrak{U}_1$ corresponds to a particular quantum system with an associated Hermitian representation. One can, in principle, confine his (her) attention to this representation which can be fully understood using the conventional QM. The main disadvantage of employing the Hermitian representation is that, in general, the Hamiltonian h is a terribly complicated nonlocal operator. Therefore, the computation of the energy levels and the description of the dynamics are more conveniently carried out in the pseudo-Hermitian representation. In contrast, it is the Hermitian representation that facilitates the computation of the expectation values of the physical position and momentum operators as well as that of the localized states in physical position or momentum spaces. See [175, 158, 159, 162] for explicit examples.

3.2. *Pseudo-Hermitian and pseudo-metric operators*

Definition 1. A linear operator $A : \mathcal{H} \to \mathcal{H}$ acting in a separable Hilbert space $\mathcal{H}$ is said to be pseudo-Hermitian if $\mathcal{D}(A)$ is a dense subset of $\mathcal{H}$, and there is an everywhere-defined invertible Hermitian linear operator $\eta : \mathcal{H} \to \mathcal{H}$ such that

$$A^\dagger = \eta A \eta^{-1}. \tag{61}$$

We will refer to an operator η satisfying (61) as a *pseudo-metric operator associated with the operator* A and denote the set of all such operators by $\mathfrak{M}_A$. Clearly, A is pseudo-Hermitian if and only if $\mathfrak{M}_A$ is nonempty. Furthermore, for every linear operator A, $\mathfrak{M}_A \subseteq \mathfrak{M}_I$ where I is the identity operator. We will call elements of $\mathfrak{M}_I$ *pseudo-metric operators*. Because they are Hermitian and have full domain, they are necessarily bounded.[gg]

Clearly if η_1 belongs to $\mathfrak{M}_A$, then so does $\eta_r := r\eta_1$, for every nonzero real number r. The scaling $\eta_1 \to \eta_r$ of the pseudo-metric operators has no physical significance. It signifies a spurious symmetry that we will eliminate by restricting our attention to pseudo-metric operators η whose spectrum $\sigma(A)$ is bounded above by 1, i.e. $\max[\sigma(A)] = 1$.[hh] The latter form a subset of $\mathfrak{M}_A$ which we will denote by $\mathfrak{U}_A$.

[gg] The definition of a pseudo-Hermitian operator given in [143] requires η to be a Hermitian automorphism. This is equivalent to the definition given above because of the following. Firstly, an automorphism is, by definition, everywhere-defined. Hence, if it is Hermitian, it must be bounded. Secondly because the inverse of every Hermitian automorphism is a Hermitian automorphism, η^{-1} is everywhere-defined and bounded, i.e. η is invertible. The fact that every everywhere-defined invertible operator is an automorphism is obvious.

[hh] For a given $\eta_1 \in \mathfrak{M}_A$ there always exists $r_\star \in \mathbb{R}$ such that the spectrum of $\eta_{r_\star}$ is bounded above by 1. This follows from the fact that because η_1 is an invertible bounded self-adjoint operator, its spectrum $\sigma(\eta_1)$ is a compact subset of $\mathbb{R}$ excluding zero [127]. Let α_1 and α_2 be respectively the minimum and maximum values of $\sigma(\eta_1)$. If $\alpha_2 > 0$, we take $r_\star := \alpha_2^{-1}$; if $\alpha_2 < 0$, we take $r_\star := -\alpha_1^{-1}$.

In general, either $\mathfrak{U}_A$ is the empty set and A is not pseudo-Hermitian or $\mathfrak{U}_A$ is an infinite set[ii]; *the pseudo-metric operator associated with a pseudo-Hermitian operator is not unique.* To see this, let $\eta \in \mathfrak{U}_A$, $B : \mathcal{H} \to \mathcal{H}$ be an everywhere-defined invertible bounded operator commuting with A, and $\tilde{\eta} := B^\dagger \eta B$. Then $B^\dagger$ is an everywhere-defined bounded operator [235] commuting with $A^\dagger$. These in turn imply that $\tilde{\eta}$ is an everywhere-defined invertible Hermitian operator which in view of (61) satisfies $\tilde{\eta} A \tilde{\eta}^{-1} = B^\dagger \eta B A B^{-1} \eta^{-1} B^{-1\dagger} = B^\dagger A^\dagger B^{-1\dagger} = A^\dagger$, i.e. $\tilde{\eta} \in \mathfrak{M}_A$. Clearly there is an infinity of choices for B defining an infinite set of pseudo-metric operators of the form $B^\dagger \eta B$. It is not difficult to observe that upon making appropriate scaling of these pseudo-metric operators one can construct an infinite set of elements of $\mathfrak{U}_A$, i.e. $\mathfrak{U}_A$ is an infinite set.

The nonuniqueness of pseudo-metric operators associated with a pseudo-Hermitian operator motivates the following definition.

Definition 2. Let A be a pseudo-Hermitian operator acting in $\mathcal{H}$ and $\eta \in \mathfrak{M}_I$ be a pseudo-metric operator. Then A is said to be η-pseudo-Hermitian if $\eta \in \mathfrak{M}_A$.

Clearly, in order to determine whether a pseudo-Hermitian operator A is η-pseudo-Hermitian one must know both A and η. It is quite possible that a pseudo-Hermitian operator fails to be η-pseudo-Hermitian for a given $\eta \in \mathfrak{M}_I$.[jj]

Given a pseudo-Hermitian operator A, the set $\mathfrak{M}_A$ may or may not include a positive-definite element η_+. If such a positive-definite element exists, we can use it to construct the inner product

$$\langle \cdot \,|\, \cdot \rangle_{\eta_+} := \langle \cdot \,|\, \eta_+ \cdot \rangle \tag{62}$$

that renders A Hermitian,

$$\langle \cdot \,|\, A \cdot \rangle_{\eta_+} = \langle A \cdot \,|\, \cdot \rangle_{\eta_+}. \tag{63}$$

This means that if we endow the underlying vector space $\mathcal{V}$ of $\mathcal{H}$ with the inner product (62), we find a separable Hilbert space $\mathcal{H}_{\eta_+}$ such that $A : \mathcal{H}_{\eta_+} \to \mathcal{H}_{\eta_+}$ is Hermitian. In particular the spectrum $\sigma(A)$ of A is real. If $\sigma(A)$ happens to be discrete, we can construct an orthonormal basis $\{\psi_n\}$ of $\mathcal{H}_{\eta_+}$ consisting of the eigenvectors of A. As a sequence of elements of $\mathcal{H}$, $\{\psi_n\}$ is a Riesz basis. Hence $A : \mathcal{H} \to \mathcal{H}$ is diagonalizable. This shows that for a densely-defined operator having a discrete spectrum, the condition that it is a diagonalizable operator having a real spectrum is necessary for the existence of a metric operator η_+ among the elements of $\mathfrak{M}_A$. The existence of η_+, in particular, implies that $\mathfrak{M}_A$ is nonempty. Hence, A is necessarily pseudo-Hermitian.

[ii] This is true unless the Hilbert space is one-dimensional.

[jj] The term "η-pseudo-Hermitian operator" is used to emphasize that one works with a particular pseudo-metric operator. It coincides with the notion of a "J-Hermitian operator" used by mathematicians [192, 18] and the old notion of a "pseudo-Hermitian operator" used occasionally in the context of indefinite-metric quantum theories [65, 223].

It is not difficult to show that the same conditions are also sufficient for the inclusion of a metric operator in $\mathfrak{M}_A$ [144, 145]. Suppose that $A : \mathcal{H} \to \mathcal{H}$ is a densely-defined diagonalizable operator having a real spectrum. Let $\{\psi_n\}$ be a Riesz basis consisting of the eigenvectors of A and $\{(\psi_n, \phi_n)\}$ be its biorthonormal extension. Then, in view of the spectral representation of A, i.e. $A = \sum_{n=1}^{N} a_n |\psi_n\rangle\langle\phi_n|$ where a_n are eigenvalues of A, and the basic properties of the biorthonormal system $\{(\psi_n, \phi_n)\}$, we can easily show that η_+, as defined by

$$\eta_+ := \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n|, \tag{64}$$

is a positive-definite operator belonging to $\mathfrak{M}_A$. As we explained in Subsec. 2.4, this is the unique metric operator whose inner product makes $\{\psi_n\}$ orthonormal.

Again if $\mathfrak{M}_A$ includes a metric operator η_+, then $\tilde{\eta}_+ = B^\dagger \eta_+ B$ for any everywhere-defined, bounded, invertible operator B commuting with A is also a metric operator belonging to $\mathfrak{M}_A$. This shows that the subset $\mathfrak{M}_A^+$ of $\mathfrak{M}_A$ that consists of metric operators is either empty or has an infinity of elements [146, 148]. The same holds for $\mathfrak{U}_A^+ := \mathfrak{M}_A^+ \cap \mathfrak{U}_A$. In summary, *for a Hilbert space with dimension $N > 1$, either there is no metric operator η_+ satisfying* (63) *or there is an infinite set of such metric operators that in addition fulfil* $\max[\sigma(\eta_+)] = 1$.

One may generalize the notion of the inner product by replacing condition (i) of Subsec. 2.1 by the following weaker condition.

($\tilde{\text{i}}$) $\langle\cdot\,|\,\cdot\rangle$ is *nondegenerate*, i.e. given $\psi \in \mathcal{H}$ the condition "$\langle\phi\,|\,\psi\rangle = 0$ for all $\phi \in \mathcal{H}$" implies "$\psi = 0$".

A function $\prec\cdot\,|\,\cdot\succ : \mathcal{H}\times\mathcal{H} \to \mathbb{C}$ which satisfies conditions ($\tilde{\text{i}}$), (ii) and (iii) is called a *pseudo-inner product*. Clearly every inner product on $\mathcal{H}$ is a pseudo-inner product. The converse is not true, because in general there are pseudo-inner products $\prec\cdot\,|\,\cdot\succ$ that fail to satisfy (i). This means that there may exist nonzero $\psi \in \mathcal{H}$ such that $\prec\psi\,|\,\psi\succ \leq 0$. Such a pseudo-inner product is called an *indefinite inner product*. It is not difficult to see that given a pseudo-metric operator $\eta \in \mathfrak{M}_I$, the following relation defines a pseudo-inner product on $\mathcal{H}$.

$$\prec\cdot\,|\,\cdot\succ = \langle\cdot\,|\,\eta\cdot\rangle =: \langle\cdot\,|\,\cdot\rangle_\eta. \tag{65}$$

Let $A : \mathcal{H} \to \mathcal{H}$ be a densely-defined operator, $\eta : \mathcal{H} \to \mathcal{H}$ be a pseudo-metric operator, and $A_\eta^\dagger := \eta^{-1} A^\dagger \eta$. Then for all $\psi_1 \in \mathcal{D}(A)$ and $\psi_2 \in \mathcal{D}(A_\eta^\dagger)$, we have $\langle\psi_1\,|\,A_\eta^\dagger\psi_2\rangle_\eta = \langle A\psi_1\,|\,\psi_2\rangle_\eta$. In particular, if A is η-pseudo-Hermitian, $A_\eta^\dagger = A$ and

$$\langle\psi_1\,|\,A\psi_2\rangle_\eta = \langle A\psi_1\,|\,\psi_2\rangle_\eta. \tag{66}$$

This means that every pseudo-Hermitian operator A is Hermitian with respect to the pseudo-inner product $\langle\cdot\,|\,\cdot\rangle_\eta$ defined by an arbitrary element η of $\mathfrak{M}_A$. It is not difficult to see that the converse is also true: If ηA and $A^\dagger\eta$ have the same domains and A satisfies (66) for some $\eta \in \mathfrak{M}_I$, then A is pseudo-Hermitian and $\eta \in \mathfrak{M}_A$.

An *indefinite-metric space* is a complex vector space $\mathcal{V}$ endowed with a function $\prec\cdot|\cdot\succ\colon \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ satisfying (i$\tilde{}$), (ii) and (iii) [53, 18]. One can turn a Hilbert space into an indefinite-metric space by endowing the underlying vector space with an indefinite inner product $\langle\cdot\,|\,\cdot\rangle_\eta$ whose pseudo-metric operator η is not positive-definite. The latter is called an *indefinite metric operator*. It is important to realize that the study of general indefinite-metric spaces is not the same as the study of consequences of endowing a given Hilbert space with an indefinite inner product. The latter, which is known as the η-formalism, avoids a host of subtle questions such as the nature of the topology of indefinite-metric spaces [183, 185].

The indefinite-metric quantum theories [190, 223, 183, 185] involve the study of particular indefinite-metric spaces having a fixed indefinite-inner product. In this sense they share the philosophy adopted in conventional QM; *the indefinite-inner product is fixed from the outset and the theory is built upon this choice.* The situation is just the opposite in pseudo-Hermitian QM where the space of state-vectors is supposed to have the structure of a (separable) Hilbert space with an inner product which is neither indefinite nor fixed *a priori*.[kk]

In pseudo-Hermitian QM, the physical Hilbert space is constructed using the following prescription. First one endows the vector space of state-vectors with a fixed auxiliary (positive-definite) inner product. This defines the reference Hilbert space $\mathcal{H}$ in which all the relevant operators act. Next, one chooses a Hamiltonian operator that acts in $\mathcal{H}$, is diagonalizable, has a real spectrum, but need not be Hermitian. Finally, one determines the (positive-definite) inner products on $\mathcal{H}$ that render the Hamiltonian Hermitian. Because there is an infinity of such inner products, one obtains an infinite class of kinematically different but dynamically equivalent quantum systems. The connection to indefinite-metric theories is that for the specific $\mathcal{PT}$-symmetric models whose study motivated the formulation of pseudo-Hermitian QM, there is a simple and universal choice for an indefinite inner product, namely the $\mathcal{PT}$-inner product (3), which makes the Hamiltonian Hermitian. But this indefinite inner product does not define the physical Hilbert space of the theory.

Clearly the basic ingredient in both the indefinite-metric and pseudo-Hermitian QM is the pseudo-metric operator. In general the spectrum of a pseudo-metric operator need not be discrete. However, for simplicity, we first consider a pseudo-metric operator $\eta\in\mathfrak{M}_I$ that has a discrete spectrum. We can express it using its spectral representation as

$$\eta=\sum_{n=1}^{N} e_n|\varepsilon_n\rangle\langle\varepsilon_n|, \tag{67}$$

Because η is a bounded invertible Hermitian operator, its eigenvalues e_n are nonzero and its eigenvectors $|\varepsilon_n\rangle$ form a complete orthonormal basis of the Hilbert space

[kk]Failure to pay attention to this point is responsible for confusing pseudo-Hermitian QM with indefinite-metric quantum theories. See for example [126].

$\mathcal{H}$. Therefore, we can define

$$B := \sum_{n=1}^{N} |e_n|^{-\frac{1}{2}} |\varepsilon_n\rangle\langle\varepsilon_n| = |\eta|^{-\frac{1}{2}}, \tag{68}$$

and use it to obtain a new pseudo-metric operator, namely

$$\tilde{\eta} := B^\dagger \eta B = \sum_{n=1}^{N} \mathrm{sgn}(e_n) |\varepsilon_n\rangle\langle\varepsilon_n|. \tag{69}$$

The presence of a continuous part of the spectrum of η does not lead to any difficulty as far as the above construction is concerned. Because η is Hermitian, one can always define $|\eta| := \sqrt{\eta^2}$ and set $B := |\eta|^{-\frac{1}{2}}$. Both of these operators are bounded, positive-definite, and invertible. Hence $\tilde{\eta} := B^\dagger \eta B$ is an element of $\mathfrak{M}_A$ whose spectrum is a subset of $\{-1, 1\}$.

If we perform the transformation $\eta \to \tilde{\eta}$ on a (positive-definite) metric operator η_+, we find $\tilde{\eta} = I$ and $\langle\cdot\,|\,\cdot\rangle_{\tilde{\eta}} = \langle\cdot\,|\,\cdot\rangle$. This observation is used by Pauli to argue that we would only gain "something essentially new if we take into consideration indefinite bilinear forms…," [190].[ll] To provide a precise justification for this assertion, let η_+ be a (positive-definite) metric operator and $\mathcal{H}_{\eta_+}$ be the Hilbert space having the inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$. Then, for all $\psi_1, \psi_2 \in \mathcal{H}$,

$$\langle B\psi_1\,|\,B\psi_2\rangle_{\eta_+} = \langle B\psi_1\,|\,\eta_+ B\psi_2\rangle = \langle\psi_1\,|\,B^\dagger \eta B\psi_2\rangle = \langle\psi_1\,|\,\tilde{\eta}_+\psi_2\rangle = \langle\psi_1\,|\,\psi_2\rangle, \tag{70}$$

where we have used the identities $B := |\eta_+|^{-\frac{1}{2}} = {\eta_+}^{-\frac{1}{2}}$ and $\tilde{\eta}_+ := B^\dagger \eta_+ B = I$. Equations (70) show that B is a unitary operator mapping $\mathcal{H}$ onto $\mathcal{H}_{\eta_+}$. As a result, the quantum system s_{η_+} whose state-vectors belong to $\mathcal{H}_{\eta_+}$ is unitary-equivalent to the quantum system s_I whose Hilbert space is the reference Hilbert space $\mathcal{H}$. They describe the same physical system. This is the conclusion reached by Pauli in 1943 [190]. There is a simple objection to this argument. It ignores the dynamical aspects of the theory. As we will see below, the description of the Hamiltonian and the time-evolution operator can be very complicated in the "*Hermitian representation*" of the physical system. Therefore, although considering $\mathcal{H}_{\eta_+}$ with a (positive-definite) metric operator η_+ generally yields an equivalent "*pseudo-Hermitian representation*" of the conventional QM, a clever choice of η_+ may be of practical significance in deriving the physical properties of the system under investigation. As we discuss in Subsec. 9.2, it turns out that indeed these new representations play a key role in the resolution of one of the oldest problems of modern physics, namely the problem of negative probabilities in relativistic QM of Klein–Gordon fields [150, 151, 161, 179] and certain quantum field theories [35].

We end this subsection with the following remarks.

- Strictly speaking Pauli's above-mentioned argument does not hold, if one keeps η_+ to be positive-definite but does not require it to be invertible or bounded

[ll] Pauli uses the term "bilinear form" for what we call a "pseudo-inner product".

[123, 211]. For example, one might consider the case that η_+^{-1} exists but is unbounded. In this case, η_+ is not onto and B fails to be a unitary operator. This type of generalized metric operators and the corresponding non-unitary transformations B have found applications in the description of resonances [133, 12, 196]. They also appear in the application of pseudo-Hermitian quantum mechanics for typical $\mathcal{PT}$-symmetric and non-$\mathcal{PT}$-symmetric models. For these models the Hamiltonian operator is a second-order differential operator H acting in an appropriate function space $\mathcal{F}$ that renders the eigenvalue problem for H well-posed. As discussed in great detail in [160], if H is to serve as the Hamiltonian operator for a unitary quantum system, one must construct an appropriate reference Hilbert space $\mathcal{H}$ in which H acts as a quasi-Hermitian operator. This, in particular, implies the existence of an associated metric operator that satisfies the boundedness and other defining conditions of the metric operators.

Suppose H' is a differential operator acting in a function space $\mathcal{F}$ and having a discrete spectrum, i.e. there is a countable set of linearly-independent eigenfunctions of H' with isolated non-degenerate or finitely degenerate eigenvalues. We can use H' and $\mathcal{F}$ to define a unitary quantum system as follows [149, 175].

First, we introduce $\mathscr{F}$ to be the subset of $\mathcal{F}$ that contains the eigenfunctions of H' with real eigenvalues, and let $\mathcal{L}$ be the span of $\mathscr{F}$, i.e. $\mathcal{L} := \{\sum_{m=1}^{M} c_m\psi_m \,|\, M \in \mathbb{Z}^+, c_m \in \mathbb{C}, \psi_m \in \mathscr{F}\}$. Next, we endow $\mathcal{L}$ with the inner product [129]

$$\left\langle \sum_{j=1}^{J} c_j\psi_j \,\middle|\, \sum_{k=1}^{K} d_k\psi_k \right\rangle := \sum_{m=1}^{\min(J,K)} c_m^* d_m, \tag{71}$$

and Cauchy-complete[mm] the resulting inner product space into a Hilbert space $\mathcal{K}$. We can then identify the restriction of H' onto $\mathcal{L}$, that we denote by H, with the Hamiltonian operator of a quantum system. It is a densely-defined operator acting in $\mathcal{K}$, because its domain has a subset $\mathcal{L}$ that is dense in $\mathcal{K}$ [195]. In fact, in view of (71) and the fact that $\mathcal{L}$ is dense in $\mathcal{K}$, the eigenvectors of H form an orthonormal basis of $\mathcal{K}$. Moreover, $H : \mathcal{K} \to \mathcal{K}$ has, by construction, a real spectrum. Therefore, it is a Hermitian operator.

This construction is quite difficult to implement in practice. Instead, one takes the reference Hilbert space $\mathcal{H}$ to be an L^2-space, ensures that the given differential operator that is now denoted by H has a real spectrum, and that the set of its eigenfunctions $\mathscr{F}$ is dense in $\mathcal{H}$. Then, one constructs an invertible positive operator η_+ satisfying the pseudo-Hermiticity condition,

$$H^\dagger = \eta_+ H \eta_+^{-1}, \tag{72}$$

[mm] Every separable inner product space N can be extended to a separable Hilbert space $\mathcal{K}$, called its Cauchy completion, in such a way that N is dense in $\mathcal{K}$ and there is no proper Hilbert subspace of $\mathcal{K}$ with the same properties [195].

and uses it to construct the physical Hilbert space and the Hermitian representation of the system.

For most of the concrete models that have so far been studied, the obtained η_+ turns out not to be everywhere-defined or bounded. But, these qualities are highly sensitive to the choice of the reference Hilbert space that may also be considered as a degree of freedom of the formalism. The mathematical data that have physical content are the eigenfunctions of H and their linear combinations, i.e. elements of $\mathcal{L}$. Therefore, the only physical restriction on the reference Hilbert spaces $\mathcal{H}$ is that $\mathcal{L}$ be a dense subset of $\mathcal{H}$. This means that the question of the existence of a genuine metric operator associated with H requires addressing the problem of the existence of a (reference) Hilbert space $\mathcal{H}$ such that

(1) $\mathcal{L}$ is a dense subset of $\mathcal{H}$, and
(2) there is metric operator $\eta_+ : \mathcal{H} \to \mathcal{H}$ satisfying (72).

It is also possible that given a Hilbert space $\mathcal{H}$ fulfilling the first of these conditions and an unbounded invertible positive operator $\eta_+ : \mathcal{H} \to \mathcal{H}$ satisfying (72), one can construct a genuine bounded metric operator fulfilling the latter condition. These mathematical problems require a systematic study of their own. Following physicists' tradition, we shall ignore mathematical subtleties related to these problems when we deal with specific models that allow for an explicit investigation.

- Let A be a densely-defined linear operator with a nonempty $\mathfrak{U}_A^+$ and $\eta_+ \in \mathfrak{U}_A^+$. Because $B^{-1} := \eta_+^{\frac{1}{2}} : \mathcal{H}_{\eta_+} \to \mathcal{H}$ is a unitary operator and $A : \mathcal{H}_{\eta_+} \to \mathcal{H}_{\eta_+}$ is Hermitian, the operator $a := B^{-1}AB$ is a Hermitian operator acting in $\mathcal{H}$. This shows that $A : \mathcal{H} \to \mathcal{H}$ is related to a Hermitian operator $a : \mathcal{H} \to \mathcal{H}$ via a similarity transformation,

$$A = BaB^{-1}. \tag{73}$$

  Such an operator is called *quasi-Hermitian* [207].[nn]
- Let $B := \eta_+^{-\frac{1}{2}}, B' : \mathcal{H} \to \mathcal{H}_{\eta_+}$ be an arbitrary unitary operator, and $a' := {B'}^{-1}AB'$. Then in view of (73), $a' = U^{-1}aU$, where $U : \mathcal{H} \to \mathcal{H}$ is defined by $U := B^{-1}B'$. Because both B and B' are unitary operators mapping $\mathcal{H}$ onto $\mathcal{H}_{\eta_+}$, a' and U are, respectively, Hermitian and unitary operators acting in $\mathcal{H}$. Conversely, for every unitary operator $U : \mathcal{H} \to \mathcal{H}$ the operator $B' := BU$ is a unitary operator mapping $\mathcal{H}$ onto $\mathcal{H}_{\eta_+}$ and $a' := {B'}^{-1}AB'$ is a Hermitian

[nn] A linear densely-defined operator $A : \mathcal{H} \to \mathcal{H}$ acting in a Hilbert space $\mathcal{H}$ is said to be *quasi-Hermitian* if there exists an everywhere-defined, bounded, invertible linear operator $B : \mathcal{H} \to \mathcal{H}$ and a Hermitian operator $a : \mathcal{H} \to \mathcal{H}$ such that $A = BaB^{-1}$. The above analysis shows that A is quasi-Hermitian if and only if it is pseudo-Hermitian and $\mathfrak{U}_A^+$ is nonempty. In mathematical literature, the term quasi-Hermitian is used for bounded operators A satisfying $A^\dagger T = TA$ for a positive but possibly non-invertible linear operator T [76]. These and their various generalizations and special cases have been studied in the context of symmetrizable operators [197, 131, 213, 239, 125]. For a more recent review see [109].

operator acting in $\mathcal{H}$. These observations show that the most general Hermitian operator $a' : \mathcal{H} \to \mathcal{H}$ that is related to A via a similarity transformation,

$$A = B' a' B'^{-1}, \tag{74}$$

has the form

$$B' = BU = \eta_+^{-\frac{1}{2}} U, \tag{75}$$

where U is an arbitrary unitary transformation acting in $\mathcal{H}$, i.e. $U \in \mathcal{U}(\mathcal{H})$. If we identify A with the Hamiltonian operator for a quantum system and employ the formalism of pseudo-Hermitian QM, the metric operator η_+ defines the physical Hilbert space as $\mathcal{H}_{\rm phys} := \mathcal{H}_{\eta_+}$. Being Hermitian operators acting in $\mathcal{H}_{\rm phys}$, the observables O can be constructed using the unitary operator $B : \mathcal{H} \to \mathcal{H}_{\eta_+}$ and Hermitian operators $o : \mathcal{H} \to \mathcal{H}$ according to

$$O = BoB^{-1} = \eta_+^{-\frac{1}{2}} o \eta_+^{\frac{1}{2}}. \tag{76}$$

One can use any other unitary operator $B' : \mathcal{H} \to \mathcal{H}_{\eta_+}$ for this purpose. Different choices for B' correspond to different one-to-one mappings of the observables O to Hermitian operators o. According to (75), if $o = B^{-1}OB$, then $o' := B'^{-1}OB' = U^{-1}oU$. Therefore making different choices for B' corresponds to performing quantum canonical transformations in $\mathcal{H}$. This in turn means that, without loss of generality, we can identify the physical observables of the system in its pseudo-Hermitian representation using (76).

3.3. *Spectral properties of pseudo-Hermitian operators*

Consider a pseudo-Hermitian operator A acting in an N-dimensional separable Hilbert space $\mathcal{H}$, with $N \leq \infty$, and let $\eta \in \mathfrak{M}_A$. The spectrum of A is the set $\sigma(A)$ of complex numbers λ such that the operator $A - \lambda I$ is not invertible. Let $\lambda \in \sigma(A)$, then $A - \lambda I$ is not invertible and because η is invertible, $\eta(A - \lambda I)\eta^{-1} = A^\dagger - \lambda I$ must not be invertible. This shows that $\lambda \in \sigma(A^\dagger)$. But the spectrum of $A^\dagger$ is the complex-conjugate of the spectrum of A, i.e. $\lambda \in \sigma(A^\dagger)$ if and only if $\lambda^* \in \sigma(A)$ [123]. This argument shows that as a subset of the complex plane $\mathbb{C}$, the spectrum of a pseudo-Hermitian operator is symmetric under the reflection about the real axis [18, 53]. In particular, the eigenvalues a_n of A (for which $A - a_n I$ is not one-to-one) are either real or come in complex-conjugate pairs [190, 143].

Let A be a diagonalizable pseudo-Hermitian operator with a discrete spectrum [195].[oo] Then, one can use a Riesz basis $\{\psi_n\}$ consisting of a set of eigenvectors of A and the associated biorthonomal basis $\{\phi_n\}$ to yield the following spectral representation of A and a pseudo-metric operator $\eta \in \mathfrak{M}_A$ [143, 146].

$$A = \sum_{n_0=1}^{N_0} a_{n_0} |\psi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (\alpha_\nu |\psi_\nu\rangle\langle\phi_\nu| + \alpha_\nu^* |\psi_{-\nu}\rangle\langle\phi_{-\nu}|), \tag{77}$$

[oo]This, in particular, implies that the eigenvalues of A have finite multiplicities.

$$\eta := \sum_{n_0=1}^{N_0} \sigma_{n_0} |\phi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\phi_\nu\rangle\langle\phi_{-\nu}| + |\phi_{-\nu}\rangle\langle\phi_\nu|), \tag{78}$$

where n_0 labels the real eigenvalues a_{n_0} (if any), ν labels the complex eigenvalues α_ν with positive imaginary part (if any), $-\nu$ labels the complex eigenvalues $\alpha_{-\nu} = \alpha_\nu^*$ with negative imaginary part, the eigenvalues with different spectral labels $n \in \{n_0, \nu, -\nu\}$ need not be distinct, $0 \leq N_0, \mathcal{N} \leq \infty$, $\sigma_{n_0} \in \{-1, 1\}$ are arbitrary, and we have

$$A|\psi_{n_0}\rangle = a_{n_0}|\psi_{n_0}\rangle, \quad A|\psi_{\pm\nu}\rangle = \alpha_{\pm\nu}|\psi_{\pm\nu}\rangle, \tag{79}$$

$$\langle\phi_{m_0}\,|\,\psi_{n_0}\rangle = \delta_{m_0,n_0} \qquad \text{for all } m_0, n_0 \in \{1, 2, 3, \ldots, N_0\}, \tag{80}$$

$$\langle\phi_{\mathfrak{g}\mu}\,|\,\psi_{\mathfrak{h}\,\nu}\rangle = \delta_{\mathfrak{g},\mathfrak{h}}\delta_{\mu,\nu} \qquad \text{for all } \mathfrak{g}, \mathfrak{h} \in \{-, +\} \text{ and } \mu, \nu \in \{1, 2, 3, \ldots, \mathcal{N}\}. \tag{81}$$

Consider the set $\mathcal{L}(\{\psi_n\})$ of finite linear combinations of ψ_n's, as defined by (14). According to (77), elements of $\mathcal{L}(\{\psi_n\})$ belong to the domain of A, i.e. $\mathcal{L}(\{\psi_n\}) \subseteq \mathcal{D}(A)$. But because $\{\psi_n\}$ is a basis, $\mathcal{L}(\{\psi_n\})$ is a dense subset of $\mathcal{H}$. This implies that $\mathcal{D}(A)$ is a dense subset of $\mathcal{H}$.

Next, we show that the operator η defined by (78) does actually define a pseudo-metric operator, i.e. it is an everywhere-defined, bounded, invertible, Hermitian operator.

Let $\{\chi_n\}$ be an orthonormal basis of $\mathcal{H}$ and $B : \mathcal{H} \to \mathcal{H}$ be the everywhere-defined, bounded, invertible operator that maps $\{\chi_n\}$ onto the Riesz basis $\{\psi_n\}$, i.e. $\psi_n = B\chi_n$ for all n. It is not difficult to see that the biorthonormal basis $\{\phi_n\}$ may be mapped onto $\{\chi_n\}$ by $B^\dagger$, $\chi_n = B^\dagger\phi_n$ for all n. We can use this relation and (78) to compute

$$\tilde{\eta} := B^\dagger\eta B = \sum_{n_0=1}^{N_0} \sigma_{n_0} |\chi_{n_0}\rangle\langle\chi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\chi_\nu\rangle\langle\chi_{-\nu}| + |\chi_{-\nu}\rangle\langle\chi_\nu|). \tag{82}$$

It is not difficult to show that $\tilde{\eta}$ is a pseudo-metric operator, $\tilde{\eta} \in \mathfrak{M}_I$. To see this, let $\psi \in \mathcal{H}$ be arbitrary. Then because $\{\chi_n\}$ is orthonormal,

$$\psi = \sum_{n=1}^{N} \langle\chi_n\,|\,\psi\rangle\chi_n = \sum_{n_0=1}^{N_0} \langle\chi_{n_0}\,|\,\psi\rangle\chi_{n_0} + \sum_{\nu=1}^{\mathcal{N}} (\langle\chi_\nu\,|\,\psi\rangle\chi_\nu + \langle\chi_{-\nu}\,|\,\psi\rangle\chi_{-\nu}). \tag{83}$$

In view of (82) and (83), we have

$$\tilde{\eta}\psi = \sum_{n_0=1}^{N_0} \sigma_{n_0} \langle\chi_{n_0}\,|\,\psi\rangle\chi_{n_0} + \sum_{\nu=1}^{\mathcal{N}} (\langle\chi_{-\nu}\,|\,\psi\rangle\chi_\nu + \langle\chi_\nu\,|\,\psi\rangle\chi_{-\nu}). \tag{84}$$

In particular,

$$\|\tilde{\eta}\psi\|^2 = \sum_{n_0=1}^{N_0} |\,\langle\chi_{n_0}|\psi\rangle|^2 + \sum_{\nu=1}^{\mathcal{N}} (|\langle\chi_{-\nu}\,|\,\psi\rangle|^2 + |\langle\chi_\nu\,|\,\psi\rangle|^2) = \|\psi\|^2. \tag{85}$$

This shows that not only $\tilde{\eta}$ is everywhere-defined but it is bounded. Indeed, we have $\|\tilde{\eta}\| = 1$. Because $\tilde{\eta}$ is a bounded everywhere-defined operator, $\tilde{\eta}^\dagger$ is also everywhere-defined and as is obvious from (82), it coincides with $\tilde{\eta}$, i.e. $\tilde{\eta}$ is Hermitian. Finally, in view of (82), we can easily show that $\tilde{\eta}^2 = I$. In particular, $\tilde{\eta}^{-1} = \tilde{\eta}$ is bounded and $\tilde{\eta}$ is invertible. This completes the proof of $\tilde{\eta} \in \mathfrak{M}_I$.

Next, we observe that $\tilde{\eta} \in \mathfrak{M}_I$ implies $\eta \in \mathfrak{M}_I$. This is because according to (82), $\eta = {B^\dagger}^{-1}\tilde{\eta}B^{-1}$ and B^{-1} and ${B^\dagger}^{-1}$ are bounded everywhere-defined invertible operators. Therefore, η as defined by (78) is a pseudo-metric operator. Let us also note that the inverse of η is given by

$$\eta^{-1} = B\tilde{\eta}B^\dagger = \sum_{n_0=1}^{N_0} \sigma_{n_0}|\psi_{n_0}\rangle\langle\psi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}}(|\psi_\nu\rangle\langle\psi_{-\nu}| + |\psi_{-\nu}\rangle\langle\psi_\nu|). \tag{86}$$

We can easily show that η belongs to $\mathfrak{M}_A$ by substituting (77), (78), and (86) in $\eta A\eta^{-1}$ and checking that the result coincides with $A^\dagger$.

In Reference [146], it is shown that any element $\eta \in \mathfrak{M}_A$ can be expressed in the form (78) where $\{\psi_n\}$ is the biorthonormal basis associated with some (Riesz) basis $\{\psi_n\}$ consisting of the eigenvectors of A. As any two Riesz bases are related by a bounded everywhere-defined invertible operator $L : \mathcal{H} \to \mathcal{H}$ one may conclude that the elements of $\mathfrak{M}_A$ have the following general form.

$$\eta' = L^\dagger\eta L, \tag{87}$$

where η is the pseudo-metric operator (78) that is defined in terms of a fixed (but arbitrary) (Riesz) basis $\{\psi_n\}$ consisting of the eigenvectors of A and σ_{n_0} are a set of arbitrary signs. The operator L appearing in (87) maps eigenvectors ψ_n of A to eigenvectors $L\psi_n$ of A in such a way that ψ_n and $L\psi_n$ have the same eigenvalue [146]. This, in particular, implies that L commutes with A.

