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Time-dependent version of crypto-Hermitian quantum theory

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For many quantum models an apparent non-Hermiticity of observables just corresponds to their hidden Hermiticity in another, physical Hilbert space. For these models we show that the existence of observables which are manifestly time-dependent may require the use of a manifestly time-dependent representation of the physical Hilbert space of states.

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I. INTRODUCTION

In standard textbooks one finds numerous examples of an elementary quantum Hamiltonian $H = p^2 + V(x)$ which describes a particle (or quasiparticle) moving in a time-independent external field $V(x)$ in one dimension, $x \in \mathbb{R}$. The time evolution of its wave function $\Phi(x, t)$ is determined by the time-dependent Schrödinger equation

$$\mathrm{i}\,\partial_t \Phi(x, t) = H\Phi(x, t). \qquad (1)$$

Tacitly, it is understood that all of the operators of observables Λ_j with $j = 1, 2, \ldots$ (including also the Hamiltonian itself at $j = 0$, $H = \Lambda_0$) are self-adjoint, $\Lambda_j = \Lambda_j^\dagger$, $j = 0, 1, \ldots$. Even if the external field becomes manifestly time dependent, $V = V(x, t)$, the generalized model with $H = H(t) = H^\dagger(t)$ (and, optionally, with an appropriate experimental background for the time dependence of $\Lambda_1 = \Lambda_1(t) = \Lambda_1^\dagger(t)$, etc.) does not necessitate any modification of the time-evolution law (1).

Bender and Boettcher [1] conjectured (and, subsequently, Dorey, Duncan and Tateo proved [2]) that certain manifestly non-Hermitian Hamiltonians $H = p^2 + V(x) \neq H^\dagger$ may also generate a purely real, i.e., in principle, observable spectrum of bound-state energies. This reattracted attention to several older works where the similar ideas appeared in the context of field theory [3] or relativistic quantum mechanics [4] or nuclear physics [5]. Empirically, the reality of spectra of similar Hamiltonians has been attributed to their $\mathcal{PT}$ symmetry [6], $\mathcal{CPT}$ symmetry [7], quasi-Hermiticity [5,8,9], or crypto-Hermiticity [10]. The related innovation of methods led to a new round of perceivable progress in relativistic quantum mechanics [11], quantum cosmology [12], statistics [13] and scattering theory [14], and even in classical electrodynamics [15] and magnetohydrodynamics [16]. In this context, the title, "Making sense of non-Hermitian Hamiltonians" of the recent review paper [17] written by Carl Bender gives the name to one of the most remarkable recent projects in theoretical physics.

In Refs. [18,19] the idea has tentatively been extended to the time-dependent non-Hermitian Hamiltonians

$$H = H(t) \neq H^\dagger(t). \qquad (2)$$

Unexpectedly, a number of conceptual difficulties has been encountered. Serious problems have arisen, first of all, in connection with the probabilistic and unitary-evolution interpretation of the generalized models. For this reason, just a very special linear time dependence of $H(t)$ has been admitted in [18] and the so-called quasistationary generalization of this constraint has been accepted in [19]. The resulting theories of time dependence with constraints looked incomplete and deeply unsatisfactory.

In our present paper, we intend to reanalyze the problem. In essence, we shall reveal that all of the specific and constrained, quasistationary models are based on the same, purely intuitive and unfounded *assumption* that even for all of the models with property (2) the time-dependent Schrödinger equation must remain valid in its naive, noncovariant form (1). We shall show here that after this assumption is relaxed, the theory becomes transparent again. We shall point out that the time-dependent non-Hermitian Hamiltonians (2) may simply *cease* to play the role of the generators of time evolution in general.

In the preliminary part of our text, Sec. II will summarize a few basic mathematical features of crypto-Hermitian operators, i.e., of the Hamiltonians H and/or other operators of observables $\Lambda_1, \Lambda_2, \ldots$ with real spectra which are manifestly non-Hermitian in an *auxiliary* Hilbert space $\mathcal{H}^{(A)}$. We shall emphasize that the reality of the respective spectra is to be understood as a direct consequence of the standard Hermiticity requirements imposed in *another*, *physical* Hilbert space of states $\mathcal{H}^{(P)}$.

Our main results will be presented in Sec. III where we shall show how the crypto-Hermitian time-evolution law has to be modified in order to preserve the consistency of the theory in $\mathcal{H}^{(P)}$. These observations will be complemented by their brief discussion and summary in Sec. IV.

II. CRYPTO-HERMITIAN HAMILTONIANS

For models with property (2) a striking contrast emerges between their innovative mathematics and conservative

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physics. In [17], Carl Bender identifies a deeper source of interest in Hamiltonians $H \neq H^\dagger$ in the theoretical weakness of the current practice where among all of the eligible representations of the quantum Hilbert space of states $\mathcal{H}$ people most often choose the most friendly one, viz., the space $\mathcal{H}^{(A)} = \mathbb{L}^2(\mathbb{R})$ composed of the square-integrable complex functions of the single real variable $x \in \mathbb{R}$. In this representation the inner product between two equal-time wave functions $\psi_a(x, t)$ and $\psi_b(x, t)$ is trivial,

$$(\psi_a, \psi_b)^{(A)} = \int_{\mathbb{R}} \psi_a^*(x, t)\psi_b(x, t)dx \tag{3}$$

but its use seems to exclude, as unphysical, any complex potential $V(x)$. Still, for many concrete non-Hermitian Hamiltonians $H = p^2 + V(x) \neq H^\dagger$ exhibiting the standard kinetic energy + potential energy structure *and* leading to the real spectrum of bound states one *can* admit a complex $V(x)$. Naturally, the representation of the physical Hilbert space of states must be changed. Such a change of space from auxiliary to physical,

$$\mathcal{H}^{(A)} \to \mathcal{H}^{(P)}$$

is usually nontrivial. At the same time, the innovated Hilbert space $\mathcal{H}^{(P)}$ need not necessarily be substantially different from its unphysical partner $\mathcal{H}^{(A)}$. In the majority of applications the latter two spaces even coincide as vector spaces while the second one merely requires a modified definition of the inner product using the following double integral,

$$(\psi_a, \psi_b)^{(P)} = \int_{\mathbb{R}^2} \psi_a^*(x, t)\Theta(x, x', t)\psi_b(x', t)dxdx'. \tag{4}$$

The time t is considered fixed and the integral kernel $\Theta(x, x', t)$ itself is usually called "metric."

One of the most visible features shared by virtually all of the quantum models defined within any anomalous, non-Dirac [17] Hilbert space $\mathcal{H}^{(P)}$ with metric $\Theta \neq I$ is that the underlying Hamiltonian H *looks* non-Hermitian,

$$H \neq H^\dagger \quad \text{in } \mathcal{H}^{(A)} = \mathcal{H}^{(\text{unphysical})}. \tag{5}$$

The same Hamiltonian H remains safely self-adjoint (and, hence, standard and physical) in $\mathcal{H}^{(P)}$. Unfortunately, the definition of the Hermitian conjugation $H \to H^\ddagger$ derived from Eq. (4) is more complicated and depends on the metric,

$$H = H^\ddagger = \Theta^{-1}H^\dagger\Theta \quad \text{in } \mathcal{H}^{(P)} = \mathcal{H}^{(\text{physical})}. \tag{6}$$

A certain complementarity is encountered between physics which is correct in $\mathcal{H}^{(P)}$ and mathematics which usually proves much easier in $\mathcal{H}^{(A)}$ [5]. Thus, one is only allowed to speak about a loss of Hermiticity of the Hamiltonian in the irrelevant, auxiliary space $\mathcal{H}^{(A)}$ with, typically,

$$\Theta^{(\text{Dirac})}(x, x', t) = \delta(x - x')$$

in Eq. (4). All the postulates of quantum theory remain unchanged in the correct space $\mathcal{H}^{(P)}$.