Suppose that A has a complex-conjugate pair of nonreal eigenvalues $\alpha_{\pm\nu}$. Let $\psi_{\pm\nu}$ be a corresponding pair of eigenvectors, $\eta' \in \mathfrak{M}_A$ be an arbitrary pseudo-metric operator associated with A, L be an everywhere-defined, bounded, invertible operator commuting with A and satisfying (87), and $\xi := L^{-1}\psi_\nu$. Then $\langle\xi\,|\,\eta'\xi\rangle = \langle\psi_\nu\,|\,\eta\psi_\nu\rangle = 0$. Because L is invertible $\xi \neq 0$, this is an indication that η' is not a positive-definite operator. Similarly suppose that one of the signs σ_{n_0} appearing in (78) is negative and let $\zeta := L^{-1}\psi_{n_0}$. Then $\langle\zeta\,|\,\eta'\zeta\rangle = \langle\psi_{n_0}\,|\,\eta\psi_{n_0}\rangle = \sigma_{n_0} = -1$, and again η' fails to be positive-definite. These observations show that in order for η' to be a positive-definite operator, the spectrum of A must be real and all the signs σ_{n_0} appearing in (78) must be positive. In this case, we have $\eta' = \eta'_+$, where

$$\eta'_+ := L^\dagger\eta_+ L, \quad \eta_+ = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n|. \tag{88}$$

The choice of the signs σ_{n_0} is not dictated by the operator A itself. Therefore it is the reality of the spectrum of A that ensures the existence of positive-definite

elements of $\mathfrak{M}_A$. By definition, such elements are metric operators belonging to $\mathfrak{M}_A^+$. Their general form is given by (88).

3.4. *Symmetries of pseudo-Hermitian Hamiltonians*

Consider a pseudo-Hermitian operator $A : \mathcal{H} \to \mathcal{H}$ and let η_1 and η_2 be a pair of associated pseudo-metric operators; $\eta_1 A \eta_1^{-1} = A^\dagger = \eta_2 A \eta_2^{-1}$. Then it is a trivial exercise to show that the invertible linear operator $S := \eta_2^{-1}\eta_1$ commutes with A [143]. If we identify A with the Hamiltonian of a quantum system, which we shall do in what follows, S represents a linear symmetry of A.

Next, consider a diagonalizable pseudo-Hermitian operator A with a discrete spectrum, ψ_n be eigenvectors of A, and $\{(\psi_n, \phi_n)\}$ be the complete biorthonormal extension of $\{\psi_n\}$ so that A admits a spectral representation of the form (77):

$$A = \sum_{n_0=1}^{N_0} a_{n_0} |\psi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (\alpha_\nu |\psi_\nu\rangle\langle\phi_\nu| + \alpha_\nu^* |\psi_{-\nu}\rangle\langle\phi_{-\nu}|). \tag{89}$$

Moreover, for every sequence $\sigma = (\sigma_{n_0})$ of signs ($\sigma_{n_0} \in \{-1, +1\}$), let

$$\eta_\sigma := \sum_{n_0=1}^{N_0} \sigma_{n_0} |\phi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\phi_\nu\rangle\langle\phi_{-\nu}| + |\phi_{-\nu}\rangle\langle\phi_\nu|), \tag{90}$$

$$\mathcal{C}_\sigma := \sum_{n_0=1}^{N_0} \sigma_{n_0} |\psi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\psi_\nu\rangle\langle\phi_\nu| + |\psi_{-\nu}\rangle\langle\phi_{-\nu}|), \tag{91}$$

and $\eta_1, \mathfrak{S} : \mathcal{H} \to \mathcal{H}$ be defined by

$$\eta_1 := \sum_{n_0=1}^{N_0} |\phi_{n_0}\rangle\langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\phi_\nu\rangle\langle\phi_{-\nu}| + |\phi_{-\nu}\rangle\langle\phi_\nu|), \tag{92}$$

$$\mathfrak{S} := \sum_{n_0=1}^{N_0} |\psi_{n_0}\rangle \star \langle\phi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\psi_\nu\rangle \star \langle\phi_\nu| + |\psi_{-\nu}\rangle \star \langle\phi_{-\nu}|), \tag{93}$$

where for every $\psi, \phi \in \mathcal{H}$ the symbol $|\psi\rangle \star \langle\phi|$ denotes the following antilinear operator acting in $\mathcal{H}$.

$$|\psi\rangle \star \langle\phi|\zeta := \langle\zeta \,|\, \phi\rangle\psi = \langle\phi \,|\, \zeta\rangle^* \, \psi, \quad \text{for all } \zeta \in \mathcal{H}. \tag{94}$$

As we discussed in Subsec. 3.3, η_σ and η_1 are pseudo-metric operators associated with A. The operators $\mathcal{C}_\sigma$ and $\mathfrak{S}$ have the following remarkable properties [148].

- In view of the fact that $\eta_1^{-1} = \sum_{n_0=1}^{N_0} |\psi_{n_0}\rangle\langle\psi_{n_0}| + \sum_{\nu=1}^{\mathcal{N}} (|\psi_\nu\rangle\langle\psi_{-\nu}| + |\psi_{-\nu}\rangle\langle\psi_\nu|)$, we have

$$\mathcal{C}_\sigma = \eta_1^{-1}\eta_\sigma. \tag{95}$$

Therefore, $\mathcal{C}_\sigma$ is a linear invertible operator that generates a symmetry of A:

$$[\mathcal{C}_\sigma, A] = 0. \tag{96}$$

- Using (94) and the biorthonormality and completeness properties of $\{(\psi_n, \phi_n)\}$, we can check that $\mathfrak{S}$ is an invertible antilinear operator that also commutes with A,

$$[\mathfrak{S}, A] = 0. \tag{97}$$

- $\mathcal{C}_\sigma$ and $\mathfrak{S}$ are commuting involutions, i.e.

$$[\mathcal{C}_\sigma, \mathfrak{S}] = 0, \quad \mathcal{C}_\sigma^2 = \mathfrak{S}^2 = I. \tag{98}$$

In summary, we have constructed an involutive antilinear symmetry generator $\mathfrak{S}$ and a class of involutive linear symmetry generators $\mathcal{C}_\sigma$ that commute with $\mathfrak{S}$.

It turns out that if a given diagonalizable operator A with a discrete spectrum commutes with an invertible antilinear operator, then A is necessarily pseudo-Hermitian. Therefore, for such operators pseudo-Hermiticity and the presence of (involutive) antilinear symmetries are equivalent conditions [145, 219]. Furthermore, each of these conditions is also equivalent to the *pseudo-reality* of the spectrum of A. The latter means that the complex-conjugate of every eigenvalue of A is an eigenvalue with the same multiplicity [145, 219]. These observations are the key for understanding the role of $\mathcal{PT}$-symmetry in the context of our study. They admit extensions for a certain class of non-diagonalizable operators with discrete spectrum [147, 208, 218, 62] and some operators with continuous spectrum [150, 159, 165].

The reality of the spectrum of A is the necessary and sufficient condition for the existence of an associated metric operator and the corresponding positive-definite inner product that renders A Hermitian [144]. For the case that the spectrum of A is real, the expressions for $\eta_\sigma, \eta_1, \mathcal{C}_\sigma$, and $\mathfrak{S}$ simplify:

$$\eta_\sigma := \sum_{n=1}^{N} \sigma_n |\phi_n\rangle\langle\phi_n|, \quad \eta_1 = \sum_{n=1}^{N} |\phi_n\rangle\langle\phi_n| = \eta_+, \tag{99}$$

$$\mathcal{C}_\sigma = \sum_{n=1}^{N} \sigma_n |\psi_n\rangle\langle\phi_n|, \quad \mathfrak{S} = \sum_{n=1}^{N} |\psi_n\rangle \star \langle\phi_n|, \tag{100}$$

and we find

$$\mathcal{C}_\sigma \psi_n = \sigma_n \psi_n, \quad \mathfrak{S}\psi_n = \psi_n. \tag{101}$$

Hence, $\mathcal{C}_\sigma$ and $\mathfrak{S}$ generate exact symmetries of A.

In order to make the meaning of $\mathcal{C}_\sigma$ more transparent, we use the basis expansion of an arbitrary $\psi \in \mathcal{H}$, namely $\psi = \sum_{n=1}^{N} c_n \psi_n$, to compute

$$\mathcal{C}_\sigma \psi = \sum_{n=1}^{N} c_n \mathcal{C}\psi_n = \sum_{n=1}^{N} \sigma_n c_n \psi_n = \psi_+ - \psi_-, \tag{102}$$

where $\psi_\pm := \sum_{n\in\mathfrak{N}_\pm} c_n \psi_n$ and $\mathfrak{N}_\pm := \{n \in \{1, 2, 3, \ldots, N\} \,|\, \sigma_n = \pm 1\}$. According to (102), for every $\psi \in \mathcal{H}$ there are unique state-vectors $\psi_\pm$ belonging to the

eigenspaces $\mathcal{H}_\pm := \{\psi \in \mathcal{H} \,|\, \mathcal{C}_\sigma\psi = \pm\psi\}$ of $\mathcal{C}_\sigma$ such that $\psi = \psi_+ - \psi_-$. This identifies $\mathcal{C}_\sigma$ with a ($\mathbb{Z}_2$-) grading operator for the Hilbert space.

If $\sigma_n = \pm 1$ for all n, we find $\mathcal{C}_\sigma = \pm I$. In the following we consider the nontrivial cases: $\mathcal{C} \neq \pm I$. Then $\mathcal{H}_\pm$ are proper subspaces of $\mathcal{H}$ satisfying

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-, \tag{103}$$

$\mathcal{C}_\sigma$ is a genuine grading operator, both η_σ and $-\eta_\sigma$ fail to be positive-definite, and $\langle\cdot\,|\,\cdot\rangle_{\eta_\sigma}$ is indefinite. Furthermore, in view of (102), the operators $\Pi_\pm := \frac{1}{2}(I \pm \mathcal{C}_\sigma)$, satisfy $\Pi_\pm\psi = \psi_\pm$, i.e. they are projection operators onto $\mathcal{H}_\pm$.

Next, consider computing $\langle\psi_\mathfrak{g}\,|\,\phi_\mathfrak{h}\rangle_{\eta_\sigma}$ for arbitrary $\mathfrak{g},\mathfrak{h} \in \{-,+\}$ and $\psi_\pm, \phi_\pm \in \mathcal{H}_\pm$. Using the basis expansion of $\psi_\pm$ and $\phi_\pm$, i.e. $\phi_\pm = \sum_{n\in\mathfrak{N}_\pm} d_n\psi_n$ and $\psi_\pm = \sum_{n\in\mathfrak{N}_\pm} c_n\psi_n$, and (99), we have $\eta_\sigma\phi_\pm = \pm\sum_{n\in\mathfrak{N}_\pm} d_n\phi_n$ and

$$\langle\psi_\mathfrak{g}\,|\,\phi_\mathfrak{h}\rangle_{\eta_\sigma} = \langle\psi_\mathfrak{g}\,|\,\eta_\sigma\phi_\mathfrak{h}\rangle = \mathfrak{g}\delta_{\mathfrak{g},\mathfrak{h}}\sum_{n\in\mathfrak{N}_\mathfrak{g}} c_n^* d_n. \tag{104}$$

Therefore, with respect to the indefinite inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_\sigma}$, the subspaces $\mathcal{H}_+$ and $\mathcal{H}_-$ are orthogonal, and (103) is an orthogonal direct sum decomposition.

Another straightforward implication of (104) is that, for all $\psi, \phi \in \mathcal{H}$,

$$\begin{aligned}\langle\psi\,|\,\phi\rangle_{\eta_\sigma} &= \langle\psi_+\,|\,\phi_+\rangle_{\eta_\sigma} + \langle\psi_-\,|\,\phi_-\rangle_{\eta_\sigma}\\ &= \sum_{n\in\mathfrak{N}_+} c_n^* d_n - \sum_{n\in\mathfrak{N}_-} c_n^* d_n = \langle\psi_+\,|\,\phi_+\rangle_{\eta_+} - \langle\psi_-\,|\,\phi_-\rangle_{\eta_+},\end{aligned} \tag{105}$$

where $\psi_\pm := \Pi_\pm\psi, \phi_\pm := \Pi_\pm\phi, c_n := \langle\phi_n\,|\,\psi\rangle$ and $d_n := \langle\phi_n\,|\,\phi\rangle$. Similarly, we have

$$\begin{aligned}\langle\psi\,|\,\mathcal{C}_\sigma\phi\rangle_{\eta_\sigma} &= \langle\psi_+\,|\,\phi_+\rangle_{\eta_\sigma} - \langle\psi_-\,|\,\phi_-\rangle_{\eta_\sigma}\\ &= \sum_{n\in\mathfrak{N}_+} c_n^* d_n + \sum_{n\in\mathfrak{N}_-} c_n^* d_n = \sum_{n=1}^{N} c_n^* d_n = \langle\psi\,|\,\phi\rangle_{\eta_+}.\end{aligned} \tag{106}$$

This calculation shows that the positive-definite inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$ can be expressed in terms of the indefinite inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_\sigma}$ and the grading operator $\mathcal{C}_\sigma$ according to

$$\langle\cdot\,|\,\cdot\rangle_{\eta_+} = \langle\cdot\,|\,\mathcal{C}_\sigma\cdot\rangle_{\eta_\sigma}. \tag{107}$$

Conversely, one can use (107) to define a positive-definite inner product that makes H Hermitian. The latter scheme may be traced back to a similar construction developed in the 1950's in the context of indefinite-metric quantum theories [187]. See [183, 185] for reviews. In the context of $\mathcal{PT}$-symmetric quantum mechanics, it was proposed (with a specific choice for the sequence σ) in [37] and coined the name $\mathcal{CPT}$-inner product.

To see the connection with the treatment of [37], consider the case that A, which is now viewed as the Hamiltonian operator for a quantum system, is symmetric, i.e. $A^T := \mathcal{T}A^\dagger\mathcal{T} = A$, where $\mathcal{T}$ is the time-reversal operator.[pp] Then given the

[pp]Recall that $\mathcal{T}$ is an antilinear Hermitian (and unitary) involution [233, 139].

spectral representation of A and $A^\dagger$, we can easily choose a biorthonormal system $\{(\psi_n, \phi_n)\}$ such that

$$\phi_n = \sigma_n \mathcal{T} \psi_n. \tag{108}$$

Using this relation together with the biorthonormality and completeness properties of $\{(\psi_n, \phi_n)\}$, we can obtain the following spectral representation of $\mathcal{T}$.

$$\mathcal{T} = \sum_{n=1}^{N} \sigma_n |\phi_n\rangle \star \langle \phi_n|. \tag{109}$$

In view of Eqs. (99), (100), (109), and $\mathcal{T}^2 = I$, we have

$$\langle \psi_m \,|\, \psi_n \rangle = \sigma_m \sigma_n \langle \phi_n \,|\, \phi_m \rangle, \tag{110}$$

$$\mathfrak{S} = \mathcal{T} \eta_\sigma. \tag{111}$$

Clearly, we could use (109) to define an invertible antilinear operator satisfying (108) for an arbitrary possibly nonsymmetric A, namely

$$\mathcal{T}_\sigma := \sum_{n=1}^{N} \sigma_n |\phi_n\rangle \star \langle \phi_n|. \tag{112}$$

But in this more general case, (110) may not hold and $\mathcal{T}_\sigma$ may not be an involution.

In fact, condition (110) is not only a necessary condition for $\mathcal{T}_\sigma^2 = I$ but it is also sufficient [148]. An analogous necessary and sufficient condition for $\eta_\sigma^2 = I$ is [148]

$$\langle \psi_m \,|\, \psi_n \rangle = \sigma_m \sigma_n \langle \phi_m \,|\, \phi_n \rangle. \tag{113}$$

If both (110) and (113) hold,

$$\mathcal{T}_\sigma^2 = \eta_\sigma^2 = I, \tag{114}$$

and as a result

$$\mathfrak{S} = \mathcal{T}_\sigma \eta_\sigma. \tag{115}$$

By virtue of this relation and $\mathfrak{S}^2 = I$,

$$[\eta_\sigma, \mathcal{T}_\sigma] = 0. \tag{116}$$

Therefore,

$$\mathfrak{S} = \eta_\sigma \mathcal{T}_\sigma. \tag{117}$$

For the symmetric and $\mathcal{PT}$-symmetric Hamiltonians (1) that are considered in [37], we can find a biorthonormal system $\{(\psi_n, \phi_n)\}$ satisfying (110)–(113) [148]. Moreover, setting $\sigma_n := (-1)^{n+1}$ for all $n \in \mathbb{Z}^+$, we have

$$\eta_\sigma = \mathcal{P}. \tag{118}$$

Therefore, in light of (111) and (116), the antilinear symmetry generator $\mathfrak{S}$ coincides with $\mathcal{PT}$,

$$\mathfrak{S} = \mathcal{PT}, \tag{119}$$

and the linear symmetry generator $\mathcal{C}_\sigma$ is the "charge-conjugation" operator $\mathcal{C}$ of [37]. In view of (95), (97), (99), (98) and (118), it satisfies

$$\mathcal{C}^2 = I, \quad [\mathcal{C}, A] = [\mathcal{C}, \mathcal{PT}] = 0, \quad \mathcal{C} = \eta_+^{-1}\mathcal{P}. \tag{120}$$

Furthermore, because in the position representation of the state-vectors $(\mathcal{T}\psi)(x) = \psi(x)^*$, the positive-definite inner product (107) coincides with the $\mathcal{CPT}$-inner product.

This completes the demonstration that the $\mathcal{CPT}$-inner product is an example of the positive-definite inner products $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$ that we explored earlier.

We conclude this subsection by noting that, although in general we can introduce a pair of *generalized time-reversal and parity operators*, η_σ and $\mathcal{T}_\sigma$, they may fail to be involutions.

3.5. *A two-level toy model*

In this subsection, we demonstrate the application of our general results in the study of a simple two-level model which, as we will see in Subsec. 9.2, admits physically important infinite-dimensional generalizations [150, 161, 151].

Let $\mathcal{H}$ be the (reference) Hilbert space obtained by endowing $\mathbb{C}^2$ with the Euclidean inner product and $\{e_1, e_2\}$ be the standard basis of $\mathbb{C}^2$, i.e. $e_1 := \binom{1}{0}$, $e_2 := \binom{0}{1}$. Then we can represent every linear operator K acting in $\mathcal{H}$ in the basis $\{e_1, e_2\}$ by a 2×2 matrix which we denote by $\underline{\mathrm{K}}$; the entries of $\underline{\mathrm{K}}$ have the form $\underline{\mathrm{K}}_{ij} := \langle e_i\,|\,Ke_j\rangle$ where $i, j \in \{1, 2\}$.

Now, consider a linear operator $A : \mathbb{C}^2 \to \mathbb{C}^2$ represented by

$$\underline{\mathrm{A}} := \frac{1}{2}\begin{pmatrix} D+1 & D-1 \\ -D+1 & -D-1 \end{pmatrix}, \tag{121}$$

where D is a real constant. $A : \mathcal{H} \to \mathcal{H}$ is a Hermitian operator if and only if $D = 1$. We can easily solve the eigenvalue problem for A. Its eigenvalues a_n and eigenvectors ψ_n have the form

$$a_1 = -a_2 = D^{\frac{1}{2}}, \quad \psi_1 = c_1\begin{pmatrix} 1+D^{\frac{1}{2}} \\ 1-D^{\frac{1}{2}} \end{pmatrix}, \quad \psi_2 = c_2\begin{pmatrix} 1-D^{\frac{1}{2}} \\ 1+D^{\frac{1}{2}} \end{pmatrix}, \tag{122}$$

where c_1, c_2 are arbitrary nonzero complex numbers. Clearly, for $D = 0$, $a_1 = a_2 = 0$, the eigenvectors become proportional, and A is not diagonalizable. For $D \neq 0$, A has two distinct eigenvalues and $\{\psi_1, \psi_2\}$ forms a basis of $\mathbb{C}^2$. This shows that $D = 0$ marks an exceptional spectral point [123, 103], for $D > 0$ the eigenvalues are real and for $D < 0$ they are imaginary.

It is an easy exercise to show that A is Σ_3-pseudo-Hermitian where $\Sigma_3 : \mathbb{C}^2 \to \mathbb{C}^2$ is the linear operator represented in the standard basis by the Pauli matrix $\sigma_3 := \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. Hence $\mathfrak{M}_A$ includes Σ_3, and A is Σ_3-pseudo-Hermitian for all $D \in \mathbb{R}$. This is consistent with the fact that Σ_3 is not a positive-definite operator, because otherwise A could not have imaginary eigenvalues. According to our general results, for $D > 0$, $\mathfrak{M}_A$ must include positive-definite operators. To construct these we first construct the biorthonormal basis $\{\phi_1, \phi_2\}$ associated with $\{\psi_1, \psi_2\}$. For $D > 0$, the basis vectors ϕ_n are given by

$$\phi_1 = (4c_1^*)^{-1} \begin{pmatrix} 1 + D^{-\frac{1}{2}} \\ 1 - D^{-\frac{1}{2}} \end{pmatrix}, \quad \phi_2 = (4c_2^*)^{-1} \begin{pmatrix} 1 - D^{-\frac{1}{2}} \\ 1 + D^{-\frac{1}{2}} \end{pmatrix}. \tag{123}$$

Inserting these relations in (78) we find the following expression for the matrix representation of the most general pseudo-metric operator $\eta \in \mathfrak{M}_A$.

$$\underline{\eta} = r_1\sigma_1 \begin{pmatrix} (1 + D^{-\frac{1}{2}})^2 & 1 - D^{-1} \\ 1 - D^{-1} & (1 - D^{-\frac{1}{2}})^2 \end{pmatrix} + r_2\sigma_2 \begin{pmatrix} (1 - D^{-\frac{1}{2}})^2 & 1 - D^{-1} \\ 1 - D^{-1} & (1 + D^{-\frac{1}{2}})^2 \end{pmatrix}, \tag{124}$$

where $r_1 := |4c_1|^{-2}$ and $r_2 := |4c_2|^{-2}$ are arbitrary positive real numbers and σ_1, σ_2 are arbitrary signs.

The choice $\sigma_1 = -\sigma_2 = 1$ and $r_1 = r_2 = \frac{D^{\frac{1}{2}}}{4}$ yields $\eta = \Sigma_3$. The choice $\sigma_1 = \sigma_2 = 1$ yields the form of the most general positive-definite element of $\mathfrak{M}_A$. A particularly simple example of the latter is obtained by taking $c_1 = c_2 = \frac{D^{-\frac{1}{4}}}{2}$ which implies $r_1 = r_2 = \frac{D^{\frac{1}{2}}}{4}$. It has the form

$$\underline{\eta}_+ = \frac{1}{2} \begin{pmatrix} D^{\frac{1}{2}} + D^{-\frac{1}{2}} & D^{\frac{1}{2}} - D^{-\frac{1}{2}} \\ D^{\frac{1}{2}} - D^{-\frac{1}{2}} & D^{\frac{1}{2}} + D^{-\frac{1}{2}} \end{pmatrix}. \tag{125}$$

We can simplify this expression by introducing[qq] $\theta := \frac{1}{2} \ln D$, and using the fact that the Pauli matrix $\sigma_1 := \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$ squares to the identity matrix $\underline{\mathrm{I}}$. This yields

$$\underline{\eta}_+ = \begin{pmatrix} \cosh\theta & \sinh\theta \\ \sinh\theta & \cosh\theta \end{pmatrix} = \cosh\theta \underline{\mathrm{I}} + \sinh\theta\, \sigma_1 = e^{\theta\sigma_1}. \tag{126}$$

The metric operator represented by (125) and (126) defines the following (positive-definite) inner product on $\mathbb{C}^2$ with respect to which A is a Hermitian operator.

$$\langle \vec{z} \,|\, \vec{w} \rangle_{\eta_+} := \langle \vec{z} \,|\, \eta_+ \vec{w} \rangle = (z_1^* w_1 + z_2^* w_2) \cosh\theta + (z_1^* w_2 + z_2^* w_1) \sinh\theta, \tag{127}$$

where $\vec{z} = (z_1, z_2)^T, \vec{w} = (w_1, w_2)^T \in \mathbb{C}^2$ are arbitrary. The inner product (127) has a more complicated form than both the reference (Euclidean) inner product,

[qq]This was pointed out to me by Professor Haluk Beker.

$\langle\vec{z}\,|\,\vec{w}\rangle = z_1^* w_1 + z_2^* w_2$, and the indefinite inner product defined by Σ_3,

$$\langle\vec{z}\,|\,\vec{w}\rangle_{\Sigma_3} := \langle\vec{z}\,|\,\Sigma_3\vec{w}\rangle = z_1^* w_1 - z_2^* w_2. \tag{128}$$

Furthermore, unlike $\langle\cdot\,|\,\cdot\rangle$ and $\langle\cdot\,|\,\cdot\rangle_{\Sigma_3}$, the inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$ depends on θ and consequently D. In particular, as $D \to 0$ it degenerates. In fact, a quick inspection of Eq. (124) shows that every D-independent pseudo-metric operator is proportional to Σ_3 and hence necessarily indefinite; $\pm\Sigma_3$ are the only D-independent elements of $\mathfrak{U}_A$.

Now, suppose that A is the Hamiltonian operator of a two-level quantum system. If we employ the prescription provided by the indefinite-metric quantum theories, we should endow $\mathbb{C}^2$ with an indefinite inner product from the outset. The simplest choice that is historically adopted and viewed, according to the above-mentioned argument due to Pauli, as being the unique choice is $\eta = \Sigma_3$. In this case the system has a physical state corresponding to the state-vector e_1 and a hypothetical state or ghost corresponding to e_2. Unfortunately, the subspace of physical state-vector, i.e. the span of $\{e_1\}$, is not invariant under the action of A unless $D = 1$. Hence, for $D \neq 1$, such an indefinite-metric quantum theory suffers from interpretational problems and is inconsistent. In contrast, pseudo-Hermitian quantum mechanics provides a consistent description of a unitary quantum theory based on the Hamiltonian A. This is done by endowing $\mathbb{C}^2$ with the (positive-definite) inner product $\langle\cdot\,|\,\cdot\rangle_{\eta'_+}$, where η'_+ is given by the right-hand side of (124) with $\sigma_1 = \sigma_2 = 1$. It involves the free parameters r_1 and r_2 that can be fixed from the outset or left as degrees of freedom of the formulation of the theory. We can represent this most general metric operator by

$$\underline{\eta'}_+ = r\begin{pmatrix}\cosh\theta + s & \sinh\theta\\ \sinh\theta & \cosh\theta - s\end{pmatrix}, \tag{129}$$

where $r := 2(r_1 + r_2)D^{-\frac{1}{2}} \in \mathbb{R}^+$ and $s := \frac{r_1 - r_2}{r_1 + r_2} \in (-1, 1)$ are arbitrary. We can use (129) to determine the most general inner product on $\mathbb{C}^2$ that makes A Hermitian. This is given by

$$\langle\vec{z}\,|\,\vec{w}\rangle_{\eta'_+} := \langle\vec{z}\,|\,\eta'_+\vec{w}\rangle = r[\langle\vec{z}\,|\,\vec{w}\rangle_{\eta_+} + s\langle\vec{z}\,|\,\vec{w}\rangle_{\Sigma_3}], \tag{130}$$

where $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$ and $\langle\cdot\,|\,\cdot\rangle_{\Sigma_3}$ are respectively defined by (127) and (128).

We can relate η'_+ to η_+ using a linear operator $L : \mathbb{C}^2 \to \mathbb{C}^2$ commuting with A via $\eta'_+ = L^\dagger\eta_+ L$. This operator has the following general form $L = 2D^{-\frac{1}{4}}[\sqrt{r_1}e^{i\varphi_1}|\psi_1\rangle\langle\phi_1| + \sqrt{r_2}e^{i\varphi_2}|\psi_1\rangle\langle\phi_1|]$, where $\varphi_1, \varphi_2 \in [0, 2\pi)$ are arbitrary. We can represent it by

$$\underline{\mathrm{L}} = \begin{pmatrix}\lambda_-\cosh\theta + \lambda_+ & \lambda_-\sinh\theta\\ -\lambda_-\sinh\theta & -\lambda_-\cosh\theta + \lambda_+\end{pmatrix}, \tag{131}$$

where $\lambda_\pm := D^{-\frac{1}{4}}(\sqrt{r}_1 e^{i\varphi_1} \pm \sqrt{r}_2 e^{i\varphi_2})$. With the help of (126), (129) and (131), we have checked that indeed $\underline{\eta'}_+ = \underline{\mathrm{L}}^\dagger\underline{\eta}_+\underline{\mathrm{L}}$.

Next, we wish to establish the quasi-Hermiticity of A for $D > 0$, i.e. show that it can be expressed as $A = BaB^{-1}$ for an invertible operator $B : \mathbb{C}^2 \to \mathbb{C}^2$ and a Hermitian operator $a : \mathcal{H} \to \mathcal{H}$. As we explained in Subsec. 3.2, we can identify B with the inverse of the positive square root of a metric operator belonging to $\mathfrak{M}_A^+$. A convenient choice is $B = \eta_+^{-\frac{1}{2}}$, for in light of (126) we have

$$\underline{\mathrm{B}}^{\pm 1} = e^{\mp\frac{\theta}{2}}\sigma_1 = \begin{pmatrix} \cosh\frac{\theta}{2} & \mp\sinh\frac{\theta}{2} \\ \mp\sinh\frac{\theta}{2} & \cosh\frac{\theta}{2} \end{pmatrix}.$$

This leads to the following remarkably simple expression for the matrix representation of a.

$$\underline{\mathrm{a}} = \underline{\mathrm{B}}^{-1}\underline{\mathrm{A}}\underline{\mathrm{B}} = \begin{pmatrix} D^{\frac{1}{2}} & 0 \\ 0 & -D^{\frac{1}{2}} \end{pmatrix} = D^{\frac{1}{2}}\sigma_3. \tag{132}$$

Hence, $a = D^{\frac{1}{2}}\Sigma_3$.

Because every Hermitian operator $o : \mathcal{H} \to \mathcal{H}$ is a linear combination, with real coefficients, of the identity operator I and the operators Σ_1, Σ_2, and Σ_3 that are respectively represented by Pauli matrices σ_1, σ_2, and σ_3, we can express every physical observable $O : \mathcal{H}_{\eta_+} \to \mathcal{H}_{\eta_+}$ as $O = \mathfrak{a}_0 I + \sum_{j=1}^3 \mathfrak{a}_j S_j$, where $\mathfrak{a}_0, \mathfrak{a}_1, \mathfrak{a}_2, \mathfrak{a}_3$ are some real numbers and $S_j := B\Sigma_j B^{-1} = \eta_+^{-\frac{1}{2}}\Sigma_j\,\eta_+^{\frac{1}{2}}$ for all $j \in \{1, 2, 3\}$. The observables S_j are represented by $\underline{\mathrm{S}_1} = \sigma_1$, $\underline{\mathrm{S}_2} = \cosh\theta\sigma_1 - i\sinh\theta\sigma_3$, and $\underline{\mathrm{S}_3} = i\sinh\theta\sigma_2 + \cosh\theta\sigma_3$.

Next, we repeat the calculation of the Hermitian Hamiltonian and the physical observables for the case that we choose the general metric operator η'_+ to construct the physical Hilbert space, i.e. set $\mathcal{H}_{\rm phys} = \mathcal{H}_{\eta'_+}$. The matrix representation of the Hermitian Hamiltonian $a' : \mathcal{H} \to \mathcal{H}$ is then given by

$$\begin{aligned} \underline{\mathrm{a}'} &= \underline{\eta'_+}^{\frac{1}{2}}\underline{\mathrm{A}}\,\underline{\eta'_+}^{-\frac{1}{2}} = D^{\frac{1}{2}}\begin{pmatrix} u(\theta,s) & v(\theta,s) \\ v(\theta,s) & -u(\theta,s) \end{pmatrix} \\ &= D^{\frac{1}{2}}[v(\theta,s)\sigma_1 + u(\theta,s)\sigma_3], \end{aligned} \tag{133}$$

where $u(\theta,s) := \frac{\sqrt{1-s^2}\,\sinh^2\theta + s^2\cosh\theta}{\sinh^2\theta + s^2}$ and $v(\theta,s) := \frac{s(\cosh\theta - \sqrt{1-s^2})\sinh\theta}{\sinh^2\theta + s^2}$. We can similarly express the physical observables in the form

$$O' = \mathfrak{a}_0 I + \sum_{j=1}^3 \mathfrak{a}_j S'_j, \tag{134}$$

where $S'_j := {\eta'_+}^{-\frac{1}{2}}\Sigma_j{\eta'_+}^{\frac{1}{2}}$.

As seen from (133) the Hermitian Hamiltonian a' describes the interaction of a spin $\frac{1}{2}$ particle with a magnetic field that is aligned along the unit vector $(u, 0, v)^T$ in $\mathbb{R}^3$. As one varies s the magnetic field rotates in the x–z plane. It lies on the z-axis for $s = 0$ which corresponds to using η_+ to define the physical Hilbert space. Clearly, there is no practical advantage of choosing $s \neq 0$. Furthermore, for all $s \in (-1, 1)$ and in particular for $s = 0$, the Hermitian representation of the physical

system is actually less complicated than its pseudo-Hermitian representations. This seems to be a common feature of a large class of two-level systems [149].

Next, we compute the symmetry generator $\mathcal{C}_\sigma$ for $\sigma_1 = -\sigma_2 = 1$. Denoting this operator by $\mathcal{C}$ for simplicity, realizing that $\mathcal{C} = |\psi_1\rangle\langle\phi_1| - |\psi_2\rangle\langle\phi_2|$, and using (122), (123), and $D = e^{2\theta}$, we find

$$\underline{\mathcal{C}} = \begin{pmatrix} \cosh\theta & \sinh\theta \\ -\sinh\theta & -\cosh\theta \end{pmatrix}. \tag{135}$$

Observing that in view of (121), $A^2 = DI$, and making use of this relation and (135) we are led to the curious relation [161]

$$\mathcal{C} = \frac{A}{\sqrt{A^2}}. \tag{136}$$

It is important to note that in performing the above calculation, we have not fixed the normalization constants c_1 and c_2 appearing in (122) and (123). Therefore, up to an unimportant sign, $\mathcal{C}$ is unique.

As we mentioned above, setting $c_1 = c_2 = \frac{D^{-\frac{1}{4}}}{2}$ and $\sigma_1 = -\sigma_2 = 1$, we find the pseudo-metric operator $\eta_\sigma = |\phi_1\rangle\langle\phi_1| - |\phi_2\rangle\langle\phi_2| = \Sigma_3$. Because Σ_3 is a linear involution we can identify it with $\mathcal{P}$. It is a simple exercise to show that $\mathcal{P}, \mathcal{C}$ and η_+ actually satisfy

$$\mathcal{C} = \eta_+^{-1}\mathcal{P}. \tag{137}$$

We can similarly construct the antilinear symmetry generator $\mathfrak{S}$. It turns out that unlike $\mathcal{C}$, $\mathfrak{S}$ depends on (the phase of) normalization constants c_1 and c_2 that appear in (122) and (123). Setting $c_1 = c_2 = \frac{D^{-\frac{1}{4}}}{2}$, we find

$$\mathfrak{S} = \mathcal{T}, \tag{138}$$

where $\mathcal{T}$ denotes complex conjugation, $\mathcal{T}\vec{z} = \vec{z}^*$. In view of (138), the symmetry condition $[\mathfrak{S}, A] = 0$ corresponds to the statement that A is a real operator, i.e. $\underline{A}$ is a real matrix, which is a trivial observation.

Similarly, we can introduce an antilinear operator $\mathcal{T}_\sigma$ according to (112). This yields $\mathcal{T}_\sigma := |\phi_1\rangle\star\langle\phi_1| - |\phi_2\rangle\star\langle\phi_2|$, which in general depends on the choice of c_1 and c_2. For $c_1 = c_2 = \frac{D^{-\frac{1}{4}}}{2}$, we have $\mathcal{T}_\sigma = \mathcal{P}\mathcal{T}$. Combining this relation with (138) yields $\mathfrak{S} = \mathcal{P}\mathcal{T}_\sigma$. It is not difficult to see that indeed $\mathcal{T}_\sigma$ is an involution. But it differs from the usual time-reversal operator $\mathcal{T}$. Let us also point out that we could construct the pseudo-Hermitian quantum system defined by A without going through the computation of $\mathcal{C}$, $\mathcal{P}$ and $\mathcal{T}_\sigma$ operators. What is needed is a metric operator that defines the inner product of the physical Hilbert space.

The construction of the $\mathcal{C}$ operator for two-level systems with a symmetric Hamiltonian has been initially undertaken in [50]. The $\mathcal{C}$ operator for general two-level systems and its relation to the metric operators of pseudo-Hermitian quantum mechanics are examined in [149]. See also [243]. A comprehensive treatment of the most general pseudo-Hermitian two-level system that avoids the use of the $\mathcal{C}$ operator is offered in [178].

4. Calculation of Metric Operator

A pseudo-Hermitian quantum system is defined by a (quasi-Hermitian) Hamiltonian operator and an associated metric operator η_+. This makes the construction of η_+ the central problem in pseudo-Hermitian quantum mechanics. There are various methods of calculating a metric operator. In this section, we examine some of the more general and useful of these methods.