III. TIME-DEPENDENT SCHRÖDINGER EQUATION

A. A Hermitization of the Hamiltonian in $\mathcal{H}^{(A)}$

Inside the physical Hilbert space of states $\mathcal{H}^{(A)}$ let us contemplate an *arbitrary* auxiliary invertible operator $\Omega = \Omega(t)$ and replace the non-Hermitian "uppercase" Hamiltonian H by its "lowercase" isospectral partner

$$h = \Omega H \Omega^{-1}. \tag{7}$$

Whenever needed, we must apply the same mapping also to all of the other operators of observables $\Lambda_j = \Lambda_j(t)$ in $\mathcal{H}^{(A)}$. It is well-known that a simple change of the basis is obtained when Ω is chosen unitary. In an opposite direction we now intend to choose such a nonunitary map Ω that the resulting new representation $h = h(t)$ of our Hamiltonian becomes Hermitian,

$$\begin{aligned} h = h(t) &= \Omega(t)H(t)\Omega^{-1}(t) = h^\dagger(t) \\ &= [\Omega^{-1}(t)]^\dagger H(t)\Omega^\dagger(t). \end{aligned} \tag{8}$$

This must be complemented by an observation that *both* the representations $H(t)$ and $h(t)$ of the energy operator *need not* play the role of the generator of the time evolution *simultaneously*. There exists no mathematical or physical principle which would force us to insist on the validity of Eq. (1) when $H \neq H^\dagger$. We are allowed to restrict our attention to the lowercase generators $h(t)$ of the safely unitary time evolution and to the related lowercase wave functions defined by the integral containing the kernel of Ω,

$$\varphi(x, t) = \int_{\mathbb{R}} \Omega(x, x', t)\Phi(x', t)dxdx'. \tag{9}$$

When we use the current Dirac bracket notation the latter relation can be abbreviated as $|\varphi(t)\rangle = \Omega(t)|\Phi(t)\rangle$. Thus, we may characterize the state of our physical quantum system, at any time t, by the very standard elementary projector

$$\pi(t) = |\varphi(t)\rangle \frac{1}{\langle\varphi(t)|\varphi(t)\rangle}\langle\varphi(t)|. \tag{10}$$

The evolution of this expression in time is controlled by the usual time-dependent Schrödinger equation

$$\mathrm{i}\,\partial_t|\varphi(t)\rangle = h(t)|\varphi(t)\rangle. \tag{11}$$

For any state $\varphi(x, t) = \langle x|\varphi(t)\rangle$ prepared at $t = 0$ and measured at $t > 0$ the operator $h(t)$ plays the role of its self-adjoint generator of evolution in time.

Our knowledge of this generator enables us to introduce the evolution operator $u(t)$ defined by the following operator alternative to Eq. (11),

$$\mathrm{i}\,\partial_t u(t) = h(t)u(t). \tag{12}$$

The formal solution of Eq. (11) then reads

$$|\varphi(t)\rangle = u(t)|\varphi(0)\rangle \tag{13}$$

and, obviously, it satisfies the identity

$$\langle\varphi(t)|\varphi(t)\rangle = \langle\varphi(0)|\varphi(0)\rangle.$$

This identity is a guarantee that the evolution of the system is unitary.

B. The doublet of pullbacks of wave function

For a sufficiently general kernel $\Omega(t)$ in Eq. (9) the Hermitian representation $h(t)$ of the Hamiltonian is a complicated integro-differential operator. A return to $H(t) = p^2 + V(x, t) \neq H^\dagger(t)$ makes good sense, therefore. One of the most immediate consequences of the resulting parallel work in $\mathcal{H}^{(A)}$ and $\mathcal{H}^{(P)}$ is that we must carefully distinguish between the respective bra vectors. In the usual Dirac notation, for example, Mostafazadeh [9] recommends the two-letter notation where $[|\Phi(t)\rangle]^\ddagger \equiv \langle\Psi(t)|$ and where, in the light of Eq. (4),

$$\langle x|\Phi_b(t)\rangle \equiv \psi_b(x, t) \in \mathcal{H}^{(P)},$$

$$\langle\Psi_a(t)|x\rangle \equiv \int_{\mathbb{R}} \psi_a^*(y, t)\Theta(y, x, t)dy \in [\mathcal{H}^{(P)}]'.$$

This convention well reflects the fact that in $\mathcal{H}^{(P)}$ there emerge two different pullbacks of the single wave function (13), viz.,

$$|\Phi(t)\rangle = \Omega^{-1}(t)|\varphi(t)\rangle, \qquad \langle\Psi(t)| = \langle\varphi(t)|\Omega(t). \tag{14}$$

One should emphasize that in spite of being marked by the two different Greek letters, these symbols still represent the *same* state of our physical system in question. Formally, this description is provided by the uppercase pullback of the projector $\pi(t)$ given by Eq. (10),

$$\Pi(t) = |\Phi(t)\rangle \frac{1}{\langle\Psi(t)|\Phi(t)\rangle}\langle\Psi(t)|. \tag{15}$$

The new projector $\Pi(t) = \Pi^\ddagger(t)$ remains non-Hermitian in the unphysical space $\mathcal{H}^{(A)}$ and its construction requires the knowledge of the *pair* of time-dependent functions or vectors (14). As long as $\Omega^{-1}(t) \neq \Omega^\dagger(t)$, these two complex functions of x are different in general.

Our knowledge of the time dependence of the latter two functions is a remarkable consequence of the construction. The Schrödinger Eq. (11) and some elementary algebra lead to the right-action evolution rule

$$|\Phi(t)\rangle = U_R(t)|\Phi(0)\rangle, \qquad U_R(t) = \Omega^{-1}(t)u(t)\Omega(0) \tag{16}$$

accompanied by its left-action parallel

$$|\Psi(t)\rangle = U_L^\dagger(t)|\Psi(0)\rangle, \qquad U_L^\dagger(t) = \Omega^\dagger(t)u(t)[\Omega^{-1}(0)]^\dagger. \tag{17}$$

The respective non-Hermitian analogues of the Hermitian evolution-operator rule (12) are obtained by the elementary differentiation and insertions yielding

$$\mathrm{i}\,\partial_t U_R(t) = -\Omega^{-1}(t)[\mathrm{i}\partial_t\Omega(t)]U_R(t) + H(t)U_R(t) \tag{18}$$

and

$$\mathrm{i}\,\partial_t U_L^\dagger(t) = H^\dagger(t)U_L^\dagger(t) + [\mathrm{i}\partial_t\Omega^\dagger(t)][\Omega^{-1}(t)]^\dagger U_L^\dagger(t). \tag{19}$$

We achieved our goal. In the language of mathematics the latter doublet of operator equations offers a differential-equation simplification of the equivalent integro-differential lowercase Schrödinger Eq. (12). Thus, the role of the complicated lowercase representation $u(t)$ of the evolution operator is transferred to its two uppercase maps which offer a consistent description of quantum dynamics in $\mathcal{H}^{(P)}$.

IV. DISCUSSION

Several misunderstandings concerning the pullbacks of wave functions have recently been encountered in a series of comments and replies on [20]. There, a few unexpected properties of the generalized quantum time-evolution equations have been discussed, with the final clarification of the puzzle presented in the preliminary preprint version [21] of our present paper. It makes sense, therefore, to perform an independent check of what happens with the norm $\langle\Psi(t)|\Phi(t)\rangle$ of a given state which evolves with time in $\mathcal{H}^{(P)}$. The elementary differentiation confirms that