4.1. *Spectral method*

The spectral method, which we employed in Subsec. 3.5, is based on the spectral representation of the metric operator:

$$\eta_+ = \sum_1^N |\phi_n\rangle\langle\phi_n|. \tag{139}$$

It involves the construction of a complete set of eigenvectors ϕ_n of $A^\dagger$ and summing the series appearing in (139) (or performing the integrals in case that the spectrum is continuous).

4.1.1. *$\mathcal{PT}$-symmetric infinite square well*

The first pseudo-Hermitian and $\mathcal{PT}$-symmetric model with an infinite-dimensional Hilbert space that has been treated within the framework of pseudo-Hermitian quantum mechanics is the one corresponding to the $\mathcal{PT}$-symmetric square well potential [241, 19]:

$$v(x) = \begin{cases} -i\zeta\ \mathrm{sgn}(x) & \text{for } |x| < \dfrac{L}{2}, \\ \infty & \text{for } |x| \geq \dfrac{L}{2}, \end{cases} \tag{140}$$

where ζ and L are real parameters, L is positive, and x takes real values. This was achieved in [175] using the spectral method combined with a certain approximation scheme that allowed for a reliable approximate evaluation of a metric operator as well as the corresponding equivalent Hermitian Hamiltonian and pseudo-Hermitian position and momentum operators. A more recent treatment of this model that makes use of the spectral method and obtains a perturbative expansion for a $\mathcal{C}$ operator and the corresponding metric operator η_+ in powers of ζ is given in [51].

4.1.2. *$\mathcal{PT}$-symmetric barrier*

In [159], the spectral method has been used for treating a pseudo-Hermitian quantum system defined by the scattering potential:

$$v(x) = \begin{cases} -i\zeta\ \mathrm{sgn}(x) & \text{for } |x| < \dfrac{L}{2}, \\ 0 & \text{for } |x| \geq \dfrac{L}{2}, \end{cases} \tag{141}$$

where again $\zeta, L, x \in \mathbb{R}$ and L is positive. This potential was originally used in [199] as a phenomenological tool for describing the propagation of electromagnetic waves in certain dielectric wave guides.[rr] It is the first example of a $\mathcal{PT}$-symmetric potential with a continuous spectrum that could be studied thoroughly within the context of pseudo-Hermitian quantum mechanics.

Application of the spectral method for this potential involves replacing the sum in (139) with an integral over the spectral parameter and taking into account the double degeneracy of the energy levels. The extremely lengthy calculation of a metric operator for this potential yields the following remarkably simple expression [159].

$$\langle x|\eta_+|y\rangle = \delta(x-y) + s\frac{\operatorname{im} L^2\zeta}{16\hbar^2}(2L + 2|x+y| - |x+y+L| - |x+y-L|)\operatorname{sgn}(x-y) + \mathcal{O}(\zeta^2), \tag{142}$$

where $x, y \in \mathbb{R}$, and $\mathcal{O}(\zeta^2)$ stands for terms of order ζ^2 and higher.

An unexpected feature of the scattering potential (141) is that the corresponding equivalent Hermitian Hamiltonian has an effective interaction region that is three times larger than that of the potential (141). In other words, in the physical space, which is represented by the spectrum of the pseudo-Hermitian position operator, the interaction takes place in the interval $[-\frac{3L}{2}, \frac{3L}{2}]$ rather than $[-\frac{L}{2}, \frac{L}{2}]$.

4.1.3. *Delta-function potential with a complex coupling*

Another complex scattering potential for which the spectral method could be successfully applied is the delta-function potential [165]:

$$v(x) = \mathfrak{z}\delta(x), \tag{143}$$

where $\mathfrak{z}$ is a complex coupling constant with a positive real part. For this system it has been possible to compute a metric operator and show that it is actually a bounded operator up to and including third-order terms in the imaginary part of $\mathfrak{z}$. It is given by

$$\langle x|\eta_+|y\rangle = \delta(x-y) + \frac{\operatorname{im}\zeta}{2\hbar^2}[\theta(xy)e^{-\kappa|x-y|} + \theta(-xy)e^{-\kappa|x+y|}] \times \operatorname{sgn}(y^2-x^2) + \mathcal{O}(\zeta^2), \tag{144}$$

where $\zeta := \Im(\mathfrak{z}), \kappa := m\hbar^{-2}\Re(\mathfrak{z})$, $\Re$ and $\Im$ denote the real and imaginary parts of their arguments, θ is the step function defined by $\theta(x) := \frac{[1+\operatorname{sgn}(x)]}{2}$ for all $x \in \mathbb{R}$, and we have omitted the quadratic and cubic terms for brevity.

In order to determine the physical meaning of the quantum system defined by the potential (143) and the metric operator (144), we should examine the

[rr]The use of complex potential in constructing various phenomenological models and effective theories has a long history. For a discussion that is relevant to complex scattering potentials, see the review article [181] and [2, 72, 63].

Hermitian representation of the system. The equivalent Hermitian Hamiltonian is given by [165]

$$h = \frac{p^2}{2m} + \Re(\mathfrak{z})\delta(x) + \frac{m\zeta^2}{8\hbar^2}h_2 + \mathcal{O}(\zeta^3), \tag{145}$$

where

$$(h_2\psi)(x) := \mathfrak{a}_\psi e^{-\kappa|x|} + \mathfrak{b}_\psi\delta(x), \tag{146}$$

$\psi \in L^2(\mathbb{R})$ and $x \in \mathbb{R}$ are arbitrary, $\mathfrak{a}_\psi := \psi(0)$, and $\mathfrak{b}_\psi := \int_{-\infty}^{\infty} e^{-\kappa|y|}\psi(y)dy$. As seen from (145) and (146) the nonlocal character of the Hermitian Hamiltonian h is manifested in the ψ-dependence of the coefficients $\mathfrak{a}_\psi$ and $\mathfrak{b}_\psi$.

A generalization of the delta-function potential (143) that allows for a similar analysis is the double-delta function potential: $v(x) = \mathfrak{z}_-\delta(x+a) + \mathfrak{z}_+\delta(x-a)$, where $\mathfrak{z}_\pm$ and a are complex and real parameters, respectively [177, 138]. Depending on the values of the coupling constants $\mathfrak{z}_\pm$, this potential may develop spectral singularities [184, 132]. These are the points where the eigenfunction expansion for the corresponding Hamiltonian breaks down [177]. This is a well-known mathematical phenomenon [184, 132] with an interesting and potentially useful physical interpretation: A spectral singularity is a real energy where both the reflection and transmission coefficients diverge. Therefore it corresponds to a peculiar type of scattering states that behave exactly like resonances: They are resonances with zero-width [172, 173].[ss]

4.1.4. *Other models*

The application of the spectral method for systems with an infinite-dimensional Hilbert space is quite involved. If the system has a discrete spectrum it requires summing complicated series, and if the spectrum is continuous it involves evaluating difficult integrals. This often makes use of certain approximation scheme necessary and leads to approximate expressions for the metric operator. A counterexample to this general situation is the quantum system describing a free particle confined within a closed interval on the real line and subject to a set of $\mathcal{PT}$-symmetric Robin boundary conditions [128]. For this system the spectral method may be employed to yield a closed formula for a metric operator. Other systems for which the spectral method could be employed to give an explicit and exact expression for the metric operator are the infinite-dimensional extensions of the two-level system considered in Subsec. 3.5 where D is identified with a positive-definite operator acting in an infinite-dimensional Hilbert space [150, 151]. These quantum systems appear in a certain two-component representation of the Klein–Gordon [140] and (minisuperspace) Wheeler–DeWitt fields [141].

[ss]The single delta-function potential (143) develops a spectral singularity for imaginary values of $\mathfrak{z}$. For other examples of complex potentials with a spectral singularity, see [202, 172, 173].

4.2. *Perturbation theory*

The standard perturbation theory has been employed in the determination of the spectrum of various complex potentials since long ago [60].[tt] In the present discussion we use the term "perturbation theory" to mean a particular perturbative method of constructing a metric operator for a given quasi-Hermitian Hamiltonian operator. This method involves the following steps.

(1) Decompose the Hamiltonian H in the form

$$H = H_0 + \epsilon H_1, \tag{147}$$

where ϵ is a real (perturbation) parameter, and H_0 and H_1 are respectively Hermitian and anti-Hermitian ϵ-independent operators.

(2) Use the fact that η_+ (being a positive-definite operator) has a unique Hermitian logarithm to introduce the Hermitian operator $Q := -\ln \eta_+$, so that

$$\eta_+ = e^{-Q}, \tag{148}$$

and express the pseudo-Hermiticity relation $H^\dagger = \eta_+ H \eta_+^{-1}$ in the form

$$H^\dagger = e^{-Q} H e^Q. \tag{149}$$

In view of the Backer–Campbell–Hausdorff identity [200],

$$\begin{aligned} e^{-Q} H e^Q &= H + \sum_{\ell=1}^{\infty} \frac{1}{\ell!} [H, Q]_\ell \\ &= H + [H, Q] + \frac{1}{2!}[[H, Q], Q] + \frac{1}{3!}[[[H, Q], Q], Q] + \cdots, \end{aligned} \tag{150}$$

where $[H, Q]_\ell := [[\cdots[[H, Q], Q], \ldots], Q]$ and ℓ is the number of copies of Q appearing on the right-hand side of this relation, (149) yields

$$H^\dagger = H + \sum_{\ell=1}^{\infty} \frac{1}{\ell!} [H, Q]_\ell. \tag{151}$$

(3) Expand Q in a power series in ϵ of the form

$$Q = \sum_{j=1}^{\infty} Q_j \epsilon^j, \tag{152}$$

where Q_j are ϵ-independent Hermitian operators.

(4) Insert (147) and (152) in (151) and equate terms of the same order in powers of ϵ that appear on both sides of this equation. This leads to a set of operator equations for Q_j which have the form [162]

$$[H_0, Q_j] = R_j. \tag{153}$$

[tt] For more recent developments, see [45, 61, 59] and references therein.

Here $j \in \mathbb{Z}^+$ and R_j is determined in terms of H_1 and Q_k with $k < j$ according to

$$R_j := \begin{cases} -2H_1 & \text{for } j = 1, \\ \displaystyle\sum_{k=2}^{j} q_k Z_{kj} & \text{for } j \geq 2, \end{cases} \qquad q_k := \sum_{m=1}^{k} \sum_{n=1}^{m} \frac{(-1)^n n^k m!}{k! 2^{m-1} n! (m-n)!}, \tag{154}$$

$$Z_{kj} := \sum_{\substack{s_1,\ldots,s_k \in \mathbb{Z}^+ \\ s_1+\cdots+s_k=j}} [[[\cdots[H_0, Q_{s1}], Q_{s_2}], \ldots,], Q_{s_k}]. \tag{155}$$

More explicitly we have

$$[H_0, Q_1] = -2H_1, \tag{156}$$

$$[H_0, Q_2] = 0, \tag{157}$$

$$[H_0, Q_3] = -\frac{1}{6}[H_1, Q_1]_2, \tag{158}$$

$$[H_0, Q_4] = -\frac{1}{6}([[H_1, Q_1], Q_2] + [[H_1, Q_2], Q_1]), \tag{159}$$

$$[H_0, Q_5] = \frac{1}{360}[H_1, Q_1]_4 - \frac{1}{6}([H_1, Q_2]_2 + [[H_1, Q_1], Q_3] + [[H_1, Q_3], Q_1]). \tag{160}$$

(5) Solve the above equations for Q_j iteratively by making an appropriate ansatz for their general form.

A variation of this method was originally developed in [40] to compute the $\mathcal{C}$ operator for the following $\mathcal{PT}$-symmetric Hamiltonians and some of their multidimensional and field-theoretical generalizations.

$$H = \frac{1}{2m}p^2 + \frac{1}{2}\mu^2 x^2 + i\epsilon x^3, \tag{161}$$

$$H = \frac{1}{2m}p^2 + i\epsilon x^3, \tag{162}$$

where μ and ϵ are nonzero real coupling constants.

4.2.1. *$\mathcal{PT}$-symmetric cubic anharmonic oscillator*

A perturbative calculation of a metric operator and the corresponding equivalent Hermitian Hamiltonian and pseudo-Hermitian position and momentum operators for the Hamiltonian (161) has been carried out in [158, 118].

Following [40] one can satisfy the operator equations for Q_j by taking $Q_{2i} = 0$ for all $i \in \mathbb{Z}^+$ and adopting the ansatz

$$Q_{2i+1} = \sum_{j,k=0}^{i+1} c_{ijk}\{x^{2j}, p^{2k+1}\}, \tag{163}$$

where $\{\cdot,\cdot\}$ stands for the anticommutator and c_{ijk} are real constants. Inserting (163) in (153), one can determine c_{ijk} for small values of i [158]. See also [40, 118].

Again, to determine the physical content of the system defined by the Hamiltonian (161) and the metric operator $\eta_+ = e^{-Q}$, we need to inspect the associated Hermitian Hamiltonian operator [158]:

$$\begin{aligned} h = {} & \frac{p^2}{2m} + \frac{1}{2}\mu^2 x^2 + \frac{1}{m\mu^4}\left(\{x^2, p^2\} + p\, x^2 p + \frac{3m\mu^2}{2}\, x^4\right)\epsilon^2 \\ & + \frac{2}{\mu^{12}}\left(\frac{p^6}{m^3} - \frac{63\mu^2}{16m^2}\{x^2, p^4\} - \frac{81\mu^2}{8m^2}\, p^2 x^2 p^2 - \frac{33\mu^4}{16m}\{x^4, p^2\}\right. \\ & \left. - \frac{69\mu^4}{8m}\, x^2 p^2 x^2 - \frac{7\mu^6}{4}\, x^6\right)\epsilon^4 + \mathcal{O}(\epsilon^6), \end{aligned} \tag{164}$$

and the underlying classical Hamiltonian (60):

$$\begin{aligned} H_c = {} & \frac{p_c^2}{2m} + \frac{1}{2}\mu^2 x_c^2 + \frac{3}{2\mu^4}\left(\frac{2}{m} x_c^2 p_c^2 + \mu^2 x_c^4\right)\epsilon^2 \\ & + \frac{2}{\mu^{12}}\left(\frac{p_c^6}{m^3} - \frac{18\mu^2}{m^2} x_c^2 p_c^4 - \frac{51\mu^4}{4m} x_c^4 p_c^2 - \frac{7\mu^6}{4} x_c^6\right)\epsilon^4 + \mathcal{O}(\epsilon^6). \end{aligned} \tag{165}$$

If we only consider the terms of order ϵ^2 and lower, we can express (165) in the form

$$H_c = \frac{p_c^2}{2M(x_c)} + \frac{\mu^2}{2}\, x_c^2 + \frac{3\epsilon^2}{2\mu^2}\, x_c^4 + \mathcal{O}(\epsilon^4), \tag{166}$$

where $M(x_c) := m(1 + 3\mu^{-4}\epsilon^2 x_c^2)^{-1} = m(1 - 3\mu^{-4}\epsilon^2 x_c^2) + \mathcal{O}(\epsilon^4)$. This shows that for small values of ϵ, the $\mathcal{PT}$-symmetric Hamiltonian (161) describes a position-dependent-mass quartic anharmonic oscillator [158]. This observation has motivated the use of non-Hermitian constant-mass standard Hamiltonians, $H = \frac{p^2}{(2m)+v(x)}$, in the perturbative description of a class of position-dependent-mass standard Hamiltonians [21].

As seen from (164), the fourth-order (in ϵ) contribution to the equivalent Hermitian Hamiltonian h involves p^6. It is not difficult to show that $h = \sum_{\ell=0}^{\infty} h_\ell \epsilon^{2\ell}$, where h_ℓ is a polynomial in p whose degree is an increasing function of ℓ. Therefore, the perturbative expansion of h includes arbitrarily large powers of p. This confirms the expectation that h is a nonlocal operator. The same holds for the pseudo-Hermitian position and momentum operators [158, 118].

4.2.2. *Imaginary cubic potential*

Reference [162] gives a perturbative treatment of the Hamiltonian

$$H = \frac{p^2}{2m} + i\epsilon x^3, \tag{167}$$

in which the operator equations (153) are turned into certain differential equations and solved iteratively. This method relies on the observation that for this Hamiltonian, $H_0 = \frac{p^2}{2m}$. Therefore, $\langle x|[H_0, Q_j]|y\rangle = -\frac{\hbar^2}{2m}(\partial_x^2 - \partial_y^2)\langle x|Q_j|y\rangle$. In view of this identity and (153), we find

$$(-\partial_x^2 + \partial_y^2)\langle x|Q_j|y\rangle = \frac{2m}{\hbar^2}\langle x|R_j|y\rangle. \tag{168}$$

Because R_j is given in terms of H_1 and Q_i with $i < j$, one can solve (168) iteratively for $\langle x|Q_j|y\rangle$. Note also that this equation is a non-homogeneous $(1+1)$-dimensional wave equation which is exactly solvable.

This approach has two important advantages over the earlier perturbative calculation of the metric operator for the imaginary cubic potential [40]. Firstly, it involves solving a well-known differential equation rather than dealing with difficult operator equations. Secondly, it is not restricted by the choice of an ansatz, i.e. it yields the most general expression for the metric operator. In particular, it reveals large classes of $\mathcal{CPT}$ and non-$\mathcal{CPT}$-inner products that were missed in an earlier calculation given in [40]. Here we give the form of the equivalent Hermitian Hamiltonian associated with the most general admissible metric operator:

$$\begin{aligned} h = \frac{p^2}{2m} + \frac{3m}{16}\Bigg(&\left\{x^6, \frac{1}{p^2}\right\} + 22\hbar^2\left\{x^4, \frac{1}{p^4}\right\} + \alpha_2\hbar^4\left\{x^2, \frac{1}{p^6}\right\} \\ &+ \frac{(14\alpha_2 + 1680)\hbar^6}{p^8} + \beta_2\hbar^3\left\{x^3, \frac{1}{p^5}\right\}\mathcal{P}\Bigg)\epsilon^2 \\ &+ \hbar^6\left(\alpha_3\left(\hbar\left\{x^2, \frac{1}{p^{11}}\right\} + \frac{44\hbar^3}{p^{13}}\right) + i\beta_3\left\{x^3, \frac{1}{p^{10}}\right\}\mathcal{P}\right)\epsilon^3 + \mathcal{O}(\epsilon^4), \end{aligned} \tag{169}$$

where $\alpha_2, \alpha_3, \beta_2, \beta_3$ are free real parameters characterizing the nonuniqueness of the metric operator, and $\mathcal{P}$ is the parity operator [162].

A remarkable feature of the Hamiltonian (167) is that the underlying classical Hamiltonian is independent of the choice of the metric operator (to all orders of perturbation). Up to terms of order ϵ^3 it is given by the following simple expression.

$$H_c = \frac{p_c^2}{2m} + \frac{3}{8}\, m\epsilon^2\, \frac{x_c^6}{p_c^2} + \mathcal{O}(\epsilon^4). \tag{170}$$

The presence of p_c^2 in the denominator of the second term is a clear indication that the equivalent Hermitian Hamiltonian is a nonlocal operator (and that this is the case regardless of the choice of the metric operator). Again the classical Hamiltonian (170) clarifies the meaning of the imaginary cubic potential $i\epsilon x^3$.

4.2.3. *Other models*

The perturbation theory usually leads to an infinite series expansion for the metric operator whose convergence behavior is difficult to examine. There are, however, very special models for which this method gives exact expressions for Q and consequently the metric operator $\eta_+ = e^{-Q}$. Examples of such models are given in [35, 48, 120, 49]. The simplest example is the free particle Hamiltonian studied in [162].

For other examples of the perturbative calculation of a metric operator and the corresponding equivalent Hermitian Hamiltonian, see [22] and particularly [88].

4.3. *Differential representations of pseudo-Hermiticity*

In the preceding subsection, we show how one can turn the operator equations appearing in the perturbative calculation of the metric operator into certain differential equations. In this subsection, we outline a direct application of differential equations in the computation of pseudo-metric operators for a large class of pseudo-Hermitian Hamiltonian operators H acting in the reference Hilbert space $L^2(\mathbb{R})$.

In the following we outline two different methods of identifying a differential representation of the pseudo-Hermiticity condition,

$$H^\dagger = \eta H \eta^{-1}. \tag{171}$$

4.3.1. *Field equation for the metric from Moyal product*

Consider expressing (171) in the form

$$\eta H = H^\dagger \eta, \tag{172}$$

and viewing η and H as complex-valued functions of x and p that are composed by the Moyal $*$-product:

$$f(x,p) * g(x,p) := f(x,p) e^{i\hbar \overleftarrow{\partial_x}\overrightarrow{\partial_p}} g(x,p) = \sum_{k=0}^{\infty} \frac{(i\hbar)^k}{k!} [\partial_x^k f(x,p)] \partial_p^k g(x,p). \tag{173}$$

This yields: $\eta(x,p) * H(x,p) = H(x,p)^* * \eta(x,p)$ [206]. With the help of (173) we can express this equation more explicitly as

$$\sum_{k=0}^{\infty} \frac{(i\hbar)^k}{k!} \{[\partial_p^k H(x,p)] \partial_x^k - [\partial_x^k H(x,p)^*] \partial_p^k\} \eta(x,p) = 0. \tag{174}$$

This is a linear homogeneous partial differential equation of finite order only if $H(x,p)$ is a polynomial in x and p. For example, for the imaginary cubic potential, i.e. the Hamiltonian $H = \frac{p^2}{2m} + i\epsilon x^3$, it reads

$$[\epsilon\hbar^3 \partial_p^3 - 3i\epsilon\hbar^2 x \partial_p^2 - (2m)^{-1}\hbar^2 \partial_x^2 - 3\epsilon\hbar x^2 \partial_p + im^{-1}\hbar p \partial_x + 2i\epsilon x^3] \eta(x,p) = 0. \tag{175}$$

The presence of variable coefficients in this equation is an indication that it is not exactly solvable. Particular perturbative solutions can however be constructed.

This applies more generally for other polynomial Hamiltonians. Explicit examples are given in [206, 89, 15].

We should like to note however that not every solution of (174) defines a pseudo-metric (respectively metric) operator. We need to find solutions that correspond to Hermitian (respectively positive-definite) and invertible operators η. Reference [206] suggests ways to address this problem.

The above-described method that is based on the Moyal product has two important shortcomings.

(1) If the Hamiltonian is not a polynomial of x and p, then the resulting Eq. (174) is not a differential equation with a finite order. This makes its solution extremely difficult. This is true unless $H(x,p)$ has a particularly simple form. A typical example is the exponential potential e^{ix} treated in Reference [69]. This potential is actually one of the oldest $\mathcal{PT}$-symmetric potentials whose spectral problem has been examined thoroughly [91]. For $x \in \mathbb{R}$, its spectrum includes an infinity of spectral singularities that prevent this potential from defining a genuine unitary evolution.[uu]

(2) For the polynomial Hamiltonians, for which (174) is a differential equation, the general form and even the order of this equation depends on the Hamiltonian. In particular, for the standard Hamiltonians of the form

$$H = \frac{p^2}{2m} + v(x), \tag{176}$$

they depend on the choice of the potential $v(x)$.

We shall next discuss a differential representation of the pseudo-Hermiticity that does not suffer from any of these shortcomings.

4.3.2. *Universal field equation for the metric*

Consider a pseudo-Hermitian Hamiltonian of standard form (176). Substituting (176) in the pseudo-Hermiticity relation $\eta H = H^\dagger \eta$ and evaluating the matrix elements of both sides of the resulting equation in the coordinate basis $\{|x\rangle\}$, we find [163]

$$[-\partial_x^2 + \partial_y^2 + \mu^2(x,y)]\eta(x,y) = 0, \tag{177}$$

where $\mu^2(x,y) := \frac{2m}{\hbar^2}[v(x)^* - v(y)]$, and $\eta(x,y) := \langle x|\eta|y\rangle$. Equation (177) is actually a Klein–Gordon equation for $\langle x|\eta|y\rangle$ (with a variable mass term). As such, it is much easier to handle than the equation obtained for the pseudo-metric in the preceding subsection, i.e. (174). Moreover, it applies to arbitrary polynomial and non-polynomial potentials.

[uu]For a discussion of biorthonormal systems for this potential with x taking values on a circle (a closed interval with periodic boundary condition on the eigenfunctions), see [68].

It turns out that one can actually obtain a formal series expansion for the most general solution of (177) that satisfies the Hermiticity condition: $\eta(x,y)=\eta(y,x)^*$. This solution has the form [163]

$$\eta(x,y)=\sum_{\ell=0}^{\infty}\mathcal{K}^\ell u(x,y), \tag{178}$$

where $\mathcal{K}$ is the integral operator defined by

$$\mathcal{K}f(x,y):=\frac{m}{\hbar^2}\left[\int^y dr\int_{x-y+r}^{x+y-r}dsv(r)f(s,r)+\int^x ds\int_{-x+y+s}^{x+y-s}drv(s)^*f(s,r)\right], \tag{179}$$

$f:\mathbb{R}^2\to\mathbb{C}$ is an arbitrary test function, $u:\mathbb{R}^2\to\mathbb{C}$ is defined by $u(x,y):=u_+(x-y)+u_-(x+y)$, and $u_\pm$ are arbitrary complex-valued (piecewise) smooth (generalized) functions satisfying $u_\pm(x)^*=u_\pm(\mp x)$.

For imaginary potentials, the series solution (178) provides an extremely effective perturbative method for the construction of the most general metric operator. For example, the application of this method for the $\mathcal{PT}$-symmetric square well potential that we discussed in Subsec. 4.1.1 yields, after a page-long straightforward calculation [163]

$$\eta(x,y)=\delta(x-y)+\zeta\left[w_+(x-y)+w_-(x+y)+\frac{\mathrm{im}}{2\hbar^2}|x+y|\,\mathrm{sgn}(x-y)\right]+\mathcal{O}(\zeta^2), \tag{180}$$

where $w_\pm:[-\frac{L}{2},\frac{L}{2}]\to\mathbb{C}$ are arbitrary functions satisfying $w_\pm(x)^*=w_\pm(\mp x)$ and $w_\pm(\pm L)=0$. The metric operator associated with the $\mathcal{CPT}$-inner product that is computed using the spectral method in [51] turns out to correspond to a particular choice for $w_\pm$ in (180).

A probably better evidence of the effectiveness of this method is its application in the construction of a metric operator for the $\mathcal{PT}$-symmetric barrier potential that we examined in Subsec. 4.1.2. Again, a two-page-long calculation yields [163]

$$\begin{aligned}\eta(x,y)=\delta(x-y)+\zeta\Big[&w_+(x-y)+w_-(x+y)\\&+\frac{\mathrm{im}}{4\hbar^2}(2|x+y|-|x+y+L|-|x+y-L|)\,\mathrm{sgn}(x-y)\Big]+\mathcal{O}(\zeta^2).\end{aligned} \tag{181}$$

This expression reproduces the result obtained in [159] using the spectral method (after over a hundred pages of calculations), namely (142), as a special case.

In [163], this differential representation of pseudo-Hermiticity has been used to obtain a perturbative expression for the metric operator associated with the

imaginary delta-function potentials of the form[vv]

$$v(x) = i\sum_{n=1}^{N}\zeta_n\delta(x-a_n), \tag{182}$$

where $\zeta_n, a_n \in \mathbb{R}$. The result is

$$\eta(x,y) = \delta(x-y) + \sum_{n=1}^{N}\frac{2m\zeta_n}{\hbar^2}\Big[w_{n+}(x-y) + w_{n-}(x+y) + \frac{i}{2}\theta(x+y-2a_n)\,\mathrm{sgn}(y-x)\Big] + \mathcal{O}(\zeta_n^2). \tag{183}$$

For the special case: $N = 2$, $a_1 = -a_2 > 0$ and $\zeta_1 = -\zeta_2 > 0$, where (182) is a $\mathcal{PT}$-symmetric potential, a careful application of the spectral method yields a positive-definite perturbatively bounded metric operator [24] that turns out to be a special case of (183). The general $N = 2$ case, that depending on the choice of ζ_k may or may not possess $\mathcal{PT}$-symmetry, has been examined in [177, 138].

The main difficulty with the approaches presented in this section (and its subsections) is that they may lead to a "metric" operator that is unbounded or non-invertible.[ww] For example, setting $N = 1$ in (182), one finds a delta function potential with an imaginary coupling that gives rise to a spectral singularity [165]. Therefore, the corresponding Hamiltonian is not quasi-Hermitian, and there is actually no genuine (bounded, invertible, positive-definite) metric operator for this potential. Yet, one can use (183) to obtain a formula for a "metric operator"! This observation suggests that one must employ this method with extra care.

4.4. *Lie algebraic method*

In Subsec. 4.2, we described a perturbative scheme for solving the pseudo-Hermiticity relation,

$$H^\dagger = e^{-Q}He^{Q}, \tag{184}$$

for the operator Q that yields a metric operator upon exponentiation, $\eta_+ = e^{-Q}$. In this section, we explore a class of quasi-Hermitian Hamiltonians and corresponding metric operators for which (184) reduces to a finite system of numerical equations, although the Hilbert space is infinite-dimensional. The key idea is the use of an underlying Lie algebra. In order to describe this method we first recall some basic facts about Lie algebras and their representations.

[vv]The spectral properties of $\mathcal{PT}$-symmetric potentials of this form and their consequences have been studied in [117, 1, 7, 72, 226]. In particular, see [177].

[ww]One must also restrict the free functions appearing in the formula for $\eta(x,y)$ so that the operator η they define, is at least densely-defined.

4.4.1. *Lie algebras and their representations*

Consider a matrix Lie group G, i.e. a subgroup of the general linear group $GL(N,\mathbb{C})$ for some $N\in\mathbb{Z}^+$, and let $\mathcal{G}$ denote its Lie algebra [83, 108]. A unitary representation of G is a mapping $\mathcal{U}$ of G into the group of all unitary operators acting in a separable Hilbert space $\mathcal{H}$ such that the identity element of G is mapped to the identity operator acting in $\mathcal{H}$ and for all $g_1,g_2\in G$, $\mathcal{U}(g_1g_2)=\mathcal{U}(g_1)\mathcal{U}(g_2)$. Such a unitary representation induces a unitary representation for $\mathcal{G}$, i.e. a linear mapping $\mathfrak{U}$ of $\mathcal{G}$ into the set of anti-Hermitian linear operators acting in $\mathcal{H}$ such that for all $X_1,X_2\in\mathcal{G}$, $\mathfrak{U}([X_1,X_2])=[\mathfrak{U}(X_1),\mathfrak{U}(X_2)]$ [83, 85]. The mappings $\mathcal{U}$ and $\mathfrak{U}$ are related according to: $\mathcal{U}(e^X)=e^{\mathfrak{U}(X)}$, for all $X\in\mathcal{G}$. Furthermore, because for all $X\in\mathcal{G}$, $\mathfrak{U}(X)$ is an anti-Hermitian operator acting in $\mathcal{H}$, there is a Hermitian operator $K:\mathcal{H}\to\mathcal{H}$ such that $\mathfrak{U}(X)=iK$.

Let $\{K_1,K_2,\dots,K_d\}$ be a set of Hermitian operators acting in $\mathcal{H}$ such that $\{iK_1,iK_2,\dots,iK_d\}$ is a basis of $\mathfrak{U}(\mathcal{G})$. Then K_a with $a\in\{1,2,\dots,d\}$ are called *generators* of G in the representation $\mathcal{U}$. If $\mathcal{U}$ is a faithful representation, i.e. it is a one-to-one mapping, the same holds for $\mathfrak{U}$, and d coincides with the dimension of G. In this case, we refer to the matrices

$$\underline{\mathrm{K}_a}:=\mathfrak{U}^{-1}(K_a) \tag{185}$$

as generators of G in its standard representation.

Next, consider the set of complex linear combinations of $\underline{\mathrm{K}_a}$, i.e. the *complexification* of $\mathcal{G}$: $\mathcal{G}_{\mathbb{C}}:=\{\sum_{a=1}^d \mathfrak{c}_a\underline{\mathrm{K}_a}\mid \mathfrak{c}_a\in\mathbb{C}\}$. We can extend the domain of definition of $\mathfrak{U}$ to $\mathcal{G}_{\mathbb{C}}$ by linearity: For all $\mathfrak{c}_a\in\mathbb{C}$, $\mathfrak{U}(\sum_{a=1}^d \mathfrak{c}_a\underline{\mathrm{K}_a}):=\sum_{a=1}^d \mathfrak{c}_a\mathfrak{U}(\underline{\mathrm{K}_a})=\sum_{a=1}^d \mathfrak{c}_aK_a$. Similarly, we extend the definition of $\mathcal{U}$ to the set of elements of $GL(N,\mathbb{C})$ that are obtained by exponentiation of those of $\mathcal{G}_{\mathbb{C}}$. This is done according to

$$\mathcal{U}(e^X)=e^{\mathfrak{U}(X)},\quad \text{for all } X\in\mathcal{G}_{\mathbb{C}}. \tag{186}$$

Next, we recall that according to Backer–Campbell–Hausdorff identity (150), for all $X,Y\in\mathcal{G}_{\mathbb{C}}$, $e^{-X}Ye^X\in\mathcal{G}_{\mathbb{C}}$. Furthermore, (150) and (186) imply

$$\mathcal{U}(e^{-X}Ye^X)=e^{-\mathfrak{U}(X)}\mathfrak{U}(Y)e^{\mathfrak{U}(X)}=\mathcal{U}(e^{-X})\mathfrak{U}(Y)\mathcal{U}(e^X)\quad \text{for all } X,Y\in\mathcal{G}_{\mathbb{C}}. \tag{187}$$

This completes our mathematical digression.

4.4.2. *General outline of the method*

Suppose that $H:\mathcal{H}\to\mathcal{H}$ can be expressed as a polynomial in the Hermitian generates K_a of G in a faithful unitary representation $\mathcal{U}$,[xx] i.e.

$$H=\sum_{k=1}^n\sum_{a_1,a_2,\dots,a_k=1}^d \lambda_{a_1,a_2,\dots,a_k}K_{a_1}K_{a_2}\cdots K_{a_k}, \tag{188}$$

[xx]In mathematical terms, one says that H is an element of the enveloping algebra of $\mathcal{G}$ in the representation $\mathcal{U}$.

where $n \in \mathbb{Z}^+$, d is the dimension of G, and $\lambda_{a_1,a_2,\ldots a_k} \in \mathbb{C}$. Demand that H admits a metric operator of the form $\eta_+ = e^{-Q}$ with Q given by

$$Q = \sum_{a=1}^{d} r_a K_a, \quad \text{for some } r_a \in \mathbb{R}. \tag{189}$$

Then as we will show below, the right-hand side of (184) can be evaluated using the standard representation of $\mathcal{G}$ and readily expressed as a polynomial in K_a with the same order as H. Upon imposing (184), we therefore obtain a (finite) set of numerical equations involving the coupling constants $\lambda_{a_1,a_2,\ldots a_k}$ and the parameters r_a that determine the metric operator via

$$\eta_+ := \exp\left(-\sum_{a=1}^{d} r_a K_a\right). \tag{190}$$

In order to demonstrate how this method works, we introduce the matrix $\underline{\eta_+} := \exp(-\sum_{a=1}^{d} r_a \underline{\mathrm{K}_a})$, that belongs to $\exp(\mathcal{G}_{\mathbb{c}})$ and satisfies $\eta_+ = \mathcal{U}(\underline{\eta_+})$. This together with (185) and (187) imply

$$\begin{aligned}\eta_+ H \eta_+^{-1} &= \sum_{k=1}^{n} \sum_{a_1,a_2,\ldots,a_k=1}^{d} \lambda_{a_1,a_2,\ldots a_k}\ (\eta_+ K_{a_1} \eta_+^{-1})(\eta_+ K_{a_2} \eta_+^{-1}) \cdots (\eta_+ K_{a_k} \eta_+^{-1}) \\ &= \sum_{k=1}^{n} \sum_{a_1,a_2,\ldots,a_k=1}^{d} \lambda_{a_1,a_2,\ldots a_k} \mathfrak{U}(\underline{\eta_+}\ \underline{\mathrm{K}_{a_1}}\ \underline{\eta_+^{-1}}) \cdots \mathfrak{U}(\underline{\eta_+}\ \underline{\mathrm{K}_{a_k}}\ \underline{\eta_+^{-1}})\end{aligned} \tag{191}$$

Because for all $a \in \{1, 2, \ldots, d\}$, $\underline{\eta_+}\,\underline{\mathrm{K}_a}\,\underline{\eta_+^{-1}}$ belongs to $\mathcal{G}_{\mathbb{c}}$, there are complex coefficients κ_{ab} depending on the structure constants C_{abc} of the Lie algebra $\mathcal{G}$ and the coefficients r_a such that

$$\underline{\eta_+}\ \underline{\mathrm{K}_a}\ \underline{\eta_+^{-1}} = \sum_{b=1}^{d} \kappa_{ab} \underline{\mathrm{K}_b}. \tag{192}$$

As a result, $\mathfrak{U}(\underline{\eta_+}\ \underline{\mathrm{K}_a}\ \underline{\eta_+^{-1}}) = \sum_{b=1}^{d} \kappa_{ab} \mathfrak{U}(\underline{\mathrm{K}_b}) = \sum_{b=1}^{d} \kappa_{ab} K_b$. Inserting this relation in (191), we find

$$\eta_+ H \eta_+^{-1} = \sum_{k=1}^{n} \sum_{b_1,b_2,\ldots,b_k=1}^{d} \tilde{\lambda}_{b_1 b_2 \cdots b_k} K_{b_1} K_{b_2} \cdots K_{b_k}, \tag{193}$$

where $\tilde{\lambda}_{b_1 b_2 \cdots b_k} := \sum_{a_1,a_2,\ldots,a_k=1}^{d} \lambda_{a_1,a_2,\ldots a_k} \kappa_{a_1 b_1} \kappa_{a_2 b_2} \cdots \kappa_{a_k b_k}$. Note that the coefficients $\tilde{\lambda}_{b_1 b_2 \cdots b_k}$ depend on the parameters r_a of the metric operator (190).