$$\begin{aligned}\mathrm{i}\partial_t\langle\Psi(t)|\Phi(t)\rangle &= \mathrm{i}\partial_t\langle\Psi(0)|U_L(t)U_R(t)|\Phi(0)\rangle = \langle\Psi(0)|[\mathrm{i}\partial_t U_L(t)]U_R(t)|\Phi(0)\rangle + \langle\Psi(0)|U_L(t)[\mathrm{i}\partial_t U_R(t)]|\Phi(0)\rangle \\ &= \langle\Psi(0)|U_L(t)[-H(t) + \Omega^{-1}(t)[\mathrm{i}\partial_t\Omega(t)]]U_R(t)|\Phi(0)\rangle + \langle\Psi(0)|U_L(t)[H(t) - \Omega^{-1}(t)[\mathrm{i}\partial_t\Omega(t)]]U_R(t)|\Phi(0)\rangle \\ &= 0.\end{aligned}$$

We see that irrespectively of the mapping Ω the norm does not vary so that the time evolution of the system is unitary also by this check. It reconfirms that the naive picture of the time evolution as generated by the non-Hermitian Hamiltonian $H(t)$ is incomplete.

In our present brief paper we were more constructive in showing that whenever $H \neq H^\dagger$, the time evolution must in general be prescribed by a *pair* of modified Schrödinger equations. With the purpose of making this argument fully explicit, let us abbreviate $\partial_t\Omega(t) \equiv \dot{\Omega}(t)$ and write down the following explicit specification of the time-evolution generator in $\mathcal{H}^{(P)}$,

$$H_{(\mathrm{gen})}(t) = H(t) - \mathrm{i}\Omega^{-1}(t)\dot{\Omega}(t). \qquad (20)$$

It is remarkable that this operator enters *both* the updates of the Schrödinger equation for wave functions in $\mathcal{H}^{(P)}$,

$$\mathrm{i}\,\partial_t|\Phi(t)\rangle = H_{(\mathrm{gen})}(t)|\Phi(t)\rangle, \qquad (21)$$

$$\mathrm{i}\,\partial_t|\Psi(t)\rangle = H^{\dagger}_{(\mathrm{gen})}(t)|\Psi(t)\rangle. \qquad (22)$$

Such a confirmation of the overall unitarity of the evolution comes at a very reasonable cost of the covariant redefinition $H \longrightarrow H_{(\mathrm{gen})}$ of its generator.

We can summarize that the adequate and fairly universal picture of quantum dynamics can be reinstalled in its uppercase crypto-Hermitian (i.e., typically, less nonlocal and technically simpler) representation provided only that one admits that the time evolution is *not necessarily* generated by the naive, noncovariant map $H(t)$ of a physical self-adjoint Hamiltonian $h(t)$. This confirms that the "traditional" Schrödinger Eq. (1) may cease to be valid in general. The existence of papers like [19,22] as well as of several unpublished comments on the web [20] indicates that this observation is nontrivial and that it can perceivably extend the range of applicability of crypto-Hermitian models in quantum theory.

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APPENDIX: QUASISTATIONARITY CONSTRAINT

One of the unexpected mathematical benefits of the form of operator (20) is that it is the same for both its left and right action. Still, its decisive appeal lies in the universality of its description of physics where the crypto-Hermitian (CH) observables and, in particular, crypto-Hermitian Hamiltonian operators $H = H^{(\mathrm{CH})}$ are allowed to be arbitrary (or at least arbitrary analytic) functions of time t,

$$H^{(\mathrm{CH})}(t) = H_{(0)} + tH_{(1)} + t^2H_{(2)} + \ldots. \qquad (\mathrm{A1})$$

Several aspects of the underlying idea of having the manifestly time-dependent metric $\Theta = \Theta(t)$ (i.e., the time-dependent representation of our Hilbert space of states) may look slightly counterintuitive [20]. For this reason, several authors [19,22] tried to restrict the class of the crypto-Hermitian time-dependent models by the so-called quasistationarity (QS) constraint

$$\Theta = \Theta^{(\mathrm{QS})} \neq \Theta(t). \qquad (\mathrm{A2})$$

Such a postulate is in fact rather unfortunate. In an attempt of leaving the form of Eq. (1) unchanged, it practically eliminates the possibility of a consistent application of quantum mechanics to the majority of systems with a sufficiently nontrivial time dependence of its observables $\Lambda_j(t)$.