In view of (188) and (193), the pseudo-Hermiticity relation $H^\dagger = \eta_+ H \eta_+^{-1}$ takes the form

$$\sum_{k=1}^{n} \sum_{c_1,c_2,\ldots,c_{k-1},c_k=1}^{d} (\lambda^*_{c_k c_{k-1} \cdots c_2 c_1} - \tilde{\lambda}_{c_1 c_2 \cdots c_{k-1} c_k}) K_{c_1} K_{c_2} \cdots K_{c_k} = 0. \tag{194}$$

We can use the commutation relations for the generators K_a, namely $[K_a, K_b] = i \sum_{c=1}^{d} C_{abc} K_c$, to reorder the factors $K_{c_1} K_{c_2} \cdots K_{c_k}$ and express the left-hand side

of (194) as a sum of linearly independent operators. Consequently, the coefficients of this sum must identically vanish. This yields a system of equations for r_a. In general, this system is overdetermined and a solution might not exist. However, there is a class of Hamiltonians of the form (188) for which this system has solutions. In this case, each solution determines a metric operator.

For the particular case that $n = 1$, so that

$$H = \sum_{a=1}^{d} \lambda_a K_b, \tag{195}$$

we may employ a more direct method of deriving the system of equations for r_a. This is based on the observation that, in this case, we can obtain a representation of the pseudo-Hermiticity relation $H^\dagger = \eta_+ H \eta_+^{-1}$ in $\mathcal{G}_{\mathbb{C}}$, namely

$$\underline{\mathrm{H}^{\maltese}} = \underline{\eta_+}\, \underline{\mathrm{H}}\, \underline{\eta_+^{-1}}, \tag{196}$$

where[yy]

$$\underline{\mathrm{H}} := \sum_{a=1}^{d} \lambda_a \underline{\mathrm{K}_a}, \quad \underline{\mathrm{H}^{\maltese}} := \sum_{a=1}^{d} \lambda_a^* \underline{\mathrm{K}_a}. \tag{197}$$

The matrix equation (196) is equivalent to a system of d complex equations for d real variables r_a. Therefore, it is generally overdetermined.

We can use the above Lie algebraic method to compute the equivalent Hermitian Hamiltonian h for the quasi-Hermitian Hamiltonians of the form (188). In view of the definitions: $h := \rho H \rho^{-1}$ and $\rho := \sqrt{\eta_+} = \exp(\sum_{a=1}^{d} \frac{r_a}{2} K_a)$, h is given by the right-hand side of (192) provided that we use $\frac{r_a}{2}$ in place of r_a.

An alternative Lie algebraic approach of determining metric operator and the equivalent Hermitian Hamiltonian is the following. First, we use the argument leading to (191) to obtain

$$\begin{aligned} h &= \rho H \rho^{-1} \\ &= \sum_{k=1}^{n} \sum_{a_1,a_2,\ldots,a_k=1}^{d} \lambda_{a_1,a_2,\ldots,a_k} \mathfrak{U}(\underline{\rho}\, \underline{\mathrm{K}_{a_1}}\, \underline{\rho}^{-1}) \mathfrak{U}(\underline{\rho}\, \underline{\mathrm{K}_{a_2}}\, \underline{\rho}^{-1}) \cdots \mathfrak{U}(\underline{\rho}\, \underline{\mathrm{K}_{a_k}}\, \underline{\rho}^{-1}), \end{aligned} \tag{198}$$

where $\underline{\rho} := \exp(\sum_{a=1}^{d} \frac{r_a}{2} \underline{\mathrm{K}_a})$. Then, we evaluate $\underline{\rho}\, \underline{\mathrm{K}_a}\, \underline{\rho}^{-1}$ and express it as a linear combination of $\underline{\mathrm{K}_a}$ with r_a-dependent coefficients.[zz] Substituting the result in (198) and using the linearity of $\mathfrak{U}$ and $K_a = \mathfrak{U}(\underline{\mathrm{K}_a})$ give $h = \sum_{k=1}^{n} \sum_{a_1,a_2,\ldots,a_k=1}^{d} \varepsilon_{a_1,a_2,\ldots,a_k} K_{a_1} K_{a_2} \cdots K_{a_k}$, where $\varepsilon_{a_1,a_2,\ldots,a_k}$ are r_a-dependent complex coefficients. In this approach, we obtain the desired system of equations for r_a by demanding that $h = h^\dagger$. This is the root taken in [194] where the Lie algebraic method was originally used for the construction of the metric operators

[yy] Unless G is a unitary group, $\mathfrak{U}$ is not a $*$-representation [85], and $\underline{\mathrm{H}^{\maltese}} \neq \underline{\mathrm{H}}^\dagger$.
[zz] This is possible because $\underline{\rho} \in \exp(\mathcal{G}_{\mathbb{C}})$.

and equivalent Hermitian Hamiltonians for a class of quasi-Hermitian Hamiltonians of the linear form (195) with underlying $su(1,1)$ algebra. For an application of this approach to Hamiltonians that are quadratic polynomials in generators of $SU(1,1)$, see [17].

4.4.3. *Swanson model:* $\mathcal{G} = su(1,1)$

In this section, we explore the application of the Lie algebraic method to construct metric operators for Swanson's Hamiltonian [224]:

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) + \alpha a^2 + \beta {a^\dagger}^2, \tag{199}$$

where $a := \frac{\mathrm{X}+i\mathrm{p}}{\sqrt{2}}$, $\mathrm{X} := \sqrt{\frac{m\omega}{\hbar}}\, x$, $\mathrm{p} := \frac{p}{\sqrt{m\hbar\omega}}$, α, β, ω, m are real parameters, $m > 0$, $\omega > 0$, and $\hbar^2\omega^2 > 4\alpha\beta$. The latter condition ensures the reality and discreteness of the spectrum of (199).

The problem of finding metric operators for the Hamiltonian (199) is addressed in [118, 206, 182]. The use of the properties of Lie algebras for solving this problem was originally proposed in [194].

Swanson's Hamiltonian (199) is an example of a rather trivial class of quasi-Hermitian Hamiltonians of the standard form

$$H = \frac{[p + A(x)]^2}{2M} + v(x), \tag{200}$$

where A and v are, respectively, a complex-valued vector potential and a real-valued scalar potential, and $M \in \mathbb{R}^+$ is the mass. It is easy to see that these Hamiltonians admit the x-dependent metric operator: $\eta_+ = \exp(-\frac{2}{\hbar}\int dx\, \Im[A(x)])$. This in turn yields the equivalent Hermitian Hamiltonian: $h = \frac{1}{2m}(p + \Re[A(x)])^2 + v(x)$. The subclass of the Hamiltonians (200) corresponding to imaginary vector potentials has been considered in [3]. The Swanson Hamiltonian (199) is a special case of the latter. It corresponds to the choice: $M = \frac{m}{1-\tilde\alpha-\tilde\beta}$, $A(x) = i\left(\frac{m\omega(\tilde\alpha-\tilde\beta)}{1-\tilde\alpha-\tilde\beta}\right)x$, and $v(x) = \frac{1}{2}\left(\frac{1-4\tilde\alpha\tilde\beta}{1-\tilde\alpha-\tilde\beta}\right)m\omega^2x^2$, where

$$\tilde\alpha := \frac{\alpha}{\hbar\omega}, \quad \tilde\beta := \frac{\beta}{\hbar\omega}. \tag{201}$$

As shown in [118, 182], the Hamiltonian (199) admits other exactly constructible metric operators. The Lie algebraic method considered in this section offers a systematic approach for constructing metric operators for this Hamiltonian. In order to describe the details of this construction, we begin by recalling that the operators a and $a^\dagger$ are the usual harmonic oscillator annihilation and creation operators that satisfy

$$[a, a^\dagger] = 1. \tag{202}$$

A well-known consequence of this relation is the possibility of constructing a unitary representation of the Lie algebra $su(1,1)$ using quadratic polynomials in a and $a^\dagger$.

To see this, consider the Hermitian operators: $K_1 := \frac{1}{4}(a^2+a^{\dagger 2})$, $K_2 := \frac{i}{4}(a^2-a^{\dagger 2})$ and $K_3 := \frac{1}{4}(aa^\dagger + a^\dagger a) = \frac{1}{2}(a^\dagger a + \frac{1}{2})$ that act in $\mathcal{H} := L^2(\mathbb{R})$ [142]. In view of (202), they satisfy the $su(1,1)$ algebra: $[K_1, K_2] = -iK_3$, $[K_2, K_3] = iK_1$, $[K_3, K_1] = iK_2$. Clearly the Hamiltonian (199) can be expressed as a linear combination of K_1, K_2 and K_3:

$$H = 2[(\alpha+\beta)K_1 + i(\alpha-\beta)K_2 + \hbar\omega K_3]. \tag{203}$$

This relation identifies the Hamiltonian (203) as a special case of the Hamiltonians of the form (195) with $G = SU(1,1)$, $d = 3$, $\lambda_1 = 2(\alpha+\beta)$, $\lambda_2 = 2i(\alpha-\beta)$, and $\lambda_3 = 2\hbar\omega$. We can further simplify (203) by introducing non-Hermitian generators $K_\pm := K_1 \pm iK_2$. In terms of these, we have $H = 2(\alpha K_+ + \beta K_- + \hbar\omega K_3)$.

In order to apply the above method of constructing a metric operator for (203), we need to find a set of generators $\underline{\mathrm{K}_a}$ of $SU(1,1)$ in its standard representation and a faithful unitary representation $\mathfrak{U}$ of the Lie algebra $su(1,1)$ such that $K_a = \mathfrak{U}(\underline{\mathrm{K}_a})$ for all $a \in \{1,2,3\}$. A simple choice is

$$\underline{\mathrm{K}_1} := \frac{i}{2}\sigma_1 = \frac{1}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}, \quad \underline{\mathrm{K}_2} := \frac{i}{2}\sigma_2 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \underline{\mathrm{K}_3} := \frac{1}{2}\sigma_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{204}$$

where σ_1, σ_2, and σ_3 are the Pauli matrices. We also have

$$\underline{\mathrm{K}_+} := \underline{\mathrm{K}_1} + i\underline{\mathrm{K}_2} = \begin{pmatrix} 0 & i \\ 0 & 0 \end{pmatrix}, \quad \underline{\mathrm{K}_-} := \underline{\mathrm{K}_1} - i\underline{\mathrm{K}_2} = \begin{pmatrix} 0 & 0 \\ i & 0 \end{pmatrix}, \tag{205}$$

that fulfil $\mathfrak{U}(\underline{\mathrm{K}_\pm}) = K_\pm$.

Comparing (204) and (205), we see that it is more convenient to work with the generators $K_\pm$ and K_3 rather than K_a with $a \in \{1,2,3\}$. This, in particular, suggests the following alternative parametrization of the metric operator (190).

$$\eta_+ = \exp(zK_+)\exp(2rK_3)\exp(z^*K_-), \quad \text{with } z \in \mathbb{C}, r \in \mathbb{R}. \tag{206}$$

Clearly,

$$\underline{\eta_+} = \exp(z\underline{\mathrm{K}_+})\exp(2r\underline{\mathrm{K}_3})\exp(z^*\underline{\mathrm{K}_-}) = \begin{pmatrix} e^r - e^{-r}|z|^2 & ie^{-r}z \\ ie^{-r}z^* & e^{-r} \end{pmatrix}, \tag{207}$$

$$\underline{\eta_+^{-1}} = \exp(-z^*\underline{\mathrm{K}_-})\exp(-2r\underline{\mathrm{K}_3})\exp(-z\,\underline{\mathrm{K}_+}) = \begin{pmatrix} e^{-r} & -ie^{-r}z \\ -ie^{-r}z^* & e^r - e^{-r}|z|^2 \end{pmatrix}, \tag{208}$$

where we have made use of (204) and (205). Also in view of (197), (201), (203), and $K_\pm := K_1 \pm iK_2 = K_\mp^\dagger$, we have

$$\underline{\mathrm{H}} = 2\hbar\omega[\tilde{\alpha}\underline{\mathrm{K}_+} + \tilde{\beta}\underline{\mathrm{K}_-} + \underline{\mathrm{K}_3}] = \hbar\omega \begin{pmatrix} 1 & 2i\tilde{\alpha} \\ 2i\tilde{\beta} & -1 \end{pmatrix}, \tag{209}$$

$$\underline{\mathrm{H}^\maltese} = 2\hbar\omega[\tilde{\alpha}\underline{\mathrm{K}_-} + \tilde{\beta}\underline{\mathrm{K}_+} + \underline{\mathrm{K}_3}] = \hbar\omega \begin{pmatrix} 1 & 2i\tilde{\beta} \\ 2i\tilde{\alpha} & -1 \end{pmatrix}. \tag{210}$$

Next, we insert (207)–(210) in (196). This yields the following three independent complex equations that are more conveniently expressed in terms of $s := e^r$ and $w := e^{-r}z$.

$$s(\tilde{\alpha}s - w) + \tilde{\beta}(w^2 - 1) + s|w|^2[w + \tilde{\alpha}s(|w|^2 - 2)] = 0, \tag{211}$$

$$\tilde{\beta} - \tilde{\alpha}s^2 + sw^*(1 + \tilde{\alpha}sw^*) = 0, \tag{212}$$

$$\tilde{\beta}w + sw^*[w + \tilde{\alpha}s(|w|^2 - 1)] = 0. \tag{213}$$

To solve these equations, we rewrite (213) as: $w + \tilde{\alpha}s(|w|^2 - 2) = -\tilde{\alpha}s - \frac{\tilde{\beta}w}{sw^*}$, and use this relation in (211) to obtain

$$\tilde{\alpha}s(1 - |w|^2) = \frac{\tilde{\beta}}{s} + w. \tag{214}$$

Substituting this equation back into (213), we find $\tilde{\beta}(w - w^*) = 0$. Therefore, either $\tilde{\beta} = 0$ or $w \in \mathbb{R}$. It is easy to show using (212) that the condition $\tilde{\beta} = 0$ implies $w \in \mathbb{R}$ as well. Hence, w is real and (214) reduces to a quadratic equation whose solution is

$$w = \frac{-1 \pm \sqrt{4\tilde{\alpha}^2 s^2 + 1 - 4\tilde{\alpha}\tilde{\beta}}}{2\tilde{\alpha}s}. \tag{215}$$

It turns out that (211)–(213) do not impose any further restriction on s. Therefore, (215) is the solution of the system (211)–(213). In terms of the original parameters r and z, it reads $z = -1 \pm \frac{\sqrt{4\tilde{\alpha}^2 e^{2r} + 1 - 4\tilde{\alpha}\tilde{\beta}}}{2\tilde{\alpha}} = -\hbar\omega \pm \frac{\sqrt{4\alpha^2 e^{2r} + \hbar\omega - 4\alpha\beta}}{2\alpha}$. Substituting this formula in (206), we find two one-parameter families of metric operators for Swanson's Hamiltonian.

5. Systems Defined on a Complex Contour

5.1. *Spectral problems defined on a contour*

Consider the Schrödinger operator $-\frac{d^2}{dx^2} + V(x)$, where $V : \mathbb{R} \to \mathbb{C}$ is a complex-valued piecewise real-analytic potential. The study of the spectral problem for this operator and its complex generalization, $-\frac{d^2}{dz^2} + V(z)$, with z taking values along

a contour[aaa] Γ in $\mathbb{C}$, predates the discovery of quantum mechanics.[bbb] The case of polynomial potentials have been studied thoroughly in [212]. For a more recent discussion, see [210].

The spectrum of $-\frac{d^2}{dz^2}+V(z)$ depends on the choice of the contour Γ. In the case that Γ visits the point at infinity, the spectrum is essentially determined by the boundary condition imposed on the solutions $\Psi:\Gamma\to\mathbb{C}$ of the following eigenvalue equation at infinity.

$$\left[-\frac{d^2}{dz^2}+V(z)\right]\Psi(z)=E\Psi(z). \tag{216}$$

For an extended contour Γ, that is obtained by a continuous invertible deformation of the real axis in $\mathbb{C}$, the eigenvalue problem (216) is well-posed provided that we demand $\Psi(z)$ to decay exponentially as $|z|\to\infty$ along Γ. To make this condition more explicit, we identify Γ with the graph of a parametrized curve $\zeta:\mathbb{R}\to\mathbb{C}$ in $\mathbb{C}$, i.e.

$$\Gamma=\{\zeta(s)\,|\,s\in\mathbb{R}\}. \tag{217}$$

The assumption that Γ is simple implies that ζ is a one-to-one function, and we can express the above-mentioned boundary condition as

$$|\Psi(\zeta(s))|\to 0\quad\text{exponentially as } s\to\pm\infty. \tag{218}$$

A simple consequence of this condition is

$$\int_{-\infty}^{\infty}|\Psi(\zeta(s))|^2ds<\infty. \tag{219}$$

If we view $\mathbb{C}$ as a Riemannian manifold, namely $\mathbb{R}^2$ endowed with the Euclidean metric tensor, and consider Γ as a submanifold of this manifold, we can use the embedding map $\zeta:\mathbb{R}\to\mathbb{C}$ to induce a metric tensor ($\mathfrak{g}$) on Γ. The corresponding line element is given by $d\ell:=\sqrt{\mathfrak{g}}\,ds=\sqrt{dx(s)^2+dy(s)^2}=|\zeta'(s)|\,ds$, where $x(s):=\Re(\zeta(s))$ and $y(s):=\Im(\zeta(s))$. Therefore, the integral measure defined by $\mathfrak{g}$ on Γ is the arc-length element $|\zeta'(s)|\,ds$. This in turn suggests the following parametrization-invariant definition of the L^2-inner product on Γ.

$$\prec\Psi\,|\,\Phi\succ:=\int_{-\infty}^{\infty}\Psi(\zeta(s))^*\Phi(\zeta(s))\,|\zeta'(s)|\,ds. \tag{220}$$

If we identify s with the arc-length parameter, for which $|\zeta'(s)|=1$, and let $L^2(\Gamma):=\{\Psi:\Gamma\to\mathbb{C}\,|\prec\Psi\,|\,\Psi\succ<\infty\}$, we can express (219) as

$$\Psi\in L^2(\Gamma). \tag{221}$$

This shows that the boundary condition (218) implies the square-integrability condition (221) along Γ. The converse is not generally true; the spectrum defined by

[aaa] Here by the term "contour" we mean (the graph of) a piecewise smooth simple curve that need not be closed.

[bbb] Hermann Weyl's dissertation of 1909 provides a systematic approach to this problem. For a detailed discussion of Weyl's results, see [104, §10].

the boundary condition (218) is a subset of the point spectrum[ccc] of the operator $-\frac{d^2}{dz^2}+V(z)$ viewed as acting in the Hilbert space $L^2(\Gamma)$. In the following we shall use the term spectrum to denote the subset of the point spectrum that is defined by the boundary condition (218).

In order to demonstrate the importance of the choice of the contour in dealing with the spectral problem (216), consider the imaginary cubic potential $V(z)=iz^3$. As we mentioned in Sec. 1, the spectrum defined by the boundary condition (218) along the real axis ($\zeta(s)=s$) is discrete, real and positive [79, 209]. But, the spectrum defined by the same boundary condition along the imaginary axis is empty. To see this, we parametrize the imaginary axis according to $z=\zeta(s)=is$ with $s\in\mathbb{R}$. Then the operator $-\frac{d^2}{dz^2}+iz^3$ takes the form $\frac{d^2}{ds^2}+s^3$, and we can respectively express the eigenvalue equation (216) and the boundary condition (218) as

$$\left[\frac{d^2}{ds^2}+s^3\right]\psi(s)=E\psi(s), \tag{222}$$

and

$$|\psi(s)|\to 0 \quad \text{exponentially as } s\to\pm\infty, \tag{223}$$

where $\psi(s):=\Psi(is)$ for all $s\in\mathbb{R}$.[ddd] But, it is well-known that (222) does not have any solution fulfilling (223) for either real or complex values of E.[eee]

The imaginary cubic potential belongs to the class of potentials of the form

$$V_\nu(x)=\lambda x^2(ix)^\nu, \quad \nu\in\mathbb{R}, \ \ \lambda\in\mathbb{R}^+. \tag{224}$$

As shown in [79, 209], for $\nu\geq 0$ these potentials share the spectral properties of the imaginary cubic potential, if we impose the boundary condition (218) along a contour Γ_ν that lies asymptotically in the union of the Stokes wedges [32]:

$$S_\nu^\pm:=\{re^{-i(\theta_\nu^\pm+\varphi)}\,|\,r\in[0,\infty),\ \varphi\in(-\delta_\nu,\delta_\nu)\}, \tag{225}$$

where

$$\theta_\nu^+:=\frac{\pi\nu}{2(\nu+4)}=:\theta_\nu, \quad \theta_\nu^-:=\pi-\theta_\nu, \quad \delta_\nu:=\frac{\pi}{\nu+4}. \tag{226}$$

Here by asymptotic inclusion of Γ_ν in $S_\nu^-\cup S_\nu^+$, we mean that if $\Gamma_\nu=\{\zeta_\nu(s)\,|\,s\in\mathbb{R}\}$ for a piecewise smooth one-to-one function $\zeta_\nu:\mathbb{R}\to\mathbb{C}$, then there must exist a

[ccc] By definition, the spectrum $\sigma(A)$ of an operator A acting in a Banach space is the set of complex numbers E for which the operator $A-EI$ is not invertible, i.e. one or more of the following conditions hold: (1) $A-EI$ is not one-to-one; (2) $A-EI$ is not onto; (3) $A-EI$ is one-to-one so that it has an inverse, but the inverse is not a bounded operator [105]. The *point spectrum* of A is the subset of $\sigma(A)$ consisting of the eigenvalues E of A, i.e. the numbers E for which $A-EI$ is not one-to-one [195].

[ddd] This was pointed out to me by Prof. Yavuz Nutku.

[eee] The point spectrum of $\frac{d^2}{ds^2}+s^3$ is $\mathbb{C}$, i.e. (222) admits square-integrable solutions for all $E\in\mathbb{C}$ (this was pointed out to me by Prof. Patrick Dorey). These solutions do not, however, satisfy (223). They do not represent physically acceptable bound states, because they do not belong to the domain of the observables such as position, momentum or some of their powers.

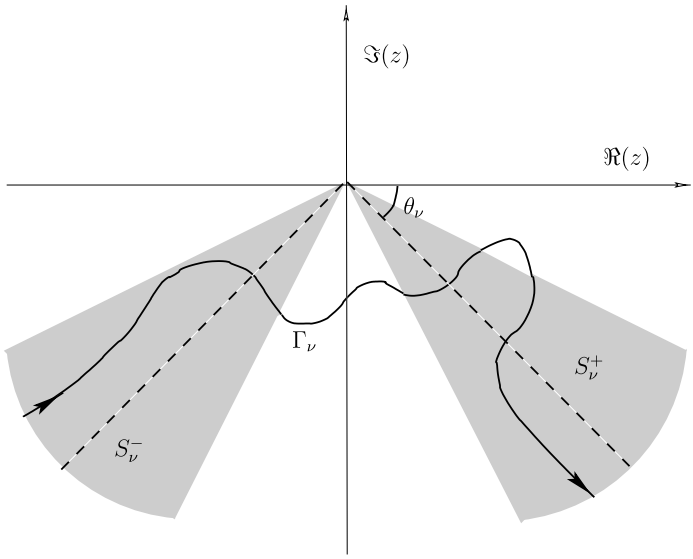

Fig. 1. A contour Γ_ν (the solid curve) lying asymptotically in the union of the Stokes wedges (the grey region). The dashed lines are the bisectors of the Stokes wedges $S_\nu^\pm$. The angle θ_ν between the positive real axis and the bisector of S_ν^+ is also depicted.

positive integer M such that for all $s \in \mathbb{R}$ the condition $\pm s > M$ implies $\zeta(s) \in S_\nu^\pm$. Figure 1 shows Stokes wedges and a typical contour lying in $S_\nu^- \cup S_\nu^+$ asymptotically.

For $\nu = 2$, (224) gives the wrong-sign quartic potential,

$$V_2(x) = -\lambda x^4, \quad \lambda \in \mathbb{R}^+, \tag{227}$$

which is known to have an empty spectrum (defined by (218) along the real axis). Setting $\nu = 2$ in (225) and (226), we have $S_2^- = \{re^{i\theta} \,|\, r \in [0,\infty), \theta \in (-\pi, -\frac{2\pi}{3})\}$ and $S_2^+ = \{re^{i\theta} \,|\, r \in [0,\infty), \theta \in (-\frac{\pi}{3}, 0)\}$. Therefore the condition that Γ_2 must lie asymptotically inside $S_2^- \cup S_2^+$ excludes the real axis as a possible choice for Γ_2. It is not difficult to see that the same holds for all $\nu \geq 2$.

5.2. *Equivalent spectral problems defined on* $\mathbb{R}$

The fact that the spectrum of the potentials (224) defined by the above-mentioned boundary condition along Γ_ν is discrete, real and positive is by no means obvious, and its proof is quite complicated [79, 209]. In this subsection, we will outline a transformation scheme that maps the spectral problem for these and similar potentials to an equivalent spectral problem that is defined on the real line [157]. This scheme provides an intuitive understanding of the spectral properties of the potentials (224) and in particular allows for a straightforward treatment of the wrong-sign quartic potential (227) that we shall consider in the following subsection.

Given an extended contour Γ, we can use $x := \Re(z)$ to parametrize it. We do this by setting $\Gamma = \{\zeta(x) \,|\, x \in \mathbb{R}\}$ where $\zeta(x) := x + if(x)$ for all $x \in \mathbb{R}$, and $f : \mathbb{R} \to \mathbb{R}$ is

a piecewise smooth function. This implies that along Γ, $dz = d\zeta(x) = [1 + if'(x)]dx$ and the eigenvalue equation (216) takes the form

$$\left[-g(x)^2\frac{d^2}{dx^2} + ig(x)^3 f''(x)\frac{d}{dx} + \tilde{v}(x)\right]\tilde{\psi}(z) = E\tilde{\psi}(z), \tag{228}$$

where for all $x \in \mathbb{R}$,

$$g(x) := \frac{1}{1 + if'(x)}, \quad \tilde{v}(x) := V(x + if(x)), \quad \tilde{\psi}(x) := \Psi(x + if(x)), \tag{229}$$

and a prime stands for the derivative of the corresponding function.

Next, we examine the consequences of using the arc-length parametrization of Γ. If we define $F : \mathbb{R} \to \mathbb{R}$ by $F(x) := \int_0^x \sqrt{1 + f'(u)^2}\, du$, we can express the arc-length parameter along Γ, which we denote by x, as $\mathrm{x} := F(x)$. Under the transformation $x \to \mathrm{x}$, the eigenvalue equation (228) takes the form

$$e^{-2i\xi(\mathrm{x})}\left[-\frac{d^2}{d\mathrm{x}^2} + ia(\mathrm{x})\frac{d}{d\mathrm{x}} + v(\mathrm{x})\right]\psi(\mathrm{x}) = E\psi(\mathrm{x}), \tag{230}$$

where[fff]

$$\xi(\mathrm{x}) := \tan^{-1}(f'(x))|_{x=F^{-1}(\mathrm{x})}, \quad a(\mathrm{x}) := \xi'(\mathrm{x}) = \left.\frac{f''(x)}{[1 + f'(x)^2]^{\frac{3}{2}}}\right|_{x=F^{-1}(\mathrm{x})}, \tag{231}$$

$$v(\mathrm{x}) := e^{2i\xi(\mathrm{x})}\tilde{v}(F^{-1}(\mathrm{x})), \quad \psi(\mathrm{x}) := \tilde{\psi}(F^{-1}(\mathrm{x})). \tag{232}$$

The arc-length parametrization of Γ is achieved by the function $G : \mathbb{R} \to \Gamma$ defined by $G(\mathrm{x}) := F^{-1}(\mathrm{x}) + if(F^{-1}(\mathrm{x}))$ for all $\mathrm{x} \in \mathbb{R}$. This is the invertible function that maps the real line $\mathbb{R}$ onto the contour Γ in such a way that the (Euclidean) distance is preserved, i.e. if $\mathrm{x}_1, \mathrm{x}_2 \in \mathbb{R}$ are respectively mapped to $z_1 := G(\mathrm{x}_1)$ and $z_2 := G(\mathrm{x}_2)$, then the length of the segment of Γ that lies between z_1 and z_2 is given by $|\mathrm{x}_1 - \mathrm{x}_2|$. In other words, $G : \mathbb{R} \to \Gamma$ is an isometry. In light of (229) and (232), G relates the solutions Ψ and ψ of the eigenvalue equations (216) and (230) according to $\psi(\mathrm{x}) = \Psi(G(\mathrm{x}))$. We can use G to express v in terms of the potential V directly:

$$v(\mathrm{x}) = e^{2i\xi(\mathrm{x})}V(G(\mathrm{x})). \tag{233}$$

Furthermore, recalling that the arc-length parametrization of Γ corresponds to identifying s and $\zeta(s)$ of (217)–(219) respectively with x and $G(\mathrm{x})$, we have

$$\prec \Psi \mid \Psi \succ = \int_{-\infty}^{\infty} |\Psi(G(\mathrm{x}))|^2 d\mathrm{x} = \int_{-\infty}^{\infty} |\psi(\mathrm{x})|^2 d\mathrm{x} = \langle \psi \mid \psi \rangle. \tag{234}$$

This observation has two important consequences. Firstly, it implies that $\Psi \in L^2(\Gamma)$ if and only if $\psi \in L^2(\mathbb{R})$. Secondly, it allows for the introduction of an induced

[fff]Because F is a monotonically increasing function, it is one-to-one. In particular, it has an inverse that we denote by F^{-1}.

unitary operator $G_* : L^2(\Gamma) \to L^2(\mathbb{R})$, namely $G_*(\Psi) := \psi$ if $\psi(\mathrm{x}) = \Psi(G(\mathrm{x}))$ for all $\mathrm{x} \in \mathbb{R}$.[ggg]

The above constructions show that a pseudo-Hermitian quantum system that is defined by a Hamiltonian operator of the form $-\frac{d^2}{dz^2} + V(z)$ acting in the reference Hilbert space $L^2(\Gamma)$ is unitary-equivalent to the one defined by the Hamiltonian operator

$$H = e^{-2i\xi(\mathrm{x})}\left[-\frac{d^2}{d\mathrm{x}^2} + ia(\mathrm{x})\frac{d}{d\mathrm{x}} + v(\mathrm{x})\right] \tag{235}$$

that is defined in the reference Hilbert space $L^2(\mathbb{R})$. In terms of the unitary operator G_*, we have $-\frac{d^2}{dz^2} + V(z) = G_*^{-1} H G_*$.

A particularly simple choice for a contour is a wedge-shaped contour: $\Gamma^{(\theta)} := \{x + if(x) \,|\, x \in \mathbb{R}\}$ where $f(x) := -\tan\theta|x|$ and $\theta \in [0, \frac{\pi}{2})$. A typical example is the contour obtained by adjoining the bisectors of the Stokes wedges (the dashed lines in Fig. 1). For such a contour,

$$\mathrm{x} = F(x) = \sec\theta x, \quad x = F^{-1}(\mathrm{x}) = \cos\theta \mathrm{x}, \tag{236}$$

$$G(\mathrm{x}) = \cos\theta\mathrm{x} - i\sin\theta|\mathrm{x}| = \begin{cases} e^{i\theta}\mathrm{x} & \text{for } \mathrm{x} < 0, \\ e^{-i\theta}\mathrm{x} & \text{for } \mathrm{x} \geq 0, \end{cases} \tag{237}$$

and in view of (231), (232) and (233) the Hamiltonian operator (235) takes the form

$$H = -e^{2i\theta\,\mathrm{sgn}(\mathrm{x})}\left[\frac{d^2}{d\mathrm{x}^2} + 2i\theta\delta(\mathrm{x})\frac{d}{d\mathrm{x}}\right] + V(\cos\theta\mathrm{x} - i\sin\theta|\mathrm{x}|). \tag{238}$$

The presence of delta-function in (238) has its root in the non-differentiability of $\Gamma^{(\theta)}$ at the origin. One can smooth out $\Gamma^{(\theta)}$ in an arbitrarily small open neighborhood of the origin and show that this delta-function singularity amounts to the imposition of a particular matching condition at $\mathrm{x} = 0$ for the solutions of the corresponding eigenvalue problem. As shown in [157], these are given by

$$\psi(0^+) = \psi(0) = \psi(0^-), \quad e^{-2i\theta}\psi'(0^-) = e^{2i\theta}\psi'(0^+), \tag{239}$$

where for every function $\phi : \mathbb{R} \to \mathbb{R}$, $\phi(0^\pm) := \lim_{\mathrm{x}\to 0^\pm} \phi(\mathrm{x})$.

In view of (238), we can express the eigenvalue equation for H in the form

$$H_\pm\psi_\pm(\mathrm{x}) = E\psi_\pm(\mathrm{x}), \quad \text{for } \mathrm{x} \in \mathbb{R}^\pm, \tag{240}$$

where

$$H_\pm := -e^{\pm 2i\theta}\frac{d^2}{d\mathrm{x}^2} + V(e^{\mp i\theta}\mathrm{x}), \tag{241}$$

and $\psi_- : (-\infty, 0] \to \mathbb{C}$, $\psi_+ : [0, \infty) \to \mathbb{C}$ are defined by $\psi_\pm(\mathrm{x}) := \psi(\mathrm{x})$ for all $\mathrm{x} \in \mathbb{R}^\pm$, $\psi_\pm(0) := \psi(0^\pm)$, and $\psi'_\pm(0) := \psi'(0^\pm)$.

[ggg] Equation (234) shows that G_* preserves the norm. This is sufficient to conclude that it is a unitary operator, for in an inner product space the norm uniquely determines the inner product [123, §6.1].

In summary, the eigenvalue problem for the Schrödinger operator $-\frac{d^2}{dz^2}+V(z)$ that is defined by the boundary condition (218) along $\Gamma^{(\theta)}$ is equivalent to finding a pair of functions $\psi_\pm$ satisfying

$$-e^{\pm 2i\theta}\psi''_\pm(\mathrm{x})+V(e^{\mp i\theta}\,\mathrm{x})\psi_\pm(\mathrm{x})=E\psi_\pm(\mathrm{x})\quad \text{for } \mathrm{x}\in\mathbb{R}^\pm, \tag{242}$$

$$\psi_-(0)=\psi_+(0),\quad e^{-2i\theta}\psi'_-(0)=e^{2i\theta}\psi'_+(0), \tag{243}$$

$$\psi_\pm(\mathrm{x})\to 0\quad \text{exponentially as } \mathrm{x}\to\pm\infty. \tag{244}$$

To elucidate the practical advantage of this formulation, we explore its application for the potentials $V_\nu(z)=\lambda z^2(iz)^\nu$ with $\lambda\in\mathbb{R}^+$.

As we explained in the preceding subsection, we need to choose a contour that belongs to the union of the Stokes wedges $S_\nu^\pm$ asymptotically. We shall choose the wedge-shaped contour $\Gamma^{(\theta_\nu)}$ that consists of the bisectors of $S_\nu^\pm$. Setting $V=V_\nu$ and $\theta=\theta_\nu$ in (241) and using (226) we find the following most surprising result.

$$H_\pm=e^{\pm 2i\theta_\nu}\left[-\frac{d^2}{d\mathrm{x}^2}+\lambda|\mathrm{x}|^{\nu+2}\right]. \tag{245}$$

Similarly, (242) becomes

$$-\psi''_\pm(\mathrm{x})+\lambda|\mathrm{x}|^{\nu+2}\psi_\pm(\mathrm{x})=E\,e^{\mp 2i\theta_\nu}\psi_\pm(\mathrm{x})\quad \text{for } \mathrm{x}\in\mathbb{R}^\pm. \tag{246}$$

The appearance of the real confining potential $\lambda|\mathrm{x}|^{\nu+2}$ in (245) and (246) allows for an alternative proof of the discreteness of the spectrum of the potentials $z^2(iz)^\nu$. See [157, Appendix] for details.[hhh]

5.3. *Wrong-sign quartic potential*

In the preceding section we showed how one can transform the spectral problem for a potential defined along a complex contour to one defined along $\mathbb{R}$. The form of the transformed Hamiltonian operator depends on the choice of the contour and its parametrization. This raises the natural question of whether one can choose an appropriate parametrized contour so that the transformed Hamiltonian admits an easily constructible metric operator. The wrong-sign quartic potential $V_2(z)=-\lambda z^4$, with $\lambda\in\mathbb{R}^+$, is a remarkable example for which the answer to this question is in the affirmative.

Let $\Gamma_2=\{\zeta(s)\,|\,s\in\mathbb{R}\}$ be the contour defined by [120]

$$\zeta(s):=-2i\sqrt{1+is},\quad \text{for all } s\in\mathbb{R}. \tag{247}$$

If we parametrize Γ_2 using $x=\Re(\zeta(s))$, we find $\Gamma_2=\{x+if(x)\,|\,x\in\mathbb{R}\}$ where f is given by $f(x):=-\sqrt{x^2+1}$ for all $x\in\mathbb{R}$. This shows that Γ_2 is a hyperbola with asymptotes $\ell_\pm:=\{\pm re^{-i\frac{\pi}{4}}\,|\,r\in\mathbb{R}^+\}$. Because $\ell_\pm$ lies in the Stokes wedge $S_2^\pm$, (247) defines an admissible contour for the potential V_2.

[hhh] It would be interesting to see if this approach can lead to an alternative proof of the reality of the spectrum.

If we perform the change of variable $z \to \zeta(s)$, we can express the eigenvalue equation: $[-\frac{d^2}{dz^2} - \lambda z^4]\Psi(z) = E\Psi(z)$, in the form

$$\left[-(1+is)\frac{d^2}{ds^2} - \frac{i}{2}\frac{d}{ds} - 16\lambda\,(1+is)^2\right]\phi(s) = E\phi(s), \tag{248}$$

where $\phi(s) := \Psi(\zeta(s))$. We can identify s with a usual (Hermitian) position operator, introduce the corresponding wave number operator $\mathfrak{K}$ as $\langle s|\mathfrak{K} := -i\frac{d}{ds}\langle s|$, and express (248) as the eigenvalue equation for the Hamiltonian

$$H := (1+is)\mathfrak{K}^2 + \frac{\mathfrak{K}}{2} - 16\lambda(1+is)^2 \tag{249}$$

that acts in $L^2(\mathbb{R})$.

As shown in [120], the application of the perturbative scheme of Subsec. 4.2 yields the following exact expressions for a metric operator and the corresponding equivalent Hermitian Hamiltonian, respectively.

$$\eta_+ = \exp\left(\frac{\mathfrak{K}^3}{48\lambda} - 2\mathfrak{K}\right), \tag{250}$$

$$h = \frac{\mathfrak{K}^4}{64\lambda} - \frac{\mathfrak{K}}{2} + 16\lambda s^2. \tag{251}$$

We shall offer an alternative derivation of these formulas momentarily.

Because h is a Hermitian operator that is isospectral to H, the spectrum of H and consequently the operator $-\frac{d^2}{dz^2} - \lambda z^4$ defined along Γ_2, is real. It is also easy to show that the common spectrum of all these operators is positive and discrete. To see this, we express h in its $\mathfrak{K}$-representation where eigenvalue equation $h\Phi = E\Phi$ reads

$$\left[-16\lambda\,\frac{d^2}{d\mathfrak{K}^2} + \frac{\mathfrak{K}^4}{64\lambda} - \frac{\mathfrak{K}}{2}\right]\tilde{\Phi}(\mathfrak{K}) = E\tilde{\Phi}(\mathfrak{K}), \tag{252}$$

and $\tilde{\Phi}(\mathfrak{K}) := \langle \mathfrak{K}\,|\,\Phi\rangle = (2\pi)^{-\frac{1}{2}}\int_{-\infty}^{\infty} ds e^{-i\mathfrak{K}s}\Phi(s)$. The operator in the square bracket in (252) is a Schrödinger operator with a confining quartic polynomial potential. Therefore its spectrum is positive and discrete [139].

We can also use the same approach to treat the quartic anharmonic oscillator, $V(z) = \omega^2 z^2 - \lambda z^4$. Using the parametrization (247), we find the following generalizations of (249)–(252).

$$H := (1+is)\mathfrak{K}^2 + \frac{\mathfrak{K}}{2} - 16\lambda(1+is)^2 - 4\omega^2(1+is) \tag{253}$$

$$\eta_+ = \exp\left[\frac{\mathfrak{K}^3}{48\lambda} - \left(2 + \frac{\omega^2}{4\lambda}\right)\mathfrak{K}\right], \tag{254}$$

$$h = \frac{(\mathfrak{K}^2 - 4\omega^2)^2}{64\lambda} - \frac{\mathfrak{K}}{2} + 16\lambda s^2. \tag{255}$$

$$\left[-16\lambda\,\frac{d^2}{d\mathfrak{K}^2} + \frac{(\mathfrak{K}^2 - 4\omega^2)^2}{64\lambda} - \frac{\mathfrak{K}}{2}\right]\tilde{\Phi}(\mathfrak{K}) = E\tilde{\Phi}(\mathfrak{K}). \tag{256}$$

Therefore, by scaling the eigenvalues according to $E \to \gamma E$ where $\gamma := \frac{1}{(16\lambda)}$, we can identify the spectrum of the operator $-\frac{d^2}{dz^2} + \omega^2 z^2 - \lambda z^4$ (defined along Γ_2) with that of the operator

$$-\frac{d^2}{dx^2} + \frac{\gamma}{4}[\gamma(x^2 - 4\omega^2)^2 - 2x] \tag{257}$$

that acts in $L^2(\mathbb{R})$ [120]. This observation has previously been made in [58]. As discussed in [11], the approach of [10] also leads to the same conclusion.

Next, we outline an alternative and more straightforward method of constructing a metric operator for the Hamiltonian (253).

If we separate the Hermitian and anti-Hermitian parts of H, we find

$$H = 16\lambda s^2 + \mathfrak{K}^2 - \frac{\mathfrak{K}}{2} - (16\lambda + 4\omega^2) + \frac{i}{2}\{s, \mathfrak{K}^2 - 4\omega^2 - 32\lambda\}. \tag{258}$$

We can combine the first and last terms on the right-hand side of this equation to express H in the form

$$H = 16\lambda\left[s + \frac{i(\mathfrak{K}^2 - 4\omega^2 - 32\lambda)}{32\lambda}\right]^2 + \frac{(\mathfrak{K}^2 - 4\omega^2)^2}{64\lambda} - \frac{\mathfrak{K}}{2}. \tag{259}$$

As seen from this relation, the term responsible for the non-Hermiticity of H may be removed by a translation of s, namely

$$s \to s - \frac{i(\mathfrak{K}^2 - 4\omega^2 - 32\lambda)}{32\lambda}. \tag{260}$$

It is not difficult to see that such a translation is affected by a $\mathfrak{K}$-dependent similarity transformation of the form $s \to e^{g(\mathfrak{K})} s e^{-g(\mathfrak{K})}$. Recalling that for any analytic function $g : \mathbb{R} \to \mathbb{R}$,

$$e^{g(\mathfrak{K})} s e^{-g(\mathfrak{K})} = s - i g'(\mathfrak{K}), \tag{261}$$

and comparing this equation with (260), we find

$$g(\mathfrak{K}) = \frac{\mathfrak{K}^3}{96\lambda} - \left(1 + \frac{\omega^2}{8\lambda}\right) + c. \tag{262}$$

Here c is an integration constant that we can set to zero without loss of generality. In view of (261), we can map H to a Hermitian Hamiltonian h according to

$$H \to h := e^{g(\mathfrak{K})} H e^{-g(\mathfrak{K})} = 16\lambda s^2 + \frac{(\mathfrak{K}^2 - 4\omega^2)^2}{64\lambda} - \frac{\mathfrak{K}}{2}. \tag{263}$$

This is precisely the equivalent Hermitian Hamiltonian given by (255). Moreover, comparing (263) with the defining relation for the equivalent Hermitian Hamiltonian, namely $h := \rho H \rho^{-1}$, and recalling that $\rho := \sqrt{\eta_+}$, where η_+ is a metric operator associated with the Hamiltonian H, we find $\eta_+ = e^{2g(\mathfrak{K})}$. In light of (262), this coincides with the metric operator given by (254).

Next, we wish to explore the underlying classical system for the pseudo-Hermitian quantum system defined by the potential $V(z) = \omega^2 z^2 - \lambda z^4$ along Γ_2.

If we view this potential as an analytic continuation of $V(x) = \omega^2 x^2 - \lambda x^4$, with x denoting the Hermitian position operator, we should identify the Hamiltonian operator for the system with

$$H_{\Gamma_2} := \frac{P_Z^2}{2m} + \Omega^2 Z^2 - \Lambda Z^4, \tag{264}$$

where $\Omega \in \mathbb{R}$ and $\Lambda \in \mathbb{R}^+$ are dimensionful coupling constants, and Z and P_Z are the dimensionful coordinate and momentum operators along Γ_2. Using an arbitrary length scale ℓ, we can introduce the corresponding dimensionless quantities:

$$\lambda := \frac{2m\ell^6\Lambda}{\hbar^2}, \quad \omega := \frac{\sqrt{2m}\,\ell^2\Omega}{\hbar}, \quad p_z := \frac{\ell P_Z}{\hbar}, \quad z := \frac{Z}{\ell}. \tag{265}$$

In terms of these the eigenvalue equation $H_{\Gamma_2}\Psi = \mathcal{E}\Psi$ takes the form

$$\left[-\frac{d^2}{dz^2} + \omega^2 z^2 - \lambda z^4\right]\Psi(z) = E\Psi(z), \tag{266}$$

where $E := \frac{2m\ell^2\mathcal{E}}{\hbar^2}$.

Now, we are in a position to apply our earlier results. Setting $z = \zeta(s) := -2i\sqrt{1+is}$, we can identify (266) with the eigenvalue equation for the pseudo-Hermitian Hamiltonian (253). One might argue that because z and p_z represent dimensionless position and momentum operators, the same should also hold for s and $\mathfrak{K}$, respectively. This suggests to identify the dimensionful position (x) and momentum (p) operators as

$$x = \alpha\ell s, \quad p = \frac{\hbar\mathfrak{K}}{\alpha\ell}, \tag{267}$$

where $\alpha \in \mathbb{R}^+$ is an arbitrary constant. In view of (255), (265), (259) and (267), we obtain the following expressions for the dimensionful pseudo-Hermitian and equivalent Hermitian Hamiltonians.

$$\begin{aligned} H' := \frac{\hbar^2 H}{2m\ell^2} &= \frac{(p^2 - 8m\tilde{\ell}^2\Omega^2)^2}{64\Lambda\tilde{\ell}^4} - \frac{\hbar\, p}{4m\tilde{\ell}} \\ &\quad + 16\Lambda\left[\tilde{\ell}\, x + \frac{i(\tilde{\ell}^{-2}p^2 - 8m\Omega^2 - 64m\ell^2\Lambda)}{64m\Lambda}\right]^2, \end{aligned} \tag{268}$$

$$h' := \frac{\hbar^2 h}{2m\ell^2} = \frac{(p^2 - 8m\tilde{\ell}^2\Omega^2)^2}{64\Lambda\tilde{\ell}^4} - \frac{\hbar p}{4m\tilde{\ell}} + 16\Lambda\tilde{\ell}^2 x^2, \tag{269}$$

where $\tilde{\ell} := \frac{\ell}{\alpha}$. Note that unlike h' that only involves the length scale $\tilde{\ell}$, H' depends on both ℓ and $\tilde{\ell}$. The same is true for the metric operator η_+. This shows that the pseudo-Hermitian quantum systems defined by the Hamiltonian H' and the metric operator η_+ with different values of the parameter α are unitary-equivalent to a Hermitian quantum system that depends on a single length scale ($\tilde{\ell}$). The latter

is not, however, fixed by the Hamiltonian (264) and the contour Γ_2 along which it is defined.[iii]

Supposing that $\tilde{\ell}$ is independent of $\hbar$, we can take $\hbar \to 0$, $x \to x_c$, and $p \to p_c$ in (269) to obtain the underlying classical Hamiltonian. The result is

$$H'_c = \frac{(p_c^2 - 8m\tilde{\ell}^2\Omega^2)^2}{64\Lambda\tilde{\ell}^4} - 16\tilde{\ell}^2\Lambda x_c^2. \tag{270}$$

We can also introduce the pseudo-Hermitian position and momentum operators (55):

$$X := \eta_+^{-\frac{1}{2}} x \eta_+^{\frac{1}{2}} = x + \frac{i(\tilde{\ell}^{-2}p^2 - 8m\Omega^2 - 64m\ell^2\Lambda)}{64m\Lambda\tilde{\ell}}, \quad P := \eta_+^{-\frac{1}{2}} p \eta_+^{\frac{1}{2}} = p. \tag{271}$$

As expected, in terms of X and P, the Hamiltonian H' takes the form

$$H' = \frac{(P^2 - 8m\tilde{\ell}^2\Omega^2)^2}{64\Lambda\tilde{\ell}^4} - \frac{\hbar P}{4m\tilde{\ell}} + 16\Lambda\tilde{\ell}^2 X^2. \tag{272}$$

Furthermore, the η_+-pseudo-Hermitian canonical quantization of the classical Hamiltonian (270) yields (272) except for the linear term in P.

The fact that the pseudo-Hermitian quantum systems defined by the Hamiltonian (264) depend on an arbitrary length scale has its root in our identification of s with the relevant dimensionless position operator. We will next consider an alternative approach that incorporates the spectral equivalence of the Hamiltonians (264) and (257). It is based on treating $\mathfrak{K}$ as the appropriate dimensionless position operator. More specifically, it involves replacing (267) with $x = \beta\ell\mathfrak{K}$ and $p = -\frac{\hbar s}{(\beta\ell)}$, where β is an arbitrary dimensionless real parameter. If we set $\beta := \frac{1}{(4\sqrt{\lambda})} = (32m\Lambda)^{-\frac{1}{2}}\ell^{-3}\hbar$, we find the following ℓ-independent expressions for the equivalent Hermitian Hamiltonian and the underlying classical Hamiltonian[jjj]: $h' = \frac{p^2}{2m} + 4\Lambda\left(x^2 - \frac{\Omega^2}{4\Lambda}\right)^2 - \hbar\sqrt{\frac{2\Lambda}{m}}\,x$ and $H'_c = \frac{p_c^2}{2m} + 4\Lambda\left(x_c^2 - \frac{\Omega^2}{4\Lambda}\right)^2$. Note, however, that H' still depends on ℓ:

$$H' = \frac{1}{2m}\left[p - i\sqrt{\frac{m}{2}}\left(4\sqrt{\Lambda}\,x^2 - \frac{\Omega^2}{\sqrt{\Lambda}} - 8\sqrt{\Lambda}\,\ell^2\right)\right]^2 + 4\Lambda\left(x^2 - \frac{\Omega^2}{4\Lambda}\right)^2 - \hbar\sqrt{\frac{2\Lambda}{m}}\,x. \tag{273}$$

This is also true for η_+. Again the quantum systems determined by H' and η_+ with different values of ℓ are unitary-equivalent to a system that is independent of ℓ. Similar to our earlier analysis, we can obtain an ℓ-independent expression for H'

[iii] If $\Omega \neq 0$, we can choose α such that $\tilde{\ell} = \frac{\Omega}{\sqrt{\Lambda}}$.

[jjj] The expression for the Hamiltonian h' was previously obtained in [36] where the last term in this expression is attributed to an anomaly in a path-integral quantization of the complex classical Hamiltonian $\frac{p_c^2}{2m} + \Omega^2 z_c^2 - \Lambda z_c^4$ along the contour Γ_2. For a more careful treatment of this problem, see [121].

in terms of the pseudo-Hermitian position and momentum operators: $X = x$ and $P = p - i\sqrt{\frac{m}{2}}\left(4\sqrt{\Lambda}\,x^2 - \frac{\Omega^2}{\sqrt{\Lambda}} - 8\sqrt{\Lambda}\,\ell^2\right)$. The result is $H' = \frac{P^2}{2m} + 4\Lambda\left(X^2 - \frac{\Omega^2}{4\Lambda}\right)^2 - \hbar\sqrt{\frac{2\Lambda}{m}}\,X$.

6. Complex Classical Mechanics versus pseudo-Hermitian QM

6.1. *Classical-quantum correspondence and observables*

In Subsec. 3.1 we outlined a procedure that assigns an underlying classical system for a given pseudo-Hermitian quantum system with reference Hilbert space $L^2(\mathbb{R}^d)$. According to this procedure that we employed in Subsecs. 4.2.1, 4.2.2 and 5.3, the classical Hamiltonian H_c may be computed using (60). In other words, to obtain H_c, we replace the standard position and momentum operators with their classical counterparts in the expression for the equivalent Hermitian Hamiltonian h and evaluate its $(\hbar \to 0)$-limit. We can quantize H_c to yield h, if we employ the standard canonical quantization scheme. We obtain the pseudo-Hermitian Hamiltonian H, if we use the pseudo-Hermitian canonical quantization scheme (58).[kkk]

By definition, a classical observable O_c is a real-valued function of the classical states $(\vec{x}_c, \vec{p}_c)$, i.e. points of the phase space $\mathbb{R}^{2d}$. If we apply the usual (Hermitian) canonical quantization program, the operator associated with a classical observable $O_c(\vec{x}_c, \vec{p}_c)$ is given by $o := O_c(\vec{x}, \vec{p})$ where $\vec{x}$ and $\vec{p}$ are the usual Hermitian position and momentum operators. If we apply the pseudo-Hermitian quantization, we find instead $O := O_c(\vec{X}, \vec{P})$ where $\vec{X}$ and $\vec{P}$ are the pseudo-Hermitian position and momentum operators, respectively (55). The common feature of both these quantization schemes is that they replace the usual classical Poisson bracket, $\{A_c, B_c\}_{\rm PB} := \sum_{j=1}^{d}\left(\frac{\partial A_c}{\partial x_{cj}}\frac{\partial B_c}{\partial p_{cj}} - \frac{\partial B_c}{\partial x_{cj}}\frac{\partial A_c}{\partial p_{cj}}\right)$, of any pair of classical observables A_c and B_c with $(i\hbar)^{-1}$ times the commutator of the corresponding operators A and B, $\{A_c, B_c\}_{\rm PB} \longrightarrow (i\hbar)^{-1}[A, B]$. Let us also recall that given a pseudo-Hermitian quantum system specified by the reference Hilbert space $\mathcal{H}$, a quasi-Hermitian Hamiltonian operator $H : \mathcal{H} \to \mathcal{H}$, and an associated metric operator $\eta_+ : \mathcal{H} \to \mathcal{H}$, the observables of the system are by definition η_+-pseudo-Hermitian operators O acting in $\mathcal{H}$,

$$O^\dagger = \eta_+ O \eta_+^{-1}. \tag{274}$$

It is absolutely essential to note that such an operator acquires its physical meaning through the classical-to-quantum correspondence:

$$O_c \to O, \tag{275}$$

where O_c is the classical observable corresponding to the operator O. For example in conventional quantum mechanics, we identify the operator $p : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ defined by $p\psi = -i\hbar\psi'$, with the momentum of a particle moving on $\mathbb{R}$, because

[kkk] Clearly this is true up to factor-ordering ambiguities/terms proportional to positive powers of $\hbar$.

p corresponds to the classical momentum p_c of the underlying classical system. Without this correspondence p is void of a physical meaning. It is merely a constant multiple of the derivative operator acting in a function space.

The situation is not different in pseudo-Hermitian quantum mechanics. Again the (η_+-pseudo-Hermitian) operators that represent observables derive their physical meaning from their classical counterparts through the pseudo-Hermitian version of the classical-to-quantum correspondence. This is also of the form (275), but the operator O is now selected from among the η_+-pseudo-Hermitian operators. As we discussed in Subsec. 3.1, if $o : \mathcal{H} \to \mathcal{H}$ denotes the Hermitian observable associated with a classical observable O_c, the corresponding pseudo-Hermitian observable is given by Eq. (54), i.e. $O := \rho^{-1} o \rho$ where $\rho := \sqrt{\eta}_+$.

Whenever one deals with a symmetric, $\mathcal{PT}$-symmetric, diagonalizable Hamiltonian H with a real spectrum, one can define the observables as operators O fulfilling the condition [39]

$$O^T = \mathcal{CPT}O\mathcal{CPT}, \tag{276}$$

where

$$O^T := \mathcal{T}O^\dagger\mathcal{T} \tag{277}$$

stands for the transpose of O, and $\mathcal{C}$, $\mathcal{P}$, $\mathcal{T}$ are respectively the charge, parity, and time-reversal operators that are assumed to satisfy

$$\mathcal{C}^2 = \mathcal{P}^2 = \mathcal{T}^2 = I, \quad [\mathcal{C}, \mathcal{PT}] = [\mathcal{P}, \mathcal{T}] = [\mathcal{C}, H] = 0. \tag{278}$$

As we explained in Subsec. 3.4, we can relate $\mathcal{C}$ to an associated metric operator η_+ according to

$$\mathcal{C} = \eta_+^{-1}\mathcal{P}. \tag{279}$$

Because $\mathcal{C}^2 = \mathcal{P}^2 = I$, we also have

$$\mathcal{C} = \mathcal{P}\eta_+. \tag{280}$$

Inserting (277) in (276) and making use of (278), we obtain $\mathcal{T}O^\dagger\mathcal{T} = \mathcal{CPT}O\mathcal{CPT} = \mathcal{PTC}O\mathcal{CPT} = \mathcal{TPC}O\mathcal{CPT}$. In view of (278), (279) and (280), this relation is equivalent to $O^\dagger = \mathcal{PC}O\mathcal{CP} = \mathcal{P}(\mathcal{P}\eta_+)O(\eta_+^{-1}\mathcal{P})\mathcal{P} = \eta_+ O \eta_+^{-1}$. Therefore (276) implies the η_+-pseudo-Hermiticity of O. The converse is also true for the cases that (276) can be applied consistently. This is actually not always the case. For example, the application of (276) for the Hamiltonian operator that commutes with $\mathcal{CPT}$ gives $H^T = H$. Therefore, unlike the η_+-pseudo-Hermiticity conditions (274), (276) cannot be employed for non-symmetric Hamiltonians. This shows that (276) has a smaller domain of application than (274).

Another advantage of the requirement of η_+-pseudo-Hermiticity (274) over the condition (276) is that it makes the dynamical consistency of the definition of observables more transparent. Recall that the main motivation for the introduction of (276) in [39] is that its original variant [37, 38], namely the requirement of $\mathcal{CPT}$-symmetry of O, i.e. $O = \mathcal{CPT}O\mathcal{CPT}$, conflicts with the Schrödinger time-evolution in the Heisenberg picture; in general the Heisenberg-picture operators

$O_H(t) := e^{-\frac{itH}{\hbar}} O e^{\frac{itH}{\hbar}}$ do not commute with $\mathcal{CPT}$ for $t \neq 0$, even if they do for $t = 0$ [153]. The reason why (276) does not suffer from this problem is that it is a restatement of the η_+-pseudo-Hermiticity of O. To see why the Heisenberg-picture operators satisfy the latter condition for all t, we first recall that because H is η_+-pseudo-Hermitian, it is a Hermitian operator acting in the physical Hilbert space $\mathcal{H}_{\rm phys}$ defined by the inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$. This implies that the time-evolution operator $e^{-\frac{itH}{\hbar}}$ is a unitary operator acting in $\mathcal{H}_{\rm phys}$. Therefore, $e^{-\frac{itH}{\hbar}} O e^{\frac{itH}{\hbar}}$ acts in $\mathcal{H}_{\rm phys}$ as a Hermitian operator for all t, i.e. it is η_+-pseudo-Hermitian for all t. Alternatively, we could argue that because H is η_+-pseudo-Hermitian, $e^{-\frac{itH}{\hbar}}$ is η_+-pseudo-unitary [4, 5, 159] and $e^{-\frac{itH}{\hbar}} O e^{\frac{itH}{\hbar}}$ is η_+-pseudo-Hermitian.

6.2. *Complex classical systems and compatible Poisson brackets*

In their pioneering article [32], Bender and Boettcher perform an asymptotic analysis of the spectral properties of the complex potentials $V_\nu(z) = z^2(iz)^\nu$ that makes use of the complex WKB-approximation. This involves the study of a certain type of complex classical dynamical system $\mathcal{S}_{\rm BBM}$ that Bender, Boettcher and Meisenger (BBM) [33] identify with the underlying classical system for the quantum system defined by V_ν. This approach, which has been the focus of attention in a number of publications [186, 43, 46, 47], is fundamentally different from the prescription we used in Subsecs. 3.1 and 6.1 to associate a classical system $\mathcal{S}$ with a pseudo-Hermitian quantum system S. In this subsection, we examine the structure of the complex classical system $\mathcal{S}_{\rm BBM}$. For simplicity, we consider complex potentials V that depend on a single complex variable $\mathfrak{z}$.[111]

According to [33] the dynamics of $\mathcal{S}_{\rm BBM}$ is determined by the Newton's equation

$$m\ddot{\mathfrak{z}} = -V'(\mathfrak{z}), \tag{281}$$

where $m \in \mathbb{R}^+$, each overdot stands for a time-derivative, and a prime marks the differentiation with respect to $\mathfrak{z}$. We can express (281) as a pair of first-order differential equations:

$$m\dot{\mathfrak{z}} = \mathfrak{p}, \quad \dot{\mathfrak{p}} = -V'(\mathfrak{z}). \tag{282}$$

This is the Hamiltonian formulation of the dynamics of $\mathcal{S}_{BBM}$; introducing the complex Hamilton function $\mathfrak{h} := \frac{\mathfrak{p}^2}{2m} + V(\mathfrak{z})$, we can express (282) as the following pair of Hamilton equations.

$$\dot{\mathfrak{z}} = \frac{\partial \mathfrak{h}}{\partial \mathfrak{p}}, \quad \dot{\mathfrak{p}} = -\frac{\partial \mathfrak{h}}{\partial \mathfrak{z}}. \tag{283}$$

The variables $\mathfrak{z}$ and $\mathfrak{p}$ are the coordinates of the phase-space of the system $\mathfrak{P}$ which is as a set identical to $\mathbb{C}^2$ and $\mathbb{R}^4$. This observation suggests that, similarly to the

[111] The use of complex phase-space variables in standard classical mechanics is an old idea [137]. See also [222]. The subject of the present study is to consider complex configuration variables.

quantum systems defined along a complex contour, the complex classical system $\mathcal{S}_{\rm BBM}$ might admit a formulation that involves real variables. This is actually quite straightforward. We can define the real variables

$$x := \Re(\mathfrak{z}), \quad y := \Im(\mathfrak{z}), \quad p := \Re(\mathfrak{p}), \quad q := \Im(\mathfrak{p}), \quad V_r := \Re(V), \quad V_i := \Im(V), \tag{284}$$

$$H_r := \Re(\mathfrak{h}) = \frac{p^2 - q^2}{2m} + V_r(x, y), \quad H_i := \Im(\mathfrak{h}) = \frac{pq}{m} + V_i(x, y), \tag{285}$$

and use the well-known relations $\frac{\partial}{\partial \mathfrak{z}} = \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)$ and $\frac{\partial}{\partial \mathfrak{p}} = \frac{1}{2}\left(\frac{\partial}{\partial p} - i\frac{\partial}{\partial q}\right)$, to turn the complex Hamilton equations (283) to a system of four real equations.

It turns out that the resulting system of equations and consequently the complex Hamilton equations (283) are not consistent with the standard symplectic structure (Poisson bracket) on the phase space $\mathbb{C}^2 = \mathbb{R}^4$ [68, 166]. To see this, let us also introduce $w_1 := x$, $w_2 := p$, $w_3 := y$, and $w_4 := q$. Then the standard Poisson bracket on $\mathbb{R}^4$ takes the form

$$\{A, B\}_{PB} = \sum_{j,k=1}^{4} J_{jk}^{(\rm st)} \frac{\partial A}{\partial w_j} \frac{\partial B}{\partial w_j}, \tag{286}$$

where $J_{jk}^{(\rm st)}$ are the entries of the standard symplectic matrix

$$J^{(\rm st)} := \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \tag{287}$$

and A and B are a pair of classical observables (real-valued functions of w_j).[mmm] Recall that given a Hamilton function H on the four-dimensional phase space obtained by endowing $\mathbb{R}^4$ with the symplectic structure corresponding to the standard Poisson bracket (286), we can express the Hamilton equations in the form $\dot{w}_j = \{w_j, H\}_{\rm PB}$. If we express (286) in terms of the complex variables $\mathfrak{z}$ and $\mathfrak{p}$, we find that $\{\mathfrak{z}, \mathfrak{h}\}_{\rm PB} = \{\mathfrak{p}, \mathfrak{h}\}_{\rm PB} = 0$ [166]. Therefore, it is impossible to formulate the dynamics defined by (283) using the standard symplectic structure on $\mathbb{C}^2$.

This observation raises the problems of the existence, uniqueness, and classification of the symplectic structures on $\mathbb{C}^2 = \mathbb{R}^4$ that are compatible with the dynamical Eq. (283). Reference [68] gives a family of dynamically compatible symplectic structures. Reference [166] offers a complete classification of such structures. The most general compatible symplectic structure is defined by the following nonstandard Poisson bracket

$$\{\{A, B\}\} = \sum_{j,k=1}^{4} J_{jk} \frac{\partial A}{\partial w_j} \frac{\partial B}{\partial w_j}, \tag{288}$$

[mmm] $\Omega := \sum_{j,k=1}^{4} J_{jk} dw_j \wedge dw_k$ is the standard symplectic form on $\mathbb{R}^4$ [137].

where J_{ij} are the entries of the symplectic matrix

$$J := \frac{1}{2}\begin{pmatrix} 0 & 1+c & -a & -d \\ -(1+c) & 0 & -d & -b \\ a & d & 0 & -1+c \\ d & b & 1-c & 0 \end{pmatrix}, \tag{289}$$

and a, b, c, d are arbitrary real parameters satisfying $c^2 + d^2 - ab \neq 1$. Regardless of the choice of these parameters, we have $\dot{\mathfrak{z}} = \{\{\mathfrak{z}, \mathfrak{h}\}\}$ and $\dot{\mathfrak{p}} = \{\{\mathfrak{p}, \mathfrak{h}\}\}$. A particularly simple choice is $a = b = c = d = 0$ that yields

$$J = J_0 := \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}. \tag{290}$$

6.3. *Real description of a complex classical system*

Among the basic results of classical mechanics is the uniqueness theorem for symplectic structures on the phase-space $\mathbb{R}^{2d}$ [13]. In order to explain the content of this theorem, first we recall that a symplectic structure on $\mathbb{R}^{2d}$ is determined by the corresponding Poisson bracket. Choosing a system of coordinates w_j, we can express the latter in the form $\{A, B\}_{\mathcal{J}} = \sum_{j,k=1}^{2d} \mathcal{J}_{jk} \frac{\partial A}{\partial w_j} \frac{\partial B}{\partial w_j}$, where $\mathcal{J}$ is a real, antisymmetric, nonsingular $2d \times 2d$ matrix. The above-mentioned theorem states that there is always a system of (so-called Darboux) coordinates in which $\{A, B\}_{\mathcal{J}}$ takes the form of the standard Poisson bracket. Application of this theorem for the Poisson bracket (288) yields a description of the dynamics defined by the complex Hamiltonian $\mathfrak{h}$ in terms of a real Hamiltonian K.

The construction of the Darboux coordinates associated with the most general symplectic matrix (289) is described in [166]. These coordinates take the following particularly simple form for $a = b = c = d = 0$.

$$\begin{aligned} x_1 &:= \sqrt{2}\, w_1 = \sqrt{2}\, x, \quad & p_1 &:= \sqrt{2}\, w_2 = \sqrt{2}\, p, \\ x_2 &:= \sqrt{2}\, w_4 = \sqrt{2}\, q, \quad & p_2 &:= \sqrt{2}\, w_3 = \sqrt{2}\, y. \end{aligned} \tag{291}$$

These are precisely the phase-space coordinates used in [234] to study the complex trajectories appearing in the semiclassical treatment of the propagator for a quartic anharmonic oscillator. They are subsequently employed in the description of $\mathcal{PT}$-symmetric models [124].

The use of the coordinates (291) together with the assumption that the potential V is an analytic function, i.e. the Cauchy–Riemann conditions, $\frac{\partial v_r}{\partial x} - \frac{\partial v_i}{\partial y} = \frac{\partial v_r}{\partial y} + \frac{\partial v_i}{\partial x} = 0$, hold, lead to the following remarkable observations.

- The equivalent real Hamiltonian K that describes the dynamics is twice the real part of the complex Hamiltonian $\mathfrak{h}$ [234, 166],

$$K = \frac{p_1^2 - x_2^2}{2m} + 2V_r\left(\frac{x_1}{2}, \frac{p_2}{2}\right) = 2H_r. \tag{292}$$

- The imaginary part of $\mathfrak{h}$, i.e.

$$H_i = \frac{x_2 p_1}{2m} + V_i\left(\frac{x_1}{2}, \frac{p_2}{2}\right) \tag{293}$$

  is an integral of motion; $\{H_i, K\}_{\rm PB} = 0$ [166].

This implies that the dynamical system defined by the Hamilton equations (283) is equivalent to a classical Hamiltonian system with phase space $\mathbb{R}^4$ and the Hamiltonian $K = 2H_r$. Furthermore, in view of Liouville's theorem on integrable systems, because the phase space is four-dimensional and H_i is an integral of motion that is functionally independent of K, this system is completely integrable [13, 228].

The integral of motion H_i generates a certain class of transformations in the phase space that leave the dynamics invariant. The infinitesimal form of these symmetry transformations is given by [166]:

$$x_1 \to x_1 + \delta x_1, \quad \delta x_1 := \xi\{x_1, H_i\}_{\rm PB} = \frac{\xi x_2}{2m}, \tag{294}$$

$$x_2 \to x_2 + \delta x_2, \quad \delta x_2 := \xi\{x_2, H_i\}_{\rm PB} = \xi\, \frac{\partial}{\partial x_1} V_r\left(\frac{x_1}{2}, \frac{p_2}{2}\right), \tag{295}$$

$$p_1 \to p_1 + \delta p_1, \quad \delta p_1 := \xi\{p_1, H_i\}_{\rm PB} = \xi\, \frac{\partial}{\partial p_2} V_r\left(\frac{x_1}{2}, \frac{p_2}{2}\right), \tag{296}$$

$$p_2 \to p_2 + \delta p_2, \quad \delta p_2 := \xi\{p_2, H_i\}_{\rm PB} = -\frac{\xi\, p_1}{2m}, \tag{297}$$

where ξ is an infinitesimal real parameter.

The existence of these symmetry transformations is related to the fact that the system involves a first class constraint. Choosing a particular value C for H_i, i.e. imposing the constraint $\Phi := H_i - C = 0$, and moding out the above symmetry transformations by identifying each orbit of these transformations with a single point, we can construct a reduced dynamical system $\mathfrak{S}$ that has a two-dimensional real phase space [166]. This procedure has been implemented for a class of monomial potentials in [217] where the above symmetry transformations have been examined in the Lagrangian formulation and the difficult issue of the quantization of these systems has been addressed in some detail.[nnn] In general, the resulting quantum system depends on whether one imposes the constraint before or after the quantization. In the former case, the prescription used to obtain the reduced classical system also affects the resulting quantum system. For the imaginary cubic potential that allows for a fairly detailed analysis, one obtains a variety of quantum systems [217]. But none of these coincides with the pseudo-Hermitian quantum system we studied in Subsec. 4.2.2.

In summary, the identification of the complex classical system $\mathcal{S}_{\rm BBM}$ with the classical limit of the pseudo-Hermitian quantum system S that is defined by a complex potential V meets two serious difficulties. Firstly, while S has a single real

[nnn] The application of this approach for some multidimensional systems is studied in [95].

degree of freedom (one-dimensional real configuration space and two-dimensional real phase space), $\mathcal{S}_{\rm BBM}$ has two real degrees of freedom (a four-dimensional real phase space). Secondly, the Hamilton equations (283) that determine the dynamics of $\mathcal{S}_{\rm BBM}$ are not consistent with the standard symplectic structure on the phase space of $\mathcal{S}_{\rm BBM}$. This, in particular, means that under the naive correspondence $\mathcal{S}_{\rm BBM} \to S$, the Hamilton equations (283) are not mapped to the Heisenberg equations for S. These problems persist regardless of whether the Hamiltonian operator for S is defined on the real line or a complex contour. In fact, the study of the systems defined on a complex contour reveals another difficulty with the naive correspondence $\mathcal{S}_{\rm BBM} \to S$, namely that while the definition of S requires making a proper choice for a contour, $\mathcal{S}_{\rm BBM}$ is independent of such a choice.[ooo]

A proper treatment of the complex dynamical systems $\mathcal{S}_{\rm BBM}$ requires the investigation of a dynamically compatible symplectic structure. Once such a structure is selected, one can adopt a corresponding set of Darboux coordinates and use them to obtain a standard (real) description of $\mathcal{S}_{\rm BBM}$. The use of the real description reveals the curious fact that this system admits an integral of motion that is functionally independent of the Hamiltonian. This has two important consequences:

(1) The system is completely integrable;
(2) The system has a first class constraint.

The choice $H_i = 0$ that is adopted in [43, 46, 47] is just one way of imposing the constraint. It corresponds to restricting the dynamics to a three-dimensional subspace of the phase space. On this subspace there acts the symmetry transformations (294)–(297) that leave the dynamics invariant. Moding out these transformations, one finds a reduced dynamical system $\mathfrak{S}$ with a two-dimensional real phase space. It is the latter that can, in principle, be related to the quantum system S. So far the existence and nature of such a relationship could not be ascertained. For the simple polynomial potentials that could be studied carefully, the various known ways of constructing and quantizing $\mathfrak{S}$ lead to quantum systems that differ from S.

Another important issue is that the above procedure of constructing complex dynamical systems $\mathcal{S}_{\rm BBM}$ and the corresponding reduced systems $\mathfrak{S}$ may be carried through for any complex analytic potential. But, not every such potential defines a unitary pseudo-Hermitian quantum system. A typical example is the exponential potential $V(x) = e^{i\kappa x}$ that is defined on $\mathbb{R}$. It is well-known that the spectrum of the Hamiltonian operator $H = \frac{p^2}{2m} + \epsilon e^{i\kappa x}$, with $m \in \mathbb{R}^+$ and $\epsilon, \kappa \in \mathbb{R} - \{0\}$, includes spectral singularities [91]. This shows that this operator cannot be mapped to a Hermitian operator by a similarity transformation, i.e. it is not quasi-Hermitian.

[ooo]The phase-space path integral formulation of the wrong-sign quartic potential defined on the contour (247) is consistent with the standard Hilbert-space formulation, if one restricts the complex classical Hamiltonian $\mathfrak{h}$ to the contour (247) [36, 121]. Whether imposing this restriction would lead to a particular reduced classical system that is identical with the classical system $\mathcal{S}$ defined by the Hamiltonian $H'_c = \frac{p_c^2}{2m} + 4\Lambda\big(x_c^2 - \frac{\Omega^2}{4\Lambda}\big)^2$ of Subsec. 5.3 is worthy of investigation.

Hence H is not capable of defining a unitary quantum system. Although the potential $V(x) = e^{i\kappa x}$ defines a complex dynamical system $\mathcal{S}_{\rm BBM}$, it cannot be related to a unitary quantum system.[ppp]

We conclude this section by underlining a rather interesting parallelism between the quantum and classical mechanics of complex (analytic) potentials. Suppose that a complex (analytic) potential V defines a unitary pseudo-Hermitian quantum system, we showed in Sec. 3 that this system admits an equivalent Hermitian representation. The above discussion reveals a classical analogue of this equivalence; the complex dynamical system defined by the complex Hamiltonian $H = \frac{p^2}{2m} + V$ admits an equivalent description involving a real Hamiltonian. What differentiates the pseudo-Hermitian and Hermitian representations of quantum mechanics is the choice of the inner product (equivalently a metric operator) on the space of state-vectors. What differentiates the complex and real representations of the classical mechanics is the choice of the symplectic structure (equivalently Poisson bracket) on the phase (state) space. Mathematically the equivalence of the pseudo-Hermitian and Hermitian representations of quantum mechanics stems from the uniqueness theorem for separable Hilbert spaces. The classical counterpart of this theorem that is responsible for the above-mentioned equivalence of the complex and real representations of the classical mechanics is the uniqueness theorem for symplectic manifolds diffeomorphic to $\mathbb{R}^{2d}$.

7. Time-Dependent Hamiltonians and Path-Integral Formulation

7.1. *Time-dependent quasi-Hermitian Hamiltonians*

Time-dependent Hamiltonian operators arise in a variety of applications of conventional quantum mechanics. Their time-dependence does not cause any difficulties except that, for the cases that the eigenvectors of the Hamiltonian are time-dependent, the time-evolution operator takes the form of a time-ordered exponential involving the Hamiltonian [54].[qqq] The situation is quite different when one deals with time-dependent quasi-Hermitian Hamiltonians.[rrr] As the following no-go theorem shows, the observability of the Hamiltonian and the unitarity of the time-evolution put a severe restriction on the way a quasi-Hermitian Hamiltonian can depend on time [167].

Theorem 2. *Let $T \in \mathbb{R}^+$ and for all $t \in [0, T]$, $H(t)$ be a time-dependent quasi-Hermitian operator acting in a reference Hilbert space $\mathcal{H}$. Suppose that $H(t)$ serves*

[ppp]For a study of the classical dynamics generated by this exponential potential, see [68].

[qqq]A rather common misconception in dealing with time-dependent Hamiltonians is to think that the time-reversal operator $\mathcal{T}$ changes the sign of the time variable t in the Hamiltonian, i.e. $H(t) \to \mathcal{T}H(t)\mathcal{T} = H(-t)$ which in view of the definition of $\mathcal{T}$, namely for all $\psi \in L^2(\mathbb{R})$, $(\mathcal{T}\psi)(x) := \psi(x)^*$, is generally false. See for example [237], where the author considers a trivial non-Hermitian time-dependent Hamiltonian that is obtained from a constant $\mathcal{PT}$-symmetric Hamiltonian through a time-dependent point transformation and a time-reparametrization.

[rrr]Time-dependent quasi-Hermitian Hamiltonians arise naturally in the application of pseudo-Hermitian quantum mechanics in quantum cosmology [150, 151]. See also [156, 88].

as the Hamiltonian operator for a pseudo-Hermitian quantum system with physical Hilbert space $\mathcal{H}_{\rm phys}$*. If the time-evolution of the system, that is determined by the Schrödinger equation*: $i\hbar\dot{\psi}(t) = H(t)\psi(t)$*, is unitary and* $H(t)$ *is an observable for all* $t \in [0,T]$*, then the metric operator defining* $\mathcal{H}_{\rm phys}$ *does not depend on time, i.e. there must exist a time-independent metric operator* η_+ *such that* $H(t)$ *is* η_+*-pseudo-Hermitian for all* $t \in [0,T]$*.*

Following [167] we call a time-dependent quasi- (pseudo-) Hermitian Hamiltonian admitting a time-independent metric (pseudo-metric) operator *quasi-stationary*. Theorem 2 states that in pseudo-Hermitian quantum mechanics we are bound to use quasi-stationary Hamiltonians. To demonstrate the severity of this restriction, consider two-level quantum systems where the Hamiltonian $H(t)$ may be represented by a 2×2 complex matrix $\underline{\mathrm{H}(t)}$ with possibly time-dependent entries. The requirement that $H(t)$ is quasi-Hermitian implies that $\underline{\mathrm{H}(t)}$ involves six independent real-valued functions (because its eigenvalues are real). The additional requirement that $H(t)$ is quasi-stationary reduces this number to four.[sss] This is also the same as the maximum number of independent real-valued functions that a general time-dependent Hermitian Hamiltonian can include.

A simple implication of Theorem 2 is that the inner product of the physical Hilbert space cannot depend on time, unless one defines the dynamics of the quantum system by an operator that is not observable or allows for nonunitary time-evolutions. In other words, insisting on observability of the Hamiltonian operator and requiring unitarity prohibit scenarios involving switching Hilbert spaces as proposed in [41].

7.2. *Path-integral formulation of pseudo-Hermitian QM*

Among the original motivations to consider $\mathcal{PT}$-symmetric quantum mechanical models is the potential applications of their relativistic and field theoretical generalizations [37, 38] in elementary particle physics. A necessary first step in trying to explore the relativistic and field theoretical generalizations of $\mathcal{PT}$-symmetric or more generally pseudo-Hermitian QM is a careful examination of its path-integral formulation. In this section we use the approach of [169] to elucidate the role of the metric operator in the path-integral formulation of pseudo-Hermitian QM and demonstrate the equivalence of the latter with the path-integral formulation of the conventional QM.

We shall first review the emergence of path integrals in dealing with a simple conventional (Hermitian) quantum system. This requires a brief discussion of the trace of a linear operator.

[sss]This can be easily inferred from the results of [178].

Let $L : \mathcal{H} \to \mathcal{H}$ be a linear operator acting in a separable Hilbert space $\mathcal{H}$ with inner product $\langle \cdot \,|\, \cdot \rangle$. Then the *trace* of L is defined by

$$\mathrm{tr}(L) := \sum_{n=1}^{N} \langle \xi_n \,|\, L\xi_n \rangle, \tag{298}$$

where $\{\xi_n\}$ is an arbitrary orthonormal basis of $\mathcal{H}$ [195]. Obviously, for $N = \infty$, the right-hand side of (298) may not converge, and $\mathrm{tr}(L)$ may not exist.

Suppose that K and L are linear operators for which $\mathrm{tr}(KL) < \infty$. Then invoking the completeness relation for ξ_n and using Dirac's bracket notation, we can show that

$$\begin{aligned} \mathrm{tr}(LK) &= \sum_{m,n=1}^{N} \langle \xi_n | L | \xi_m \rangle \langle \xi_m | K | \xi_n \rangle = \sum_{m,n=1}^{N} \langle \xi_m | K | \xi_n \rangle \langle \xi_n | L | \xi_m \rangle \\ &= \sum_{m=1}^{N} \langle \xi_m | KL | \xi_m \rangle = \mathrm{tr}(KL). \end{aligned} \tag{299}$$

A simple implication of this identity is that the right-hand side of (298) is independent of the choice of the orthonormal basis $\{\xi_n\}$.[ttt]

For a linear operator L acting in $L^2(\mathbb{R})$, we can use the position basis $\{|x\rangle\}$ to compute $\mathrm{tr}(L)$. To demonstrate how this is done, let $\{\xi_n\}$ be an orthonormal basis of $L^2(\mathbb{R})$. Using (298), the completeness relation for $|x\rangle$ and ξ_n, and Dirac's bracket notation, we have

$$\begin{aligned} \mathrm{tr}(L) &= \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dx' \langle \xi_n | x \rangle \langle x | L | x' \rangle \langle x' | \xi_n \rangle \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dx' \langle x | L | x' \rangle \sum_{n=0}^{\infty} \langle x' | \xi_n \rangle \langle \xi_n | x \rangle \\ &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx dx', \quad \langle x | L | x' \rangle \langle x' | x \rangle = \int_{-\infty}^{\infty} dx \langle x | L | x \rangle. \end{aligned} \tag{300}$$

Now, consider a quantum system defined by the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$ and a Hermitian Hamiltonian H that is an analytic (or piecewise analytic) function of the usual (Hermitian) position operator (x), momentum operator (p), and possibly time (t). The generating functional (also called partition function) for the n-point (correlation) functions of the system is given by

$$Z[J] = \mathrm{tr}\left(\mathfrak{T} \exp\left\{ -\frac{i}{\hbar} \int_{t_1}^{t_2} dt [H - Jx] \right\} \right), \tag{301}$$

[ttt]To see this, let $\{\zeta_n\}$ be another orthonormal basis of $\mathcal{H}$. Then as we described in Subsec. 2.3, ζ_n are related to ξ_n by a unitary operator $U : \mathcal{H} \to \mathcal{H}$, $\zeta_n = U\xi_n$. This in turn implies $\sum_{n=1}^{N} \langle \zeta_n \,|\, L\zeta_n \rangle = \sum_{n=1}^{N} \langle U\xi_n \,|\, LU\xi_n \rangle = \sum_{n=1}^{N} \langle \xi_n \,|\, U^\dagger (LU) \xi_n \rangle = \sum_{n=1}^{N} \langle \xi_n | (LU) U^\dagger \xi_n \rangle = \sum_{n=1}^{N} \langle \xi_n \,|\, L\xi_n \rangle$, where we have used (299) and $UU^\dagger = I$.

where "$\mathfrak{T}\exp$" denotes the time-ordered exponential, t_1 and t_2 are, respectively, the initial and final times for the evolution of the system that are taken to be $-\infty$ and ∞ in the scattering setups used particularly in quantum field theory, and J stands for the (possibly time-dependent) coupling constant for the source terms Jx [70, 231]. The latter is by definition an observable [75]. In view of the fact that x is also an observable, this implies that J must be real-valued.

One can easily justify the condition of the observability of the source term by noting that $Z[J]$ is used to compute the n-point functions according to [70]: $\big\langle\mathfrak{T}[x(\tau_1)x(\tau_2)\cdots x(\tau_n)]\big\rangle = \frac{(-i\hbar)^n}{Z[J]}\frac{\delta^n Z[J]}{\delta J(\tau_1)\delta J(\tau_2)\cdots\delta J(\tau_n)}\big|_{J=0}$, where $\tau_1,\tau_2,\ldots,\tau_n \in [t_1,t_2]$, $x(\tau)$ denotes the position operator in the Heisenberg picture, i.e. $x(\tau) := U_{\!J}(\tau,t_1)xU_{\!J}(t_1,\tau)$, and $U_{\!J}$ is the time-evolution operator associated with the interacting system; for all $\mathfrak{t}_1,\mathfrak{t}_2\in\mathbb{R}$,

$$U_{\!J}(\mathfrak{t}_1,\mathfrak{t}_2) := \mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{\mathfrak{t}_1}^{\mathfrak{t}_2} dt[H-Jx]\right\}. \tag{302}$$

The n-point functions are essentially the expectation values of the observables $\mathfrak{T}[x(\tau_1)\cdots x(\tau_n)]$ (in the groundstate of the system if $t_2=-t_1\to\infty$). Therefore, the observability of the source term Jx is linked to the observability of the Heisenberg-picture position operators $x(\tau_i)$. The latter is ensured by the unitarity of the time-evolution operator $U_{\!J}(\mathfrak{t}_1,\mathfrak{t}_2)$ and the observability of the Schrödinger-picture position operator x.

In view of (300), we can express the partition function (301) in the form

$$\begin{aligned} Z[J] &= \int_{-\infty}^{\infty} dx\,\left\langle x\left|\mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H-Jx]\right\}\right|x\right\rangle \\ &= \int_{-\infty}^{\infty} dx\langle x,t_1\,|\,x,t_2\rangle, \end{aligned} \tag{303}$$

where

$$|x,t\rangle := U_{\!J}(0,t)^\dagger|x\rangle, \tag{304}$$

are the (generalized) eigenfunctions of the Heisenberg-picture position operator $x(t)$. In light of (302) and (304), we also have, for all $x_1,x_2\in\mathbb{R}$, $\langle x_1,t_1|x_2,t_2\rangle = \langle x_1|U_{\!J}(t_1,t_2)|x_2\rangle = \langle x_1|\mathfrak{T}\exp\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H-Jx]\}|x_2\rangle$. Computing this quantity as a phase-space path integral and substituting the result in (303), we find the following phase-space path integral expression for the generating functional.

$$Z[J] = \iint \mathcal{D}(x)\mathcal{D}(p)e^{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H(x,p;t)-J(t)x]}. \tag{305}$$

If H is a quadratic polynomial in p, we can perform the momentum path integral in (305) and convert it into a configuration-space (Lagrangian) path integral. This yields

$$Z[J] = \int \mathcal{D}(x)e^{\frac{i}{\hbar}\int_{t_1}^{t_2} dtL_{\!J}(x,\dot{x};t)}, \tag{306}$$

where $L_J(x,\dot{x};t) := \dot{x}p - H(x,p;t) + J(t)x$, and p is to be identified with its expression obtained by solving $\dot{x} = \frac{\partial H(x,p;t)}{\partial p}$ for p as a function of x, $\dot{x}$ and t.

Next, we consider the extension of the above constructions to a system defined by the reference Hilbert space $\mathcal{H} = L^2(\mathbb{R})$, a metric operator $\eta_+ : L^2(\mathbb{R}) \to L^2(\mathbb{R})$, and an η_+-pseudo-Hermitian Hamiltonian $H : L^2(\mathbb{R}) \to L^2(\mathbb{R})$ that is again a (piecewise) analytic function of x, p, and possibly t. According to the Theorem 2, in order for H to be an observable that generates a unitary time-evolution, it must be quasi-stationary. As discussed in [167], this puts a severe restriction on the form of allowed time-dependent Hamiltonians.[uuu]

We can certainly work in the Hermitian representation $(\mathcal{H}, h)$ of the system where $h := \rho H \rho^{-1}$ (with $\rho := \sqrt{\eta_+}$) is the equivalent Hermitian Hamiltonian (59). In this representation the generating functional has the form

$$Z[J] = \mathrm{tr}\left(\mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[h - Jx]\right\}\right). \tag{307}$$

As we showed above this quantity admits a phase-space path integral expression. But even for the case that H is a quadratic polynomial in p, the equivalent Hermitian Hamiltonian h does not share this property, and we cannot convert the right-hand side of (307) into a Lagrangian path integral in general. This provides a concrete motivation for the derivation of the path-integral expression for the generating functional in the pseudo-Hermitian representation of the system, i.e. $(\mathcal{H}_{\rm phys}, H)$.

In [44] the authors use the expression (306) (with $t_2 = -t_1 \to \infty$) to perform a perturbative calculation of the generating functional and the one-point function for the $\mathcal{PT}$-symmetric cubic anharmonic oscillator (161).[vvv] As a result, they find an imaginary value for the one-point function. This is simply because the one-point function they calculate corresponds to the groundstate expectation value of the usual position operator that is indeed not an observable of the system. The physically meaningful generating functional is [169]

$$Z[J] = \mathrm{tr}_{\eta_+}\left(\mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H - JX]\right\}\right), \tag{308}$$

where for every linear operator $K : \mathcal{H} \to \mathcal{H}$,

$$\mathrm{tr}_{\eta_+}(K) := \sum_{n=1}^{N} \langle\psi_n \,|\, K\psi_n\rangle_{\eta_+} = \sum_{n=1}^{N} \langle\psi_n \,|\, \eta_+ K\psi_n\rangle, \tag{309}$$

$\{\psi_n\}$ is an arbitrary orthonormal basis of $\mathcal{H}_{\rm phys}$, and X is the η_+-pseudo-Hermitian position operator (55). The n-point functions generated by (308) correspond to the

[uuu] In relativistic field theories, H is obtained by integrating the Hamiltonian density over a space-like hypersurface. This makes the time-dependence of H quite arbitrary and renders the imposition of the condition of quasi-stationarity of H an extremely difficult task.

[vvv] See also [34].

expectation value of time-ordered products of the physical position operators and the resulting numerical values are necessarily real.

It is not difficult to show that $\mathrm{tr}_{\eta_+} = \mathrm{tr}$. To do this, we first recall that because $\rho := \sqrt{\eta} : \mathcal{H}_{\rm phys} \to \mathcal{H}$ is a unitary operator, it maps orthonormal bases of $\mathcal{H}_{\rm phys}$ onto orthonormal bases of $\mathcal{H}$. In particular, $\xi_n := \rho\,\psi_n$ form an orthonormal basis of $\mathcal{H}$. This together with $\rho^2 = \eta_+$, $\rho^\dagger = \rho$, (309), (298) and (299) imply

$$\begin{aligned}\mathrm{tr}_{\eta_+}(K) &= \sum_{n=1}^{N}\langle\psi_n\,|\,\rho^2 K\psi_n\rangle = \sum_{n=1}^{N}\langle\rho\,\psi_n\,|\,\rho K\psi_n\rangle\\ &= \sum_{n=1}^{N}\langle\xi_n\,|\,\rho K\rho^{-1}\xi_n\rangle = \mathrm{tr}(\rho K\rho^{-1}) = \mathrm{tr}(K).\end{aligned}\tag{310}$$

This relation allows us to express (308) in the form

$$Z[J] = \mathrm{tr}\left(\mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H - JX]\right\}\right).\tag{311}$$

Next, we employ the definitions of h and X, namely $h := \rho H\rho^{-1}$ and $X := \rho^{-1}x\rho$, and the fact that η_+ and consequently ρ do not dependent on time, to establish $\mathfrak{T}\exp\{-\frac{i}{\hbar}\int_{t_1}^{t_2}[h - Jx]\} = \rho\mathfrak{T}\exp\{-\frac{i}{\hbar}\int_{t_1}^{t_2}[H - JX]\}\rho^{-1}$. In view of this relation and (299) the right-hand sides of (307) and (311) coincide. This is another manifestation of the physical equivalence of Hermitian and pseudo-Hermitian representations of the system.

As we emphasized in the preceding sections the metric operator plays a fundamental role in the operator formulation of pseudo-Hermitian quantum mechanics. The same is true about the path-integral formulation of this theory. To elucidate this point we examine the nature of the dependence of the generating functional on the choice of a metric operator η_+.

A simple consequence of (300) and (311) is

$$Z[J] = \int_{-\infty}^{\infty} fx\left\langle x\right|\mathfrak{T}\exp\left\{-\frac{i}{\hbar}\int_{t_1}^{t_2} dt[H - JX]\right\}\left|x\right\rangle.\tag{312}$$

Clearly, $Z[0]$ does not depend on η_+ [169]. This explains the results of [113] pertaining the metric-independence of thermodynamical quantities associated with non-interacting pseudo-Hermitian statistical mechanical models. However, in contrast to the view expressed in [122], the metric-independence of $Z[0]$ does not extend to $Z[J]$ with $J \neq 0$. This is actually to be expected because the knowledge of $Z[J]$ allows for the calculation of the n-point functions that are expectation values of the time-ordered products of the Heisenberg-picture η_+-pseudo-Hermitian position operators $X(\tau_i)$.

The dependence of $Z[J]$ on the choice of η_+ is rather implicit. In the Hermitian representation, η_+ enters the expression for $Z[J]$ through the equivalent Hermitian Hamiltonian h. In the pseudo-Hermitian representation, this is done through the source term JX. The presence of X in (312) prevents one from

obtaining a Lagrangian path integral for $Z[J]$ even for the cases that H is a quadratic polynomial in p. Therefore, contrary to claims made in [44], in general, the pseudo-Hermitian representation is not practically superior to the Hermitian representation. There are certain calculations that are performed more easily in the pseudo-Hermitian representation, and there are others that are more straightforward to carry out in the Hermitian representation [154].

8. Geometry of the State-Space and the Quantum Brachistochrone

8.1. *State-space and its geometry in conventional QM*

In conventional quantum mechanics the states are not elements of the Hilbert space $\mathcal{H}$, but the rays (one-dimensional subspaces) of the Hilbert space.[www] The space of all rays that is usually called the *projective Hilbert space* and denoted by $\mathcal{P}(\mathcal{H})$ has the structure of a manifold. For an N-dimensional Hilbert space $\mathcal{H}$, $\mathcal{P}(\mathcal{H})$ is the complex projective space $\mathbb{C}P^{N-1}$. This is a compact manifold for finite N and a well-known infinite-dimensional manifold with very special and useful mathematical properties for infinite N [54].

The projective Hilbert space $\mathcal{P}(\mathcal{H})$ is usually endowed with a natural geometric structure that is of direct relevance to physical phenomena such as geometric phases [189] and optimal-speed unitary evolutions in quantum mechanics [9]. To describe this structure, we need an appropriate representation of the elements of $\mathcal{P}(\mathcal{H})$. This is provided by the projection operators associated with the states.

Consider a state λ_ψ represented by a state-vector $\psi \in \mathcal{H} - \{0\}$, i.e. $\lambda_\psi = \{c\psi \,|\, c \in \mathbb{C}\}$, and the projection operator

$$\Lambda_\psi := \frac{|\psi\rangle\langle\psi|}{\langle\psi \,|\, \psi\rangle}. \tag{313}$$

Clearly the relation between states λ_ψ and state-vectors $c\psi$ is one to (infinitely) many. But the relation between the states λ_ψ and the projection operators Λ_ψ is one-to-one. This suggests using the latter to identify the elements of the projective Hilbert space $\mathcal{P}(\mathcal{H})$. This parametrization of $\mathcal{P}(\mathcal{H})$ has the advantage of allowing us to use the algebraic properties of the projection operators (313) in the study of states.

An important property of (313) is that it is a positive operator having a unit trace. The positivity of Λ_ψ is a simple consequence of the identities

$$\Lambda_\psi^\dagger = \Lambda_\psi, \quad \Lambda_\psi^2 = \Lambda_\psi. \tag{314}$$

We recall from Subsec. 7.2 that the trace of a linear operator $J : \mathcal{H} \to \mathcal{H}$ is defined by

$$\mathrm{tr}(J) := \sum_{n=1}^{N} \langle\xi_n \,|\, J\xi_n\rangle, \tag{315}$$

[www]Throughout this article the word "state" is used to mean "pure state".

where $\{\xi_n\}$ is an arbitrary orthonormal basis of $\mathcal{H}$ [195]. If $L : \mathcal{H} \to \mathcal{H}$ is a linear operator such that $\mathrm{tr}(L^\dagger L) < \infty$, L is said to be a *Hilbert–Schmidt operator*. In view of (313)–(315) and (19), we have

$$\mathrm{tr}(\Lambda_\psi^\dagger \Lambda_\psi) = \mathrm{tr}(\Lambda_\psi^2) = \mathrm{tr}(\Lambda_\psi)$$

$$= \sum_{n=1}^{N} \frac{\langle \xi_n \,|\, \psi\rangle\langle \psi \,|\, \xi_n\rangle}{\langle \psi \,|\, \psi\rangle} = \frac{\sum_{n=1}^{N} |\langle \xi_n \,|\, \psi\rangle|^2}{\langle \psi \,|\, \psi\rangle} = \frac{\|\psi\|^2}{\langle \psi \,|\, \psi\rangle} = 1. \tag{316}$$

Therefore, Λ_ψ is a Hilbert–Schmidt operator with unit trace.

The set $\mathfrak{B}_2(\mathcal{H})$ of Hilbert–Schmidt operators forms a subspace of the vector space of bounded linear operators acting in $\mathcal{H}$. We can use "tr" to define the following inner product on $\mathfrak{B}_2(\mathcal{H})$.

$$(L \,|\, J) := \mathrm{tr}(L^\dagger J) \quad \text{for all } L, J \in \mathfrak{B}_2(\mathcal{H}). \tag{317}$$

This is called the *Frobenius* or *Hilbert–Schmidt inner product* [106, 195]. It has the appealing property that given an orthonormal set $\{\chi_n\}$ of state-vectors the corresponding set of projection operators $\{\Lambda_{\chi_n}\}$ forms an orthonormal subset of $\mathfrak{B}_2(\mathcal{H})$; $\langle \chi_m \,|\, \chi_n\rangle = \delta_{mn}$ implies $(\Lambda_{\chi_n} \,|\, \Lambda_{\chi_m}) = \delta_{mn}$.

The set $\mathfrak{H}_2(\mathcal{H})$ of Hermitian Hilbert–Schmidt operators to which the projection operators Λ_ψ belong is a subset of $\mathfrak{B}_2(\mathcal{H})$ that forms a real vector space with the usual addition of linear operators and their scalar multiplication. It is not difficult to see, with the help of (299), that (317) reduces to a real inner product on $\mathfrak{H}_2(\mathcal{H})$, namely

$$(L \,|\, J) := \mathrm{tr}(LJ) \quad \text{for all } L, J \in \mathfrak{H}_2(\mathcal{H}). \tag{318}$$

Therefore endowing $\mathfrak{H}_2(\mathcal{H})$ with this inner product produces a real inner product space.

By identifying states λ_ψ with the projection operators Λ_ψ, we can view the projective Hilbert space $\mathcal{P}(\mathcal{H})$ as a subset of $\mathfrak{H}_2(\mathcal{H})$ and use the inner product (318) to endow $\mathcal{P}(\mathcal{H})$ with a natural metric tensor. The corresponding line element ds at Λ_ψ is given by

$$ds^2(\Lambda_\psi) := \frac{1}{2}(d\Lambda_\psi \,|\, d\Lambda_\psi) = \frac{\langle \psi \,|\, \psi\rangle\langle d\psi \,|\, d\psi\rangle - |\langle \psi \,|\, d\psi\rangle|^2}{\langle \psi \,|\, \psi\rangle^2}, \tag{319}$$

where we have inserted a factor of $\frac{1}{2}$ to respect a mathematical convention and used (313), (315), (318), and the fact that $\{\xi_n\}$ is an orthonormal basis of $\mathcal{H}$.

For $N < \infty$, we can identify ψ with a nonzero complex column vector $\vec{\mathfrak{z}}$ with components $\mathfrak{z}_1, \mathfrak{z}_2, \ldots, \mathfrak{z}_N$. In terms of these we can express (319) in the form $ds^2 = \sum_{a,b=1}^{N} g_{ab^*} d\mathfrak{z}_a d\mathfrak{z}_b^*$ where

$$g_{ab^*} := \frac{|\vec{\mathfrak{z}}|^2 \delta_{ab} - \mathfrak{z}_a^* \mathfrak{z}_b}{|\vec{\mathfrak{z}}|^4}. \tag{320}$$

This is precisely the Fubini-Study metric on the complex projective space $\mathbb{C}P^{N-1}$ [82].

As a concrete example, consider the case that $\mathcal{H}$ is two-dimensional, i.e. $N = 2$. Then using the standard basis representation of operators acting in $\mathbb{C}^2$, and noting that in this case all operators are Hilbert–Schmidt, we can infer that $\mathfrak{H}_2(\mathcal{H})$ is equivalent to the set of all Hermitian matrices. This is a four-dimensional real vector space which we can identify with $\mathbb{R}^4$. Specifically, we can represent each $J \in \mathfrak{H}_2(\mathcal{H})$ using its standard matrix representation:

$$\underline{\mathrm{J}} = \begin{pmatrix} z & x - iy \\ x + iy & w \end{pmatrix}, \tag{321}$$

and observe that these matrices are in one-to-one correspondence with $(x, y, z, w) \in \mathbb{R}^4$.

The projective Hilbert space $\mathcal{P}(\mathcal{H})$ is a two-dimensional subset of the four-dimensional real vector space $\mathfrak{H}_2(\mathcal{H})$. To see this let us choose an arbitrary state-vector $\psi \in \mathbb{C}^2 - \{\vec{0}\}$. Then $\psi = \binom{\mathfrak{z}_1}{\mathfrak{z}_2}$ for some $\mathfrak{z}_1, \mathfrak{z}_2 \in \mathbb{C}$ such that $|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2 \neq 0$, and in view of (313) we can represent Λ_ψ by

$$\underline{\Lambda_\psi} = \frac{1}{|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2} \begin{pmatrix} |\mathfrak{z}_1|^2 & \mathfrak{z}_1\mathfrak{z}_2^* \\ \mathfrak{z}_1^*\mathfrak{z}_2 & |\mathfrak{z}_2|^2 \end{pmatrix}. \tag{322}$$

Using the parametrization (321), we find that for $J = \Lambda_\psi$,

$$x = \frac{\mathfrak{z}_1\mathfrak{z}_2^* + \mathfrak{z}_1^*\mathfrak{z}_2}{2(|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2)}, \quad y = \frac{i(\mathfrak{z}_1\mathfrak{z}_2^* - \mathfrak{z}_1^*\mathfrak{z}_2)}{2(|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2)}, \quad z = \frac{|\mathfrak{z}_1|^2}{|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2}, \quad w = \frac{|\mathfrak{z}_2|^2}{|\mathfrak{z}_1|^2 + |\mathfrak{z}_2|^2}. \tag{323}$$

Therefore as expected, $w = 1 - z$, so that

$$\underline{\Lambda_\psi} = \begin{pmatrix} z & x - iy \\ x + iy & 1 - z \end{pmatrix}, \tag{324}$$

and the condition $\Lambda_\psi^2 = \Lambda_\psi$ takes the form

$$x^2 + y^2 + \left(z - \frac{1}{2}\right)^2 = \frac{1}{4}. \tag{325}$$

This defines a two-dimensional sphere S^2 that we can use to represent $\mathcal{P}(\mathcal{H})$.

If we endow $\mathbb{R}^3$, that is parametrized by the Cartesian coordinates (x, y, z), with the Euclidean metric, we can identify S^2 with a round sphere of unit diameter. We will next obtain an expression for the metric induced on S^2 by the embedding Euclidean space $\mathbb{R}^3$.

Let $\mathbf{N}$ and $\mathbf{S}$ respectively denote the north and south poles of S^2, i.e. $\mathbf{N} := (x = 0, y = 0, z = 1)$ and $\mathbf{S} := (x = 0, y = 0, z = 0)$, and consider the stereographic projection of S^2 onto the tangent plane $\Pi_{\mathbf{N}}$ at $\mathbf{N}$, as depicted in Fig. 2. The line connecting $\mathbf{S}$ to an arbitrary point $p = (x, y, z)$ on $S^2 - \{\mathbf{S}\}$ intersects $\Pi_{\mathbf{N}}$ at a point p. If we set up a Cartesian coordinate system in $\Pi_{\mathbf{N}}$ with $\mathbf{N}$ as its origin

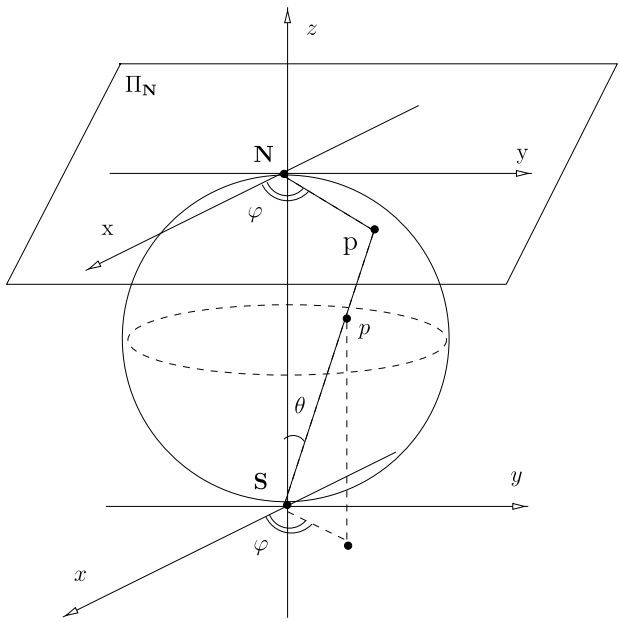

Fig. 2. Stereographic projection of the sphere S^2 defined by $x^2+y^2+(z-\frac{1}{2})^2=\frac{1}{4}$: **N** and **S** are respectively the north and south poles of S^2. $\Pi_{\mathbf{N}}$ is the tangent plane at **N**. p is a point on $S^2-\{\mathbf{S}\}$, and p is its stereographic projection on $\Pi_{\mathbf{N}}$.

and axes parallel to the x- and y-axes, and denote by (x,y) the coordinates of p in this coordinates system, we can uniquely identify the points $p\in S^2-\{\mathbf{S}\}$ with $(\mathrm{x},\mathrm{y})\in\mathbb{R}^2$. Using simple methods of analytic geometry, we can easily verify that

$$\mathrm{x}=\frac{x}{z},\quad \mathrm{y}=\frac{y}{z},\quad x=\frac{\mathrm{x}}{1+\mathrm{x}^2+\mathrm{y}^2},\quad y=\frac{\mathrm{y}}{1+\mathrm{x}^2+\mathrm{y}^2},\quad z=\frac{1}{1+\mathrm{x}^2+\mathrm{y}^2}. \tag{326}$$

We can employ the last three of these relations to compute the line element over the sphere in the (x,y)-coordinates. A rather lengthy but straightforward calculation yields

$$ds^2=dx^2+dy^2+dz^2=\frac{d\mathrm{x}^2+d\mathrm{y}^2}{(1+\mathrm{x}^2+\mathrm{y}^2)^2}. \tag{327}$$

This relation together with $ds^2=\sum_{i,j=1}^2 g^{(FS)}_{ij}d\mathrm{x}^i d\mathrm{x}^j$, where $\mathrm{x}^1:=\mathrm{x}$ and $\mathrm{x}^2:=\mathrm{y}$, gives the following local coordinate expression for the Fubini-Study metric tensor [82],

$$g^{(FS)}_{ij}=\frac{\delta_{ij}}{[1+(\mathrm{x}^1)^2+(\mathrm{x}^2)^2]^2}. \tag{328}$$

Expressing x and y in terms of the spherical coordinates,

$$\varphi:=\tan^{-1}\left(\frac{y}{x}\right),\quad \theta:=\cos^{-1}(2z-1), \tag{329}$$

of S^2, we find

$$\mathrm{x} = \tan\left(\frac{\theta}{2}\right)\cos\varphi, \quad \mathrm{y} = \tan\left(\frac{\theta}{2}\right)\sin\varphi. \tag{330}$$

Substituting these in (327) leads to the following familiar relation for the line element of a sphere of unit diameter.

$$ds^2 = \frac{1}{4}(d\theta^2 + \sin^2\theta d\varphi^2). \tag{331}$$

In order to make the relationship between (319) and (327) more transparent, we recall that the south pole $\mathbf{S}$ of S^2 corresponds to the projection operator Λ_{e_2} represented by

$$\underline{\Lambda_{e_2}} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \tag{332}$$

and the state $\lambda_{e_2} := \{ce_2 \,|\, c \in \mathbb{C}\}$, where $e_2 := \binom{0}{1}$. The coordinates (x, y) parametrize all the states except λ_{e_2}. These are represented by the state-vectors

$$\psi = \begin{pmatrix} \mathfrak{z}_1 \\ \mathfrak{z}_2 \end{pmatrix} \quad \text{with } \mathfrak{z}_1 \neq 0. \tag{333}$$

Introducing $\mathrm{z} := \frac{\mathfrak{z}_2}{\mathfrak{z}_1}$, we can simplify the expression (322) for the corresponding projection operator. In terms of z, the coordinates x, y, z appearing in (324) take the form $x = \frac{\Re(\mathrm{Z})}{1+|\mathrm{Z}|^2}$, $y = \frac{\Im(\mathrm{Z})}{1+|\mathrm{Z}|^2}$, $z = \frac{1}{1+|\mathrm{Z}|^2}$. Comparing these with (326) reveals

$$\mathrm{x} = \Re(\mathrm{z}), \quad \mathrm{y} = \Im(\mathrm{z}). \tag{334}$$

Now, we are in a position to compute the line element (319). Inserting (333) in (319), setting $\mathfrak{z}_2 = \mathfrak{z}_1\mathrm{z}$, and using (334) and (330), we find

$$ds^2 = \frac{d\mathrm{z}^* d\mathrm{z}}{(1+|\mathrm{z}|^2)^2} = \frac{d\mathrm{x}^2 + d\mathrm{y}^2}{(1+\mathrm{x}^2+\mathrm{y}^2)^2} = \frac{1}{4}(d\theta^2 + \sin^2\theta d\varphi^2). \tag{335}$$

Therefore, as a Riemannian manifold the state-space $\mathcal{P}(\mathcal{H})$ is identical to a two-dimensional (round) sphere of unit diameter.[xxx]

8.2. *State-space and its geometry in pseudo-Hermitian QM*

The construction of the space of states in pseudo-Hermitian quantum mechanics is similar to that in conventional quantum mechanics. Again, the states are rays in the (reference) Hilbert space $\mathcal{H}$ which are identical with the rays in the physical Hilbert space $\mathcal{H}_{\text{phys}}$. The only difference is in the way one associates projection

[xxx]The above calculation of the metric tensor on S^2 makes use of the stereographic projection of $S^2 - \{\mathbf{S}\}$ onto the plane $\Pi_{\mathbf{N}}$ which is a copy of $\mathbb{R}^2 = \mathbb{C}$. We could also consider the stereographic projection of $S^2 - \{\mathbf{N}\}$ onto the tangent plane $\Pi_{\mathbf{S}}$ at $\mathbf{S}$. Using both the projections we are able to describe all the points on S^2. This is a manifestation of the manifold structure of S^2.

operators to states and defines an appropriate notion of distance (metric tensor) on the state-space.

In the following we shall use $\mathcal{P}(\mathcal{H}_{\rm phys})$ to denote the state-space of a pseudo-Hermitian quantum system with physical Hilbert space $\mathcal{H}_{\rm phys}$. The latter is obtained by endowing the underlying vector space of $\mathcal{H}$ with the inner product $\langle\cdot\,|\,\cdot\rangle_{\eta_+}$, where $\eta_+ : \mathcal{H} \to \mathcal{H}$ is a given metric operator rendering the Hamiltonian of the system η_+-pseudo-Hermitian. We shall also introduce the following notation that will simplify some of the calculations: For all $\xi, \zeta \in \mathcal{H}$, $|\zeta\succ := |\zeta\rangle = \zeta$, $\prec\zeta| := \langle\zeta|\eta_+$, $\prec\xi\,|\,\zeta\succ := \langle\xi|\eta_+\,|\,\zeta\rangle = \langle\xi\,|\,\eta_+\zeta\rangle = \langle\xi\,|\,\zeta\rangle_{\eta_+}$.

First we define, for each pair of linear operators $L, J : \mathcal{H} \to \mathcal{H}$,

$$(L\,|\,J)_{\eta_+} := {\rm tr}_{\eta_+}(L^\sharp J) = {\rm tr}(L^\sharp J), \tag{336}$$

where $L^\sharp$ stands for the η_+-pseudo-adjoint of L:

$$L^\sharp := \eta_+^{-1} L^\dagger \eta_+, \tag{337}$$

${\rm tr}_{\eta_+}$ is defined by (309), and we have used (310). The linear operators $A : \mathcal{H}_{\rm phys} \to \mathcal{H}_{\rm phys}$ for which $(A\,|\,A)_{\eta_+}$ is finite together with (336) form the inner product space $\mathfrak{B}_2(\mathcal{H}_{\rm phys})$ of Hilbert–Schmidt operators acting in $\mathcal{H}_{\rm phys}$. Substituting (337) in (336) and using $\rho^2 = \eta_+$ and $\rho^\dagger = \rho$, we also have

$$\begin{aligned}(L\,|\,J)_{\eta_+} &= {\rm tr}(\eta_+^{-1} L^\dagger \eta_+ J) = {\rm tr}(\rho^{-1} L^\dagger \rho^2 J \rho^{-1}) \\ &= {\rm tr}((\rho L \rho^{-1})^\dagger \rho J \rho^{-1}) = (\rho L \rho^{-1}\,|\,\rho J \rho^{-1}).\end{aligned} \tag{338}$$

These calculations show that $\rho : \mathcal{H}_{\rm phys} \to \mathcal{H}$ induces a unitary operator $U_\rho : \mathfrak{B}_2(\mathcal{H}_{\rm phys}) \to \mathfrak{B}_2(\mathcal{H})$ defined by

$$U_\rho(L) := \rho L \rho^{-1}, \quad \text{for all } L \in \mathfrak{B}_2(\mathcal{H}_{\rm phys}). \tag{339}$$

Now, consider a state $\lambda_\psi := \{c\psi\,|\,c \in \mathbb{C}\}$ for some $\psi \in \mathcal{H}_{\rm phys} - \{0\}$. Because $\prec\cdot\,|\,\cdot\succ$ is the inner product of $\mathcal{H}_{\rm phys}$, the orthogonal projection operator onto λ_ψ is given by

$$\Lambda_\psi^{(\eta_+)} := \frac{|\psi\succ\prec\psi|}{\prec\psi\,|\,\psi\succ} = \frac{|\psi\rangle\langle\psi\,|\,\eta_+}{\langle\psi\,|\,\eta_+\psi\rangle} = \frac{\langle\psi\,|\,\psi\rangle\Lambda_\psi\eta_+}{\langle\psi\,|\,\eta_+\psi\rangle}. \tag{340}$$

A quick calculation shows that ${\Lambda_\psi^{(\eta_+)}}^2 = \Lambda_\psi^{(\eta_+)}$. Furthermore, using the arguments leading to (316), we have

$$\begin{aligned}{\rm tr}_{\eta_+}(\Lambda_\psi^{(\eta_+)\sharp}\Lambda_\psi^{(\eta_+)}) &= {\rm tr}_{\eta_+}(\Lambda_\psi^{(\eta_+)}) \\ &= \frac{\sum_{n=1}^N \prec\psi_n\,|\,\psi\succ\prec\psi\,|\,\psi_n\succ}{\prec\psi\,|\,\psi\succ} = \frac{\sum_{n=1}^N |\prec\psi_n\,|\,\psi\succ|^2}{\prec\psi\,|\,\psi\succ} = 1.\end{aligned}$$

This shows that $\Lambda_\psi^{(\eta_+)} \in \mathfrak{B}_2^{(\eta_+)}$, and also, because ${\rm tr}_{\eta_+} = {\rm tr}$,

$${\rm tr}(\Lambda_\psi^{(\eta_+)}) = 1. \tag{341}$$

Another direct implication of (340) is $\Lambda_\psi^{(\eta_+)\dagger} = \eta_+ \Lambda_\psi^{(\eta_+)} \eta_+^{-1}$. Hence $\Lambda_\psi^{(\eta_+)}$ belongs to the subset $\mathfrak{H}_2(\mathcal{H}_{\rm phys})$ of η_+-pseudo-Hermitian elements of $\mathfrak{B}_2(\mathcal{H}_{\rm phys})$. We can view this as a real vector space. Equation (336) defines a real inner product on this space, and the restriction of (339) onto $\mathfrak{H}_2(\mathcal{H}_{\rm phys})$ that we also denote by U_ρ yields a unitary operator that maps $\mathfrak{H}_2(\mathcal{H}_{\rm phys})$ onto $\mathfrak{H}_2(\mathcal{H})$. In fact $\mathfrak{H}_2(\mathcal{H}_{\rm phys})$ and $\mathfrak{H}_2(\mathcal{H})$ are real separable Hilbert spaces and the existence of the unitary operator $U_\rho : \mathfrak{H}_2(\mathcal{H}_{\rm phys}) \to \mathfrak{H}_2(\mathcal{H})$ is a manifestation of the fact that real separable Hilbert spaces of the same dimension are unitary-equivalent.

The set of the projection operators (340) that is in one-to-one correspondence with the projective Hilbert space $\mathcal{P}(\mathcal{H}_{\rm phys})$ is a proper subset of $\mathfrak{H}_2(\mathcal{H}_{\rm phys})$. Similarly to the case of conventional quantum mechanics, we can define a natural metric on this space whose line element has the form

$$ds^2_{\eta_+}(\Lambda_\psi) := \frac{1}{2}(d\Lambda_\psi^{(\eta_+)} \,|\, d\Lambda_\psi^{(\eta_+)})_{\eta_+} = \frac{\prec\psi \,|\, \psi\succ\prec d\psi \,|\, d\psi\succ - |\prec\psi \,|\, d\psi\succ|^2}{\prec\psi \,|\, \psi\succ^2}$$
$$= \frac{\langle\psi \,|\, \eta_+\psi\rangle\langle d\psi \,|\, \eta_+ d\psi\rangle - |\langle\psi \,|\, \eta_+ d\psi\rangle|^2}{\langle\psi \,|\, \eta_+\psi\rangle^2}. \tag{342}$$

It is important to note that as smooth manifolds $\mathcal{P}(\mathcal{H})$ and $\mathcal{P}(\mathcal{H}_{\rm phys})$ are the same, but as Riemannian manifolds they are different. While $\mathcal{P}(\mathcal{H})$ is endowed with the Fubini-Study metric, $\mathcal{P}(\mathcal{H}_{\rm phys})$ is endowed with the metric corresponding to (342). For $N < \infty$ we can obtain a global expression for the latter in terms of the coordinates $\mathfrak{z}_1, \mathfrak{z}_2, \ldots, \mathfrak{z}_N$ of the state-vectors $\psi = \vec{\mathfrak{z}} \in \mathbb{C}^N$. This yields the following generalization of (320) that satisfies $ds^2_{\eta_+} = \sum_{a,b=1}^N g^{(\eta_+)}_{ab^*} d\mathfrak{z}_a \mathfrak{z}^*_b$.

$$g^{(\eta_+)}_{ab^*} := \frac{\sum_{c,d=1}^N (\eta_{+cd}\eta_{+ba} - \eta_{+ca}\eta_{+bd})\mathfrak{z}^*_c\mathfrak{z}_d}{\left(\sum_{r,s=1}^N \eta_{+rs}\mathfrak{z}^*_r\mathfrak{z}_s\right)^2}. \tag{343}$$

Here η_{+ab} are the entries of the standard representation $\underline{\eta_+}$ of η_+ [168].

For two-level systems where $N = 2$, we can easily obtain an explicit expression for the line element (342). In general, the metric operator η_+ is represented by

$$\underline{\eta_+} = \begin{pmatrix} a & b_1 - ib_2 \\ b_1 + ib_2 & c \end{pmatrix}, \tag{344}$$

where $a, b_1, b_2, c \in \mathbb{R}$ are such that

$$a + c = {\rm tr}(\underline{\eta_+}) > 0, \quad {\rm d} := ac - (b_1^2 + b_2^2) = \det(\underline{\eta_+}) > 0. \tag{345}$$

In view of (340) we can again parametrize $\underline{\Lambda_\psi^{(\eta_+)}}$ using the Cartesian coordinates x, y, z of the sphere S^2 defined by (325). For the states differing from λ_{e_2}, we can

alternatively choose the coordinates x and y of (334) and show using (333), (340), and (344) that

$$ds^2_{\eta_+} = \frac{\mathrm{d}(dx^2+dy^2)}{[a+2(b_1x+b_2y)+c(x^2+y^2)]^2}. \tag{346}$$

It is easy to see that for $\eta_+ = I$ where $a = c = 1$ and $b_1 = b_2 = 0$, (346) reproduces (335).

To gain a more intuitive understanding of (346), we next express its right-hand side in terms of the spherical coordinates (329). Inserting (330) in (346) and carrying out the necessary calculations, we find

$$ds^2_{\eta_+} = \frac{k_1(d\theta^2+\sin^2\theta d\varphi^2)}{[1+k_2\cos\theta+g(\varphi)\sin\theta]^2} = \frac{k_1(d\theta^2+\sin^2\theta d\tilde{\varphi}^2)}{[1+k_2\cos\theta+k_3\cos\tilde{\varphi}\sin\theta]^2} \tag{347}$$

where we have introduced

$$k_1 := \frac{\mathrm{d}}{(a+c)^2} = \frac{\det(\underline{\eta_+})}{\mathrm{tr}(\underline{\eta_+})^2}, \quad k_2 := \frac{a-c}{a+c}, \quad k_3 := \frac{2\sqrt{b_1^2+b_2^2}}{a+c}, \tag{348}$$

$$g(\varphi) := \frac{2(b_1\cos\varphi+b_2\sin\varphi)}{a+c}, \quad \tilde{\varphi} := \varphi-\beta, \quad \beta := \tan^{-1}\left(\frac{b_2}{b_1}\right). \tag{349}$$

Note that the change of coordinate $\varphi \to \tilde{\varphi}$ corresponds to a constant rotation about the z-axis, and because of (345) we have $k_1 > 0$, $-1 < k_2 < 1$ and $0 \le k_3 < 1$.

The projective Hilbert space $\mathcal{P}(\mathcal{H}_{\rm phys})$ is the Riemannian manifold obtained by endowing the sphere S^2 with the metric $\mathbf{g}^{(\eta_+)}$ corresponding to the line element (347).

Next, consider the general case where N need not be two. In order to compare the geometric structure of $\mathcal{P}(\mathcal{H}_{\rm phys})$ and $\mathcal{P}(\mathcal{H})$, we recall that $\mathcal{P}(\mathcal{H}_{\rm phys}) \subset \mathfrak{B}_2(\mathcal{H}_{\rm phys})$, $\mathcal{P}(\mathcal{H}) \subset \mathfrak{B}_2(\mathcal{H})$, and that the linear operator U_ρ of Eq. (339) maps $\mathfrak{B}_2(\mathcal{H}_{\rm phys})$ onto $\mathfrak{B}_2(\mathcal{H})$. It is easy to check that the restriction of U_ρ on $\mathcal{P}(\mathcal{H}_{\rm phys})$, i.e. the function $u_\rho : \mathcal{P}(\mathcal{H}_{\rm phys}) \to \mathcal{P}(\mathcal{H})$ defined by

$$u_\rho(\Lambda_\psi^{(\eta_+)}) := \rho\Lambda_\psi^{(\eta_+)}\rho^{-1}, \quad \text{for all } \Lambda_\psi^{(\eta_+)} \in \mathcal{P}(\mathcal{H}_{\rm phys}), \tag{350}$$

is a diffeomorphism. Furthermore, in view of (313), (340), and $\rho^\dagger = \rho = \sqrt{\eta_+}$, we have

$$u_\rho(\Lambda_\psi^{(\eta_+)}) = \frac{\rho\,|\,\psi\rangle\langle\psi\,|\,\eta_+\rho^{-1}}{\langle\psi\,|\,\rho^2\psi\rangle} = \frac{\rho\,|\,\psi\rangle\langle\psi\,|\,\rho}{\langle\rho\psi\,|\,\rho\psi\rangle} = \frac{|\Psi\rangle\langle\Psi|}{\langle\Psi\,|\,\Psi\rangle} = \Lambda_\Psi, \tag{351}$$

where $\Psi := \rho\psi \in \mathcal{H}$. A straightforward consequence of (319), (318), (338), (342), (350) and (351) is

$$\begin{aligned} ds^2(u_\rho(\Lambda_\psi^{(\eta_+)})) = ds^2(\Lambda_\Psi) &= \frac{1}{2}(d\Lambda_\Psi\,|\,d\Lambda_\Psi) = \frac{1}{2}(\rho d\Lambda_\psi^{(\eta_+)}\rho^{-1}\,|\,\rho d\Lambda_\psi^{(\eta_+)}\rho^{-1}) \\ &= \frac{1}{2}(d\Lambda_\psi^{(\eta_+)}\,|\,d\Lambda_\psi^{(\eta_+)})_{\eta_+} = ds^2_{\eta_+}(\Lambda_\psi^{(\eta_+)}). \end{aligned} \tag{352}$$

This shows that $u_\rho : \mathcal{P}(\mathcal{H}_{\rm phys}) \to \mathcal{P}(\mathcal{H})$ is an *isometry*, i.e. it leaves the distances invariant. Therefore, $\mathcal{P}(\mathcal{H}_{\rm phys})$ and $\mathcal{P}(\mathcal{H})$ have the same geometric structure. In

particular, for $N = 2$, we can identify $\mathcal{P}(\mathcal{H}_{\rm phys})$ with a sphere of unit diameter embedded in $\mathbb{R}^3$ with its standard geometry.

This result is another manifestation of the fact that pseudo-Hermitian quantum mechanics is merely an alternative representation of the conventional quantum mechanics. Because the geometry of the state space may be related to physical quantities such as geometric phases, we should not have expected to obtain different geometric structures for $\mathcal{P}(\mathcal{H}_{\rm phys})$ and $\mathcal{P}(\mathcal{H})$.

8.3. *Optimal-speed evolutions*

Let $H : \mathcal{H} \to \mathcal{H}$ be a possibly time-dependent Hermitian Hamiltonian with a discrete spectrum. Suppose that we wish to use H to evolve an initial state $\lambda_{\psi_I} \in \mathcal{P}(\mathcal{H})$ into a final state $\lambda_{\psi_F} \in \mathcal{P}(\mathcal{H})$ in some time τ. Then the evolving state-vector $\psi(t) \in \mathcal{H}$ satisfies

$$H\psi(t) = i\hbar\dot{\psi}(t), \quad \psi(0) = \psi_I, \quad \psi(\tau) = \psi_F, \tag{353}$$

and the corresponding state $\lambda_{\psi(t)}$ traverses a curve in the projective Hilbert space $\mathcal{P}(\mathcal{H})$.

The instantaneous speed for the motion of $\lambda_{\psi(t)}$ in $\mathcal{P}(\mathcal{H})$ is

$$v_\psi := \frac{ds}{dt}, \tag{354}$$

where ds is the line element given by (319). In view of this equation,

$$v_\psi^2 = \frac{\langle\psi(t)\,|\,\psi(t)\rangle\langle\dot{\psi}(t)\,|\,\dot{\psi}(t)\rangle - |\langle\psi(t)\,|\,\dot{\psi}(t)\rangle|^2}{\langle\psi(t)\,|\,\psi(t)\rangle^2} = \frac{\Delta E_\psi(t)^2}{\hbar^2}, \tag{355}$$

where

$$\Delta E_\psi(t)^2 := \frac{\langle\psi(t)\,|\,H^2\psi(t)\rangle}{\langle\psi(t)\,|\,\psi(t)\rangle} - \frac{|\langle\psi(t)\,|\,H\psi(t)\rangle|^2}{\langle\psi(t)\,|\,\psi(t)\rangle^2}, \tag{356}$$

is the square of the energy uncertainty, and we have used (353) and the Hermiticity of H. We can employ (354) and (355) to express the length of the curve traced by $\lambda_{\psi(t)}$ in $\mathcal{P}(\mathcal{H})$ in the form [9]:

$$s = \frac{1}{\hbar}\int_0^\tau \Delta E_\psi(t)dt. \tag{357}$$

Because ΔE_ψ is non-negative, s is a monotonically increasing function of τ. This makes τ a monotonically increasing function of s. Therefore, the shortest travel time is achieved for the paths of the shortest length, i.e. the geodesics of $\mathcal{P}(\mathcal{H})$.

For a time-independent Hamiltonian H we have $\psi(t) = e^{-\frac{itH}{\hbar}}\psi_I$ and as seen from (356), ΔE_ψ is also time-independent. In this case, (357) yields

$$\tau = \frac{\hbar s}{\Delta E_\psi}, \tag{358}$$

and the minimum possible travel time is achieved when s is identified with the geodesic distance between ψ_I and ψ_F.

Because of the particular structure of $\mathcal{P}(\mathcal{H})$, the geodesic(s) connecting any two states λ_{ψ_I} and λ_{ψ_F} lie entirely on a two-dimensional submanifold of $\mathcal{P}(\mathcal{H})$ that is actually the projective Hilbert space $\mathcal{P}(\mathcal{H}_{I,F})$ for the subspace $\mathcal{H}_{I,F}$ of $\mathcal{H}$ spanned by ψ_I and ψ_F. If the time evolution generated by the Hamiltonian minimizes the travel time, the evolving state λ_{ψ_I} should stay in $\mathcal{P}(\mathcal{H}_{I,F})$ during the evolution. This means that the problem of determining minimum-travel-time evolutions [90, 227, 135, 55, 64] reduces to the case that $\mathcal{H}$ is two-dimensional [56]. As we saw in Subsec. 8.1, in this case $\mathcal{P}(\mathcal{H})$ is a round sphere of unit diameter and the geodesics are the large circles on this sphere.

Next, we study, without loss of generality, the case $N = 2$. It is easy to show the existence of a time-independent Hamiltonian that evolves λ_{ψ_I} to λ_{ψ_F} along a geodesic. We will next construct such a Hamiltonian.

Consider a time-independent Hamiltonian H acting in a two-dimensional Hilbert space. We can always assume that H has a vanishing trace so that its eigenvalues have opposite sign, $E_2 = -E_1 =: E$.[yyy] Because ΔE_ψ is time-independent we can compute it at $t = 0$. Expanding $\psi(0) = \psi_I$ in an orthonormal basis $\{\psi_1, \psi_2\}$ consisting of a pair of eigenvectors of H, i.e. writing it in the form

$$\psi_I = c_1\psi_1 + c_2\psi_2, \quad c_1, c_2 \in \mathbb{C}, \tag{359}$$

we find [171]

$$\Delta E_\psi = E\sqrt{1 - \left(\frac{|c_1|^2 - |c_2|^2}{|c_1|^2 + |c_2|^2}\right)^2} \leq E. \tag{360}$$

Therefore, the travel time τ satisfies

$$\tau \geq \tau_{\rm min} := \frac{\hbar s}{E}, \tag{361}$$

where s is the geodesic distance between λ_{ψ_I} and λ_{ψ_F} in $\mathcal{P}(\mathcal{H})$. Equation (361) identifies $\tau_{\rm min}$ with a lower bound on the travel time. Next, we shall construct a Hamiltonian $H_\star$ with eigenvalues $\pm E$ for which $\tau = \tau_{\rm min}$. This will, in particular, identify $\tau_{\rm min}$ with the minimum travel time.

In order to determine $H_\star$ we only need to construct a pair of its linearly independent eigenvectors ψ_1 and ψ_2 and use its spectral resolution:

$$H_\star = E(-|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|). \tag{362}$$

As seen from (360), to saturate the lower bound on τ, we must have $|c_1| = |c_2|$. In view of time-independence of ΔE_ψ we could also use ψ_F to compute this quantity.

[yyy] This is true for general possibly time-dependent Hamiltonians $H(t)$. Under the gauge transformation $\psi(t) \to \psi'(t) \to e^{\frac{i\alpha(t)}{\hbar}}\psi(t)$ with $\alpha(t) = N^{-1}\int_0^t {\rm tr}[H(s)]ds$, the Hamiltonian $H(t)$ transforms into the traceless Hamiltonian $H'(t) := H(t) - N^{-1}{\rm tr}[H(t)]I$.

If we expand the latter as

$$\psi_F = d_1\psi_1 + d_2\psi_2, \quad d_1, d_2 \in \mathbb{C}, \tag{363}$$

we find that ΔE_ψ satisfies (360) with (c_1, c_2) replaced by (d_1, d_2). Therefore, by the same argument we find $|d_1| = |d_2|$. This in turn means that there must exist $\beta_I, \beta_F \in \mathbb{R}$ such that

$$c_2 = e^{\beta_I} c_1, \quad d_2 = e^{\beta_F} d_1. \tag{364}$$

Inserting these relations in (359) and (363) gives

$$\psi_1 + e^{i\beta_I}\psi_2 = c_1^{-1}\psi_I, \quad \psi_1 + e^{i\beta_F}\psi_2 = d_1^{-1}\psi_F. \tag{365}$$

Solving these for ψ_1 and ψ_2, we obtain

$$\psi_1 = \frac{\sqrt{2}(\hat\psi_I - e^{\frac{i\vartheta}{2}}\hat\psi_F)}{1 - e^{i\vartheta}}, \quad \psi_2 = \frac{\sqrt{2}e^{-i\beta_F}(-\hat\psi_I + e^{\frac{-i\vartheta}{2}}\hat\psi_F)}{1 - e^{i\vartheta}}, \tag{366}$$

where we have introduced

$$\vartheta := \beta_I - \beta_F, \quad \hat\psi_I := \frac{\psi_I}{\sqrt{2}c_1}, \quad \hat\psi_F := \frac{e^{\frac{i\vartheta}{2}}\psi_F}{\sqrt{2}d_1}. \tag{367}$$

Clearly $\hat\psi_n$ determines the same state as ψ_n for $n \in \{1, 2\}$. Also in view of (362), the presence of β_F in (366) does not affect the expression for $H_\star$. The only parameter that has physical significance is the angle ϑ. The orthonormality of ψ_1 and ψ_2 implies that $\hat\psi_I$ and $\hat\psi_F$ have unit norm, and more importantly, that ϑ fulfils

$$\langle\hat\psi_I \,|\, \hat\psi_F\rangle = \cos\left(\frac{\vartheta}{2}\right). \tag{368}$$

In terms of ψ_I and ψ_F this equation takes the form

$$\langle\psi_I \,|\, \psi_F\rangle = c_1^* d_1(1 + e^{-i\vartheta}). \tag{369}$$

Note that because $\hat\psi_I$ and $\hat\psi_F$ have unit norm, according to (367), $\langle\psi_I \,|\, \psi_I\rangle = 2|c_1|^2$ and $\langle\psi_F \,|\, \psi_F\rangle = 2|d_1|^2$. These relations together with (367) and (368) imply

$$\cos^2\left(\frac{\vartheta}{2}\right) = \frac{|\langle\psi_I \,|\, \psi_F\rangle|^2}{\langle\psi_I \,|\, \psi_I\rangle\langle\psi_F \,|\, \psi_F\rangle}. \tag{370}$$

Therefore whenever ψ_I and ψ_F are orthogonal, $\vartheta = \pi$. Furthermore, as discussed in [9], (370) shows that ϑ is related to the geodesic distance s between λ_{ψ_I} and λ_{ψ_F} according to[zzz]

$$\vartheta = 2s. \tag{371}$$

In the case that ψ_I and ψ_F are orthogonal, λ_{ψ_I} and λ_{ψ_F} are *antipodal* points on $\mathcal{P}(\mathcal{H})$. Therefore their geodesic distance s is half of the perimeter of a large circle. Because $\mathcal{P}(\mathcal{H})$ is a round sphere of unit diameter, we have $s = \frac{\pi}{2}$, which is consistent with (371).

[zzz] Note that the metric on $\mathcal{P}(\mathcal{H})$ that is used in [9] differs from our metric by a factor of $\sqrt{2}$.

Having calculated the eigenvectors ψ_1 and ψ_2, we can use (362) to obtain an explicit expression for the Hamiltonian $H_\star$ that evolves λ_{ψ_I} into λ_{ψ_F} in time $\tau_{\rm min}$. Substituting (366) in (362) and using (367), (368) and (371), we find [64, 56, 171]

$$H_\star = \frac{iE(|\hat\psi_F\rangle\langle\hat\psi_I| - |\hat\psi_I\rangle\langle\hat\psi_F|)}{4\sin(\frac{\vartheta}{2})} = \frac{iE\cot(s)}{4}\left(\frac{|\psi_F\rangle\langle\psi_I|}{\langle\psi_I\,|\,\psi_F\rangle} - \frac{|\psi_I\rangle\langle\psi_F|}{\langle\psi_F\,|\,\psi_I\rangle}\right). \quad (372)$$

The last equation shows that $H_\star$ depends only on the states λ_{ψ_I} and λ_{ψ_F} and not on the particular state-vectors one uses to represent these states. Note also that this equation is valid generally; it applies for quantum systems with an arbitrary finite- or infinite-dimensional $\mathcal{H}$.

This completes our discussion of the quantum Brachistochrone problem in conventional quantum mechanics. We can use the same approach to address this problem within the framework of pseudo-Hermitian quantum mechanics [168]. This amounts to making the following substitutions in the above analysis: $|\psi_n\rangle \to |\psi_n\succ$, $\langle\psi_n| \to \prec\psi_n|$, and $s \to s_{\eta_+}$. In particular, the minimum travel time is given by

$$\tau_{\rm min}^{(\eta_+)} = \frac{\hbar s_{\eta_+}}{E}, \quad (373)$$

and the η_+-pseudo-Hermitian Hamiltonian that generates minimal-travel-time evolution between λ_{ψ_I} and λ_{ψ_F} has the form

$$H_\star^{(\eta_+)} = \frac{iE\cot(s_{\eta_+})}{4}\left(\frac{|\psi_F\succ\prec\psi_I|}{\prec\psi_I\,|\,\psi_F\succ} - \frac{|\psi_I\succ\prec\psi_F|}{\prec\psi_F\,|\,\psi_I\succ}\right), \quad (374)$$

where

$$\cos^2(s_{\eta_+}) = \frac{|\prec\psi_I\,|\,\psi_F\succ|^2}{\prec\psi_I\,|\,\psi_I\succ\prec\psi_F\,|\,\psi_F\succ}. \quad (375)$$

Equation (374) gives the expression for the most general time-independent optimal-speed quasi-Hermitian Hamiltonian operator that evolves ψ_I into ψ_F. Similar to its Hermitian counterpart, it applies irrespective of the dimensionality of the Hilbert space.

In [41], the authors show, using a class of quasi-Hermitian Hamiltonians, that one can evolve an initial state λ_{ψ_I} into a final state λ_{ψ_F} in a time τ that violates the condition $\tau \geq \tau_{\rm min}$. They actually show that by appropriately choosing the form of the quasi-Hermitian Hamiltonian one can make τ arbitrarily small. This phenomenon can be easily explained using the above treatment of the problem. The minimum travel time for an η_+-pseudo-Hermitian Hamiltonian is given by (373). In view of (347), depending on the value of $k_1 = \det(\underline{\eta_+})/{\rm tr}(\underline{\eta_+})^2$ one can make s_{η_+} and consequently $\tau_{\rm min}^{(\eta_+)}$ as small as one wishes. This observation does not, however, seem to have any physically significant implications, because a physical process that involves evolving λ_{ψ_I} into λ_{ψ_F} using an η_+-pseudo-Hermitian Hamiltonian H can be described equally well by considering the evolution of $\lambda_{\rho\psi_I}$ into $\lambda_{\rho\psi_F}$ using the Hermitian Hamiltonian $h := \rho H\rho^{-1}$. In light of the existence of the isometry

$u_\rho : \mathcal{P}(\mathcal{H}_{\rm phys}) \to \mathcal{P}(\mathcal{H})$, the distance between λ_{ψ_I} and λ_{ψ_F} in $\mathcal{P}(\mathcal{H}_{\rm phys})$ is equal to the distance between $\lambda_{\rho\psi_I}$ and $\lambda_{\rho\psi_F}$ in $\mathcal{P}(\mathcal{H})$. It is also easy to show that the travel time for both the evolutions are identical. Therefore as far as the evolution speed is concerned, there is no advantage of using the η_+-pseudo-Hermitian Hamiltonian H over the equivalent Hermitian Hamiltonian h [168].

We wish to emphasize that the existence of a lower bound on travel time is significant, because it limits the speed with which one can perform unitary transformations dynamically. Such transformations play a central role in quantum computation. For example, the construction of efficient NOT-gates involves unitary transformations that map a state into its antipodal state. The distance between antipodal states in $\mathcal{P}(\mathcal{H}_{\rm phys})$ is the same as in $\mathcal{P}(\mathcal{H})$. Hence, for such states $\tau_{\rm min}^{(\eta_+)} = \tau_{\rm min}$.

The situation is quite different if we consider the evolution generated by the η_+-pseudo-Hermitian Hamiltonian $H_\star^{(\eta_+)}$ in the standard projective Hilbert space $\mathcal{P}(\mathcal{H})$. In this case, we can indeed obtain arbitrarily fast evolutions, but they will not be unitary [16]. The possibility of infinitely fast non-unitary evolutions is actually not surprising. What is rather surprising is that one can achieve such evolutions using quasi-Hermitian Hamiltonians; *there are arbitrarily fast quasi-unitary evolutions* [171].

A scenario that is also considered in [41] is to use both Hermitian and quasi-Hermitian Hamiltonians to produce an arbitrarily fast evolution of λ_{ψ_I} into λ_{ψ_F}. This is done in three stages. First, one evolves the initial state λ_{ψ_I} into an auxiliary state $\lambda_{\psi'_I}$ using a Hermitian Hamiltonian h_1 in time τ_1, then one evolves $\lambda_{\psi'_I}$ into another auxiliary state $\lambda_{\psi'_F}$ using a quasi-Hermitian Hamiltonian H in time τ', and finally one evolves $\lambda_{\psi'_F}$ into the desired final state λ_{ψ_F} using another Hermitian Hamiltonian h_2 in time τ_2. By choosing the intermediate states $\lambda_{\psi'_I}$ and $\lambda_{\psi'_F}$ appropriately, one can make τ_1 and τ_2 as small as one wishes. By choosing H to be an η_+-pseudo-Hermitian operator of the form (374) with the parameter k_1 of η_+ sufficiently small, one can make the total travel time $\tau := \tau_1 + \tau' + \tau_2$ smaller than $\tau_{\rm min}$. In this scenario, both the initial and final states belong to $\mathcal{P}(\mathcal{H})$, but to maintain unitarity of the evolution one is bound to switch (the defining metric of) the physical Hilbert space at $t = \tau_1$ and $t = \tau_1 + \tau'$. Therefore, this scheme involves a physical Hilbert space with a time-dependent inner product. As discussed in Subsec. 7.1, the latter violates the condition that the Hamiltonian is an observable. Therefore, *there seems to be no legitimate way of lowering the bound on travel time between two states of a given distance except allowing for non-unitary* (*possibly quasi-unitary*) *evolutions.*

9. Physical Applications

Since its inception in the form of $\mathcal{PT}$-symmetric models in the late 1990's and later as a consistent quantum mechanical scheme [175], pseudo-Hermitian QM has been

the subject of extensive research. The vast majority of the publications on the subject deal with issues related to formalism or various (quantum mechanical as well as field theoretical) toy models with mostly obscure physical meaning. There are however, a number of exceptions to this general situation where concrete problems are solved using the methods developed within the framework of pseudo-Hermitian QM. In this section, we outline the basic ideas upon which these recent developments rest. Before engaging into a discussion of these, however, we wish to list some of the applications that predate the recent activities in the field.

9.1. *Earlier applications*

9.1.1. *Dyson–Boson mapping*

Among the earliest manifestations of pseudo-Hermitian operators is the one appearing in the context of the Dyson mapping of Hermitian Fermionic Hamiltonians to equivalent quasi-Hermitian bosonic Hamiltonians [81]. Dyson mapping has subsequently found applications in nuclear physics [115] and provided the basic idea for the formulation of quasi-Hermitian QM [207]. For a brief review of the Dyson mapping method, see [92].

9.1.2. *Complex scaling and resonances*

Consider the one-parameter family of operators: $ru_\alpha = \exp(\frac{i\alpha}{2\hbar}\{x,p\})$ with $\alpha \in \mathbb{C}$, that act in the Hilbert space $L^2(\mathbb{R})$. We can easily use the Backer–Campbell–Hausdorff identity (150) together with the canonical computation relation $[x,p] = i\hbar$ to show that $\mathfrak{u}_\alpha$ induces a scaling of the position and momentum operators: $x \to \mathfrak{u}_\alpha x \mathfrak{u}_\alpha^{-1} = e^\alpha x$ and $p \to \mathfrak{u}_\alpha p \mathfrak{u}_\alpha^{-1} = e^{-\alpha} p$. For $\alpha \in \mathbb{R}$, $\mathfrak{u}_\alpha$ is a unitary transformation, and one can use the latter property to show that $(\mathfrak{u}_\alpha\psi)(x) = e^{-\frac{\alpha}{2}}\psi(e^\alpha x)$ for all $\psi \in L^2(\mathbb{R})$.

For $\alpha \in \mathbb{C} - \mathbb{R}$, the transformation $\psi \to \mathfrak{u}_\alpha\psi$ is called a *complex scaling* transformation. In this case, $\mathfrak{u}_\alpha$ is no longer a unitary operator. In fact, neither $\mathfrak{u}_\alpha$ nor its inverse is bounded. This implies that its action on a Hermitian Hamiltonian H, namely $H \to H' = \mathfrak{u}_\alpha H \mathfrak{u}_\alpha^{-1}$, that (neglecting the unboundedness of $\mathfrak{u}_\alpha$ and $\mathfrak{u}_\alpha^{-1}$) maps H into a quasi-Hermitian Hamiltonian H', can have dramatic effects on the nature of its continuous spectrum. This observation has applications in the treatment of resonances (where one replaces x with the radial spherical coordinate in $\mathbb{R}^3$). The main idea is to perform an appropriate complex scaling transformation so that the non-square-integrable wave functions representing resonant states of H are mapped to square-integrable eigenfunctions of H'. For details, see [214, 133, 12] and references therein.

9.1.3. *Vortex pinning in superconductors*

Consider the Hamiltonian: $H_g = \frac{(p+ig)^2}{2m} + v(x)$, where g is a real constant and v is a real-valued potential. This Hamiltonian can be mapped to the Hermitian

Hamiltonian H_0 by the similarity transformation:

$$H_g \to e^{-\frac{gx}{\hbar}} H_g e^{\frac{gx}{\hbar}} = H_0. \tag{376}$$

This in turn implies that H_g is η_+-pseudo-Hermitian for the metric operator $\eta_+ := e^{-\frac{2gx}{\hbar}}$. This is to be expected, because (376) is an example of the quasi-Hermitian Hamiltonians of the form (200) that admit x-dependent metric operators. In [101, 102] the Hamiltonian H_g (with random potential v) is used in modeling a delocalization phenomenon relevant for the vortex pinning in superconductors. A review of the ensuing developments is provided in [100].

9.2. *Relativistic QM, quantum cosmology, and QFT*

The issue of constructing an appropriate inner product for the defining Hilbert space of a quantum mechanical system, which we shall refer to as the *Hilbert-space problem*, is almost as old as quantum mechanics itself. Probably the first serious encounter with this problem is Dirac's attempts to obtain a probabilistic interpretation of the (first-quantized) Klein–Gordon fields in the late 1920's. The same problem arises in the study of other bosonic fields and particularly in the application of Dirac's method of constrained quantization for systems with first class constraints [78]. This method defines the "physical space" $\mathcal{V}$ of the state-vectors as the common null space (kernel) of the constraints, but it does not specify the inner product necessary to make $\mathcal{V}$ into a Hilbert space. Often the inner product induced from the auxiliary Hilbert space of the unconstrained system is not physically admissible, and one must find an alternative method of constructing an appropriate inner.

In trying to deal with the Hilbert-space problem for Klein–Gordon fields, Dirac was led to the discovery of the wave equation for massive spin-half particles and the antimatter that earned him the 1933 Nobel prize in physics. Another major historical development that has its root in attempts to address the Hilbert-space problem is the discovery of the method of second quantization and eventually relativistic quantum field theories. These developments did not bring a definitive resolution for the original problem, but diminished the interest in its solution considerably.

In the 1960's the discovery of the Hamiltonian formulation of the General Theory of Relativity [14] provided the necessary means to apply Dirac's method of constrained quantization to gravity. This led to the formulation of canonical quantum gravity and quantum cosmology [74, 232] and brought the Hilbert-space problem to forefront of research in fundamental theoretical physics for the second time. In this context, it emerges as the problem of finding an appropriate inner product on the space of solutions of the Wheeler–DeWitt equation. Without such an inner product, these solutions, that are often called the "wave functions of the universe", are void of a physical meaning. The lack of a satisfactory solution to this problem has been one of the major obstacles in transforming canonical quantum gravity and quantum cosmology into genuine physical theories [130, 107].

A widely used approach in dealing with the Hilbert-space problem for Klein–Gordon and Proca fields is to use the ideas of indefinite-metric quantum theories. These fields admit a conserved current density whose integral over space-like hypersurfaces yields a conserved scalar charge. This is however not positive-definite, and as a result, cannot be used to define a positive-definite inner product and make the space of all fields $\mathcal{V}$ into a genuine Hilbert space directly. This makes one pursue the following well-known scheme [230]. First, one uses the conserved charge to define an indefinite inner product on $\mathcal{V}$, and then restricts this indefinite inner product to the (so-called positive-energy) subspace of $\mathcal{V}$ where the inner product is positive-definite. The common practice is to label this subspace as "physical" and define the Hilbert space using the fields belonging to this "physical space".

This approach is not quite satisfactory, because even for physical fields the above-mentioned conserved current density can take negative values [23]. Therefore it cannot be identified with a probability density. There are also other problems related with the observables that mix "physical fields" with "unphysical fields" or "ghosts".

The application of pseudo-Hermitian QM in dealing with the Hilbert space problem in relativistic QM and quantum cosmology [150, 151, 161, 179, 114, 238], and the removal of ghosts in certain quantum field theories [35, 119] relies on the construction of an appropriate (positive-definite) inner product on the space of solutions of the relevant field equation.[aaaa]

The basic idea behind the application of pseudo-Hermitian QM in dealing with the Hilbert-space problem in relativistic QM and quantum cosmology is that the relevant field equations whose solutions constitute the state-vectors of the desired quantum theory are second-order differential equations in a "time" variable.[bbbb] These equations have the following general form.

$$\frac{d^2}{dt^2}\psi(t) + D\psi(t) = 0, \tag{377}$$

where t denotes a dimensionless time variable, $\psi : \mathbb{R} \to \mathcal{L}$ is a function taking values in some separable Hilbert space $\mathcal{L}$, and $D : \mathcal{L} \to \mathcal{L}$ is a positive-definite operator that may depend on t.

We can express (377) as a two-component Schrödinger equation [87],

$$i\frac{d}{dt}\Psi(t) = H\psi(t), \tag{378}$$

where $\Psi : \mathbb{R} \to \mathcal{L}^2$ and $H : \mathcal{L}^2 \to \mathcal{L}^2$ are defined by [140, 141]

$$\Psi(t) := \begin{pmatrix} \psi(t) + i\dot{\psi}(t) \\ \psi(t) - i\dot{\psi}(t) \end{pmatrix}, \quad H := \frac{1}{2}\begin{pmatrix} D+1 & D-1 \\ -D+1 & -D-1 \end{pmatrix}, \tag{379}$$

[aaaa] This should be distinguished with the treatment of the Pais–Uhlenbeck oscillator proposed in [49], because the latter involves changing the boundary conditions on the field equation which in turn changes the vector space of fields.

[bbbb] This is the physical time variable in an inertial frame in relativistic QM or a fictitious evolution parameter in quantum cosmology which may not be physically admissible [151].

$\mathcal{L}^2$ stands for the Hilbert space $\mathcal{L} \oplus \mathcal{L}$, and a dot denotes a t-derivative. The Hamiltonian (379) can be easily shown to be quasi-Hermitian [150].

In Subsec. 3.5, we examined in detail the quantum system defined by the Hamiltonian (379) for the case that $\mathcal{L}$ is $\mathbb{C}$ with the usual Euclidean inner product and D is multiplication by a positive number. In this case, the field equation (377) is the classical equation of motion for a (complex) harmonic oscillator with frequency $\sqrt{D}$. It turns out that most of the practical and conceptual difficulties of addressing the Hilbert-space problem for Klein–Gordon, Proca, and Wheeler–DeWitt fields can be reduced to and dealt with in the context of this simple oscillator.[cccc] In particular, the cases in which D is t-dependent (that arises in quantum cosmological models) require a more careful examination. We will not deal with these cases here. Instead, we refer the interested reader to [151] where a comprehensive discussion of these issues and their ramifications is provided.

Following the approach taken in Subsec. 3.5, one can construct a metric operator $\eta_+ : \mathcal{L}^2 \to \mathcal{L}^2$ and a new inner product $\langle \cdot \,|\, \cdot \rangle_{\eta_+}$ on $\mathcal{L}^2$ that renders H Hermitian. This defines a physical Hilbert space $\mathcal{K}$ of two-component fields $\Psi(t)$. Because $H : \mathcal{K} \to \mathcal{K}$ is Hermitian, it generates a unitary time-evolution in $\mathcal{K}$. In particular, for every initial time $t_0 \in \mathbb{R}$, every pair Ψ_1 and Ψ_2 of solutions of the Schrödinger equation (378), and all $t \in \mathbb{R}$,

$$\langle \Psi_1(t) \,|\, \Psi_2(t) \rangle_{\eta_+} = \langle \Psi_1(t_0) \,|\, \Psi_2(t_0) \rangle_{\eta_+}. \tag{380}$$

As a vector space $\mathcal{K}$ (and $\mathcal{L}^2$) are isomorphic to the space of solutions of the single-component field equation (377), i.e. $\mathcal{V} := \{\psi : \mathbb{R} \to \mathcal{L} \mid \ddot{\psi}(t) + D\psi(t) = 0 \text{ for all } t \in \mathbb{R}\}$. We can obtain an explicit realization of this isomorphism as follows. Let t_0 be an initial time and $\mathcal{U}_{t_0} : \mathcal{V} \to \mathcal{K}$ be defined by

$$\mathcal{U}_{t_0}(\psi) := \Psi(t_0). \tag{381}$$

According to (379) and (381), the effect of $\mathcal{U}_{t_0}$ on solutions ψ of the field equation (377) is to map them to the corresponding initial conditions $\psi(t_0)$ and $\dot{\psi}(t_0)$. Because the field equation is linear and second order, this mapping is a linear bijection. Therefore, $\mathcal{U}_{t_0}$ is a vector space isomorphism. This is an important observation, because it allows us to use $\mathcal{U}_{t_0}$ to induce a positive-definite inner product $(\cdot, \cdot)_{\eta_+}$ on $\mathcal{V}$ form the inner product $\langle \cdot \,|\, \cdot \rangle_{\eta_+}$ on $\mathcal{K}$. The induced inner product is defined by

$$(\psi_1, \psi_2)_{\eta_+} := \langle \mathcal{U}_{t_0}(\psi_1) \,|\, \mathcal{U}_{t_0}(\psi_2) \rangle_{\eta_+}, \quad \text{for all } \psi_1, \psi_2 \in \mathcal{V}. \tag{382}$$

Note that in view of (381) and (380), the right-hand side of (382) is independent of the value of t_0. This makes $(\cdot, \cdot)_{\eta_+}$ into a well-defined inner product on $\mathcal{V}$ and gives it the structure of a Hilbert space.[dddd]

[cccc] For a discussion of this particular quantization of the classical harmonic oscillator, see [159].

[dddd] Strictly speaking, one must also perform a Cauchy completion of the inner product space obtained by endowing $\mathcal{V}$ with $(\cdot, \cdot)_{\eta_+}$.

In principle different choices for η_+ give rise to different inner products $(\cdot,\cdot)_{\eta_+}$, but the resulting Hilbert spaces $\mathcal{H}_{\eta_+} := (\mathcal{V},(\cdot,\cdot)_{\eta_+})$ are unitary-equivalent. The arbitrariness in the choice of η_+ can be restricted by imposing additional physical conditions. For example in the case of Klein–Gordon and Proca fields, the requirement that $(\cdot,\cdot)_{\eta_+}$ be Lorentz-invariant reduces the enormous freedom in the choice of η_+ to a finite number of free numerical parameters [150, 238].

The most general Lorentz-invariant and positive-definite inner product on the space of (real or complex) Klein–Gordon fields has the following form [179]

$$(\psi_1,\psi_2)_{\eta_+} := -\frac{i\hbar\kappa}{2mc}\int_\Sigma d\sigma^\mu\,\Big[\psi_1(x)^*\overset{\leftrightarrow}{\partial_\mu}\mathcal{C}\psi_2(x)+a\psi_1(x)^*\overset{\leftrightarrow}{\partial_\mu}\psi_2(x)\Big], \tag{383}$$

where Σ is a space-like Cauchy hypersurface in the Minkowski spacetime, $x := (x^0,x^1,x^2,x^3)$ are the spacetime coordinates in an inertial frame, ψ_1 and ψ_2 are a pair of solutions of the Klein–Gordon equation: $\hbar^2[-\partial_0^2+\nabla^2]\psi(x)=m^2c^2\psi(x)$, such that for all $x^0\in\mathbb{R}$, $\psi(x^0,\vec{x})$ and $\partial_0\psi(x^0,\vec{x})$ define square-integrable functions of $\vec{x}:=(x^1,x^2,x^3)$, $\partial_\mu := \frac{\partial}{\partial x^\mu}$, $\nabla^2 := \partial_1^2+\partial_2^2+\partial_3^2$, for any pair of differentiable functions f and g, $f\overset{\leftrightarrow}{\partial_\mu}g := f\partial_\mu g - g\partial_\mu f$, $\kappa\in\mathbb{R}^+$ and $a\in(-1,1)$ are arbitrary dimensionless free parameters demonstrating the arbitrariness in the choice of η_+, and $\mathcal{C}$ is the grading operator defined by

$$(\mathcal{C}\psi)(x) := i\left(-\nabla^2+\frac{m^2c^2}{\hbar^2}\right)^{-\frac{1}{2}}\psi(x) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} dk^3dy^3\,\frac{e^{i\vec{k}\cdot(\vec{x}-\vec{y})}\psi(x^0,\vec{y})}{\sqrt{\vec{k}^2+\frac{m^2c^2}{\hbar^2}}}. \tag{384}$$

Note that $-\nabla^2+\frac{\hbar^2}{m^2c^2}$ is a positive operator acting in $\mathcal{L}=L^2(\mathbb{R}^3)$ and that $\mathcal{C}$ is Lorentz-invariant [179].

According to (382), as a linear operator mapping $\mathcal{H}_{\eta_+}$ to $\mathcal{K}$, $\mathcal{U}_{t_0}$ is a unitary operator. Similarly, $\rho := \sqrt{\eta_+}$ is a unitary operator mapping $\mathcal{K}$ to $\mathcal{L}^2$. Therefore $\rho\mathcal{U}_{\eta_+}:\mathcal{H}_{\eta_+}\to\mathcal{L}^2$ is also unitary. Usually $\mathcal{L}$ is an L^2-space with well-known self-adjoint operators. This allows for a simple characterization of the self-adjoint operators o acting in $\mathcal{L}^2$. We can use these operators and the unitary operator $\rho\mathcal{U}_{\eta_+}$ to construct the self-adjoint operators $O:\mathcal{H}_{\eta_+}\to\mathcal{H}_{\eta_+}$ that serve as the observables of the desired quantum theory. This is done using

$$O = (\rho\mathcal{U}_{\eta_+})^{-1}o\rho\mathcal{U}_{\eta_+}. \tag{385}$$

The application of this construction for Klein–Gordon [161, 179] and Proca [238] fields yields explicit expressions for the corresponding relativistic position operators and localized states, a problem that has been a subject of ongoing research since the 1940's [193, 188]. A natural consequence of these developments is the construction of a set of genuine relativistic coherent states for Klein–Gordon fields interacting with a constant magnetic field [180].

9.3. *Electromagnetic wave propagation*

An interesting application of pseudo-Hermitian QM is its role in dealing with a more than a century-old problem of the propagation of electromagnetic waves in linear dielectric media [176]. Unlike the applications we discussed in the preceding section, here it is the spectral properties of quasi-Hermitian operators and their similarity to Hermitian operators that plays a key role.

Consider the propagation of the electromagnetic waves inside a source-free dispersionless (linear) dielectric medium with dielectric and permeability tensors $\overleftrightarrow{\varepsilon} = \overleftrightarrow{\varepsilon}(\vec{x})$ and $\overleftrightarrow{\mu} = \overleftrightarrow{\mu}(\vec{x})$ that may depend on space $\vec{x} \in \mathbb{R}^3$ but not on time $t \in \mathbb{R}$. Maxwell's equations in such a medium read [111]

$$\vec{\nabla} \cdot \vec{D} = 0, \quad \vec{\nabla} \cdot \vec{B} = 0, \tag{386}$$

$$\dot{\vec{B}} + \vec{\nabla} \times \vec{E} = 0, \quad \dot{\vec{D}} - \vec{\nabla} \times \vec{H} = 0, \tag{387}$$

where $\vec{E}$ and $\vec{B}$ are the electric and magnetic fields, a dot means a time-derivative, and

$$\vec{D} := \overleftrightarrow{\varepsilon}\,\vec{E}, \quad \vec{H} := \overleftrightarrow{\mu}^{-1}\vec{B}. \tag{388}$$

Equations (386) and (387) are respectively called the constraint and dynamical equations. The former may be viewed as conditions on the initial values of the electromagnetic field, because once they are satisfied for some initial time, the dynamical equations ensure their validity for all time.

Similarly to Klein–Gordon equation, we can express the dynamical Maxwell equations (387) as first-order ordinary differential equations for state-vectors belonging to a separable Hilbert space. To achieve this, we introduce the complex vector space $\mathcal{V}$ of vector fields $\vec{F} : \mathbb{R}^3 \to \mathbb{C}^3$ and endow it with the inner product $\langle \vec{F}_1 \,|\, \vec{F}_2 \rangle := \int_{\mathbb{R}^3} d^3x \vec{F}_1(\vec{x})^* \cdot \vec{F}_2(\vec{x})$, for all $\vec{F}_1, \vec{F}_2 \in \mathcal{V}$, to define the Hilbert space of square-integrable vector fields: $\mathcal{H} := \{\vec{F} : \mathbb{R}^3 \to \mathbb{C}^3 \,|\, \langle \vec{F} \,|\, \vec{F} \rangle < \infty\}$. The operation of computing the curl of the (differentiable) elements of this Hilbert space turns out to define a linear Hermitian operator $\mathfrak{D} : \mathcal{H} \to \mathcal{H}$ according to $(\mathfrak{D}\vec{F})(\vec{x}) := \vec{\nabla} \times \vec{F}(\vec{x})$. We can use $\mathfrak{D}$ to write (387) in the form: $\dot{\vec{B}}(t) + \mathfrak{D}\vec{E}(t) = 0$ and $\dot{\vec{D}}(t) - \mathfrak{D}\vec{H}(t) = 0$. Evaluating the time-derivative of both sides of the second of these equations and using the first of these equations and (388), we find

$$\ddot{\vec{E}}(t) + \Omega^2 \vec{E}(t) = 0, \tag{389}$$

where $\Omega^2 : \mathcal{H} \to \mathcal{H}$ is defined by $\Omega^2 := \overleftrightarrow{\varepsilon}^{-1}\mathfrak{D}\,\overleftrightarrow{\mu}^{-1}\mathfrak{D}$.

In view of the fact that $\overleftrightarrow{\varepsilon}$, $\overleftrightarrow{\mu}$, and consequently Ω^2 are time-independent, we can integrate (389) to obtain the following formal solution

$$\vec{E}(t) = \cos(\Omega t)\vec{E}_0 + \Omega^{-1}\sin(\Omega t)\dot{\vec{E}}_0, \tag{390}$$

where $\vec{E}_0 := \vec{E}(0)$, $\dot{\vec{E}}_0 := \dot{\vec{E}}(0) = \overleftrightarrow{\varepsilon}^{-1}\mathfrak{D}\,\overleftrightarrow{\mu}^{-1}\vec{B}(0)$, and

$$\cos(\Omega t) := \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!}\,(t^2\Omega^2)^n, \quad \Omega^{-1}\sin(\Omega t) := t\sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!}\,(t^2\Omega^2)^n. \tag{391}$$

Given initial values of the electric and magnetic fields $\vec{E}(0)$ and $\vec{B}(0)$, we can use (390) and (391) to obtain a series expansion for the evolving electric field. One can select specific initial fields so that this expansion involves a finite number of nonzero terms, but these are of little physical significance. In general, the resulting solution is an infinite derivative series expansion that is extremely difficult to sum or provide reliable estimates for. A crucial observation which nonetheless makes this expansion useful is that, for the cases that $\overleftrightarrow{\varepsilon}$ and $\overleftrightarrow{\mu}$ are Hermitian, the operator $\Omega^2 : \mathcal{H} \to \mathcal{H}$ is $\overleftrightarrow{\varepsilon}$-pseudo-Hermitian: $\Omega^{2\dagger} = \overleftrightarrow{\varepsilon}\,\Omega^2\,\overleftrightarrow{\varepsilon}^{-1}$. In particular, for lossless material where $\overleftrightarrow{\varepsilon}$ is a positive $\vec{x}$-dependent matrix, Ω^2 is a quasi-Hermitian operator[eeee] that can be mapped to a Hermitian operator h by a similarity transformation, namely $h = \rho\Omega^2\rho^{-1}$ where $\rho := \overleftrightarrow{\varepsilon}^{\frac{1}{2}}$.

In terms of h the solution (390) takes the form: $\vec{E}(t) = \rho^{-1}[\cos(h^{\frac{1}{2}}t)\rho\vec{E}_0 + h^{-\frac{1}{2}}\sin(h^{\frac{1}{2}}t)\rho\dot{\vec{E}}_0]$. Therefore,

$$\begin{aligned}\vec{E}(\vec{x},t) &= \langle\vec{x}\,|\,\vec{E}(t)\rangle\\ &= \rho^{-1}(\vec{x})\int_{\mathbb{R}^3} d^3y\,\Big[\overleftrightarrow{C}(\vec{x},\vec{y};t)\rho(\vec{y})\vec{E}_0(\vec{y}) + \overleftrightarrow{S}(\vec{x},\vec{y};t)\rho(\vec{y})\dot{\vec{E}}_0(\vec{y})\Big],\end{aligned}\tag{392}$$

where

$$\overleftrightarrow{C}(\vec{x},\vec{y};t) := \langle\vec{x}|\cos(h^{\frac{1}{2}}t)|\vec{y}\rangle,\quad \overleftrightarrow{S}(\vec{x},\vec{y};t) := \langle\vec{x}|h^{-\frac{1}{2}}\sin(h^{\frac{1}{2}}t)|\vec{y}\rangle.\tag{393}$$

The fact that h is a Hermitian operator acting in $\mathcal{H}$ makes it possible to compute the kernels $\overleftrightarrow{C}(\vec{x},\vec{y};t)$ and $\overleftrightarrow{S}(\vec{x},\vec{y};t)$ of the operators $\cos(h^{\frac{1}{2}}t)$ and $h^{-\frac{1}{2}}\sin(h^{\frac{1}{2}}t)$ using the spectral representation of h:

$$h = \sum_{n=1}^{N}\sum_{a} E_n|\psi_{n,a}\rangle\langle\psi_{n,a}|,\tag{394}$$

where the sum over the spectral label n should be identified with an integral or a sum together with an integral whenever the spectrum of h has a continuous part, E_n and $|\psi_{n,a}\rangle$ denote the eigenvalues and eigenvectors of h respectively, and a is a degeneracy label. In view of (394), for every analytic function F of h, such as $\cos(h^{\frac{1}{2}}t)$ and $h^{-\frac{1}{2}}\sin(h^{\frac{1}{2}}t)$, we have $\langle\vec{x}|F(h)|\vec{y}\rangle = \sum_{n=1}^{N}\sum_a F(E_n)\psi_{n,a}(\vec{x})\psi_{n,a}(\vec{y})^*$. In the scattering setups where $\overleftrightarrow{\varepsilon}$ and $\overleftrightarrow{\mu}$ tend to constant values as $|\vec{x}| \to \infty$, h has a continuous spectrum and one finds integral representations for the kernels (393) that reduce the solution (392) of Maxwell's equations into performing certain integrals (after solving the eigenvalue problem for h).

Reference 176 outlines the application of this method for the cases that the medium is isotropic, the initial fields as well as the dielectric and permeability constants change only along the z-direction, and the WKB approximation is applicable

[eeee] As an operator acting in $\mathcal{H}$, the dielectric tensor $\overleftrightarrow{\varepsilon}$ plays the role of a metric operator. This is one of the rare occasions where a metric operator has a concrete physical meaning.

in dealing with the eigenvalue problem for h. Under these conditions, one can compute the kernels (393) analytically. This allows for the derivation of the following closed form expression for the propagating electromagnetic field in terms of the initial fields $\vec{E}_0$, $\dot{\vec{E}}_0$, and the z-dependent dielectric and permeability constants $\varepsilon(z)$ and $\mu(z)$.

$$\vec{E}(z,t) = \frac{1}{2}\left[\frac{\mu(z)}{\varepsilon(z)}\right]^{\frac{1}{4}}\left\{\left[\frac{\varepsilon(w_-(z,t))}{\mu(w_-(z,t))}\right]^{\frac{1}{4}}\vec{E}_0(w_-(z,t)) + \left[\frac{\varepsilon(w_+(z,t))}{\mu(w_+(z,t))}\right]^{\frac{1}{4}}\vec{E}_0(w_+(z,t)) + \int_{w_-(z,t)}^{w_+(z,t)} dw\mu(w)^{\frac{1}{4}}\varepsilon(w)^{\frac{3}{4}}\dot{\vec{E}}_0(w)\right\},$$

where $w_\pm(z,t) := u^{-1}(u(z)\pm t)$, $u(z) := \int_0^z d\mathfrak{z}\sqrt{\varepsilon(\mathfrak{z})\mu(\mathfrak{z})}$, and u^{-1} stands for the inverse function for u [176].

The possibility of the inclusion of dispersion effects in the above approach of solving Maxwell's equations is considered in [174].

9.4. *Other applications and physical manifestations*

The following are some other areas where pseudo-Hermitian operators arise and/or the methods of pseudo-Hermitian QM are used in dealing with specific physics problems.

9.4.1. *Atomic physics and quantum optics*

Effective quasi-Hermitian scattering Hamiltonians arise in the study of the bound-state scattering from spherically symmetric short-range potentials. As shown by Matzkin in [136], the use of the machinery of pseudo-Hermitian QM in the study of these Hamiltonians leads to a more reliable quantitative description of the scattering problem. It also provides a better understanding of the approximation schemes used in this context in the past and allows for their improvement.

The relevance of pseudo-Hermitian operators to two-level atomic and optical systems has been noted in [27, 26, 204], and their application in describing squeezed states is elucidated in [73, 25]. The optical systems provide an important arena for manufacturing non-Hermitian and in particular pseudo- and quasi-Hermitian effective Hamiltonians. Recent experimental studies of $\mathcal{PT}$-symmetric periodic potentials that make use of $\mathcal{PT}$-symmetric optical lattices is based on this observation [134]. See also [52].

9.4.2. *Open quantum systems*

The emergence of non-Hermitian effective Hamiltonians in the description of the resonant states, that is based on Feshbach's projection scheme [86] is a very well-known phenomenon [181]. The application of a similar idea, that replaces the projection scheme with an averaging scheme, for open quantum systems also leads to

a class of non-Hermitian effective Hamiltonians (usually called Liouvillian or Liouville's super operator) [57]. These Hamiltonians that determine the dynamics of the reduced density operators can, under certain conditions, be pseudo-Hermitian or even quasi-Hermitian. In [220, 112, 221], Stenholm and Jakob explore the application of the properties of pseudo- and quasi-Hermitian operators in the study of open quantum systems. The key development reported in these articles is the construction of a metric operator, that uses the spectral method we discussed in Subsec. 4.1, and the identification of the corresponding norm with a viable candidate for a generalized notion of entropy.

9.4.3. *Magnetohydrodynamics*

Pseudo-Hermitian effective Hamiltonians arise in the study of the dynamo effect in magnetohydrodynamics [96, 97]. These Hamiltonians are typically non-quasi-Hermitian and involve exceptional points. Therefore, they can only be treated in the framework of indefinite-metric theories and using the properties of Krein spaces [18].

9.4.4. *Quantum chaos and statistical mechanics*

In [71], Date *et al.* study the spectrum of the Hamiltonian operator: $H = \frac{1}{2}(p_x + \frac{\alpha y}{r^2})^2 + \frac{1}{2}(p_y - \frac{\alpha y}{r^2})^2$, where α is a real coupling constant and $r := \sqrt{x^2+y^2}$. This Hamiltonian that is Hermitian and $\mathcal{PT}$-symmetric describes a rectangular Aharonov–Bohm billiard. Here, note that the spectrum is obtained by imposing Dirichlet boundary condition on the boundary of the rectangular configuration space, that is defined by $|x| \leq a$ and $|y| \leq b$ for some $a, b \in \mathbb{R}^+$, and also at the location of the flux line, namely $x = y = 0$. The main result of [71] is that the nearest neighbor spacing distribution for this system has a transition that interpolates between the Poisson (level clustering) and Wigner (level repulsion) distributions. In an attempt to obtain a random matrix model with this kind of behavior, Ahmed and Jain constructed and studied certain pseudo-Hermitian random matrix models in [4, 5].

9.4.5. *Biophysics*

In [84], Eslami–Moossallam and Ejtehadi have introduced the following effective Hamiltonian for the description of the dynamics of an anisotropic DNA molecule.

$$H := \frac{J_1^2}{2A_1} + \frac{J_2^2}{2A_2} + \frac{J_3^2}{2C} + i\omega_0 J_3 - \tilde{f}\cos\beta, \tag{395}$$

where A_1, A_2, C, ω_0, and $\tilde{f}$ are real coupling constants, α, β, γ are Euler angles, and J_1, J_2, J_3, that satisfy the commutation relations for angular momentum operators, are defined by $J_1 := -i(-\frac{\cos\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} + \sin\gamma\frac{\partial}{\partial\beta} + \cot\beta\cos\gamma\frac{\partial}{\partial\gamma})$, $J_2 := -i(\frac{\sin\gamma}{\sin\beta}\frac{\partial}{\partial\alpha} + \cos\gamma\frac{\partial}{\partial\beta} - \cot\beta\sin\gamma\frac{\partial}{\partial\gamma})$, and $J_3 := -i\frac{\partial}{\partial\gamma}$. Clearly, the Hamiltonian (395) is non-Hermitian, but it is at the same time real, i.e. it commutes with the time-reversal

operator $\mathcal{T}$. In light of the fact that $\mathcal{T}$ is an antilinear operator, this implies that H is a pseudo-Hermitian operator [145]. It would be interesting to see if this observation has any physically interesting implications, besides the restriction it puts on the spectrum of H.

10. Summary and Conclusions

In this article, we addressed various basic problems related to what we call pseudo-Hermitian quantum mechanics. Our starting point was the observation that a given quantum system admits an infinity of unitary-equivalent representations in terms of Hilbert space-Hamiltonian operator pairs. This freedom in the choice of representation can be as useful as gauge symmetries of elementary particle physics.

We have surveyed a variety of mathematical concepts and tools to establish the foundations of pseudo-Hermitian quantum on a solid ground and to clarify the shortcomings of the treatment of the subject that is based on the so-called charge operator $\mathcal{C}$. We showed that it is the metric operator η_+ that plays the central role in pseudo-Hermitian quantum mechanics. Although one can in general introduce a $\mathcal{C}$ operator and express η_+ in terms of $\mathcal{C}$, the very construction of observables of the theory and the calculations of the physical quantities requires the knowledge of η_+. This motivates addressing the problem of the computation of a metric operator for a given quasi-Hermitian operator. We have described different approaches to this problem.

We have discussed a number of basic issues related to the classical-to-quantum correspondence to elucidate the status of the classical limit of pseudo-Hermitian quantum mechanics. We have also elaborated on the surprising limitation on the choice of time-dependent quasi-Hermitian Hamiltonians, the role of the metric operator in path-integral formulation of the theory, a treatment of the systems defined on complex contours, and a careful study of the geometry of the space of states that seems to be indispensable for clarifying the potential application of quasi-Hermitian Hamiltonians in generating fast quantum evolutions.

Finally, we provided a discussion of various known applications and manifestations of pseudo-Hermitian quantum mechanics.

Among the subjects that we did not cover and suffice to provide a few references for are pseudo-supersymmetry and its extensions [146, 215, 203, 216], weak pseudo-Hermiticity [219, 20, 242, 164], and the generalizations of $\mathcal{PT}$-symmetry [31, 170]. This omission was particularly because of our intention not to treat the results or methods with no direct or concrete implications for the development of pseudo-Hermitian quantum mechanics. We particularly avoided discussing purely formal results and speculative ideas.

Appendix. Reality of Expectation Values Implies Hermiticity of the Observables

Theorem 3. *Let $\mathcal{H}$ be a Hilbert space with inner product $\langle\cdot\,|\,\cdot\rangle$ and $A : \mathcal{H} \to \mathcal{H}$ be a (densely-defined, closed) linear operator satisfying $\mathcal{D}(A) = \mathcal{D}(A^\dagger)$, i.e. A and*

its adjoint $A^\dagger$ have the same domain $\mathcal{D}(A)$. Then A is a Hermitian operator if and only if $\langle\psi\,|\,A\psi\rangle$ is real for all $\psi\in\mathcal{D}(A)$.

Proof. If A is Hermitian, we have $\langle\phi\,|\,A\psi\rangle = \langle A\phi\,|\,\psi\rangle$ for all $\psi,\phi\in\mathcal{D}(A)$. Then according to property (ii) of Subsec. 2.1, $\langle\psi\,|\,A\psi\rangle\in\mathbb{R}$ for all $\psi\in\mathcal{D}(A)$. Next, suppose that for all $\psi\in\mathcal{D}(A)$, $\langle\psi\,|\,A\psi\rangle\in\mathbb{R}$. We will show that this condition implies the Hermiticity of A in two steps.

Step 1: Let $A_+ := \frac{1}{2}(A+A^\dagger)$ and $A_- := \frac{1}{2i}(A-A^\dagger)$. Then $A = A_+ + iA_-$, $\mathcal{D}(A_\pm)=\mathcal{D}(A)$, and $A_\pm$ are Hermitian operators. In view of the first part of the theorem, this implies that

$$\langle\psi\,|\,A_\pm\psi\rangle\in\mathbb{R},\quad \text{for all } \psi\in\mathcal{D}(A). \tag{396}$$

Furthermore, according to $A=A_++iA_-$ and the hypothesis of the second part of the theorem, $\langle\psi\,|\,A_+\psi\rangle + i\langle\psi\,|\,A_-\psi\rangle = \langle\psi\,|\,A\psi\rangle\in\mathbb{R}$. This relation and (396) show that

$$\langle\psi\,|\,A_-\psi\rangle = 0\quad \text{for all } \psi\in\mathcal{D}(A). \tag{397}$$

Step 2: Let ϕ,ψ be arbitrary elements of $\mathcal{D}(A)$, $\xi_\pm := \phi\pm\psi$, and $\zeta_\pm=\phi\pm i\psi$. Then a direct calculation, using the property (iii) of Subsec. 2.1, shows that $\langle\phi\,|\,A_-\psi\rangle = \frac{1}{4}(\langle\xi_+\,|\,A_-\xi_+\rangle - \langle\xi_-\,|\,A_-\xi_-\rangle - i\langle\zeta_+\,|\,A_-\zeta_+\rangle + i\langle\zeta_-\,|\,A_-\zeta_-\rangle)=0$, where the last equality follows from (397) and the fact that $\xi_\pm,\zeta_\pm\in\mathcal{D}(A)$. This establishes $\phi\,|\,A_-\psi\rangle=0$ for all $\phi,\psi\in\mathcal{D}(A)$. In particular, setting $\phi=A_-\psi$, we find $\langle A_-\psi\,|\,A_-\psi\rangle=0$ which in view of the property (i) of Subsec. 2.1 implies $A_-\psi=0$ for all $\psi\in\mathcal{D}(A)$. Hence $A_-=0$, and according to $A=A_++iA_-$, we finally have $A=A_+$. But A_+ is Hermitian. □

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