In the light of empirical results of Ref. [18], the latter statement can even be strengthened and made more quantitative since in the generic quasistationary case the infinite Taylor series of Eq. (A1) *must* degenerate to the linear polynomial

$$H^{(\mathrm{QS})}(t) = H_{(0)} + tH_{(1)}. \qquad (\mathrm{A3})$$

The preliminary, two-by-two matrix illustration of such a key drawback resulting from assumption (A2) can be found in Ref. [19]. Here, we just intend to complement this example by a less model-dependent demonstration that the linearity constraint (A3) is generic, for the finite-dimensional models at least.

In the first step of our proof we accept the assumption that a given N by N crypto-Hermitian Hamiltonian $H^{(\mathrm{CH})}$ (with $N \leq \infty$) is quasistationary, time dependent, and crypto-Hermitian, i.e.,

$$[H^{(\mathrm{CH})}(t)]^\dagger = \Theta^{(\mathrm{QS})}H^{(\mathrm{CH})}(t)[\Theta^{(\mathrm{QS})}]^{-1}. \qquad (\mathrm{A4})$$

With a constant, time-independent metric $\Theta^{(\mathrm{QS})}$ this requirement can be rewritten as an *infinite* family of equations to be satisfied by the coefficients in Eq. (A1),

$$H^{\dagger}_{(m)}\Theta^{(\mathrm{QS})} = \Theta^{(\mathrm{QS})}H_{(m)} \qquad m = 0, 1, \ldots. \qquad (\mathrm{A5})$$

Up to exceptional cases which will not be discussed here, all of the individual N by N matrix coefficients $H_{(m)} \neq H^{\dagger}_{(m)}$ in Eq. (A1) may be assumed diagonalizable,

$$H^{(\mathrm{CH})}_m = \sum_{j=1}^{N} |\Phi_{m,j}\rangle\varepsilon_{m,j}\langle\Psi_{m,j}|.$$

Each choice of $m = 0, 1, \ldots$ specifies, in general, a different biorthonormalized set of vectors together with a different real Nplet of eigenvalues $\varepsilon_{m,j}$ with $j = 1, 2, \ldots, N$.

At this moment we remind the readers that at any subscript $m = 0, 1, \ldots$ we may specify and construct the Nplet of the "left eigenvectors" $|\Psi_{n,j}\rangle$ as a set of biorthonormalized eigenvectors of the conjugate matrix $H^{\dagger}_{(m)}$. In terms of these vectors [23] we may write the Mostafazadeh's [9] most general spectral expansion

$$\Theta^{(\mathrm{QS})} = \sum_{n=1}^{N} |\Psi_{0,n}\rangle\kappa_{0,n}\langle\Psi_{0,n}|. \qquad (\mathrm{A6})$$

At any finite N this formula describes all the metrics compatible with Eq. (A5) at $m = 0$. They depend on N free parameters $\kappa_{0,n}$ which must be real and positive [24].

In the next step of our proof we contemplate the overlap matrix

$$\mathcal{A}_{jk} = \langle \Psi_{0,j} | \Phi_{1,k} \rangle,$$

and deduce that

$$\mathcal{B}_{jk} = \langle \Psi_{1,j} | \Phi_{0,k} \rangle = (\mathcal{A}^{-1})_{jk}.$$

Then, the insertion of Eq. (A6) and the use of the two diagonal real matrices T (with elements $T_{jj} = \kappa_{0,j}$) and F (with elements $F_{jj} = \varepsilon_{1,j}$) transform Eq. (A5) into a remarkably compact matrix relation at the next subscript $m = 1$,

$$T\mathcal{A}F\mathcal{A}^{-1} = (\mathcal{A}^{-1})^{\dagger} F \mathcal{A}^{\dagger} T. \tag{A7}$$

The first line of this relation has the form of a vectorial identity

$$(M_{11}\kappa_{0,1}, M_{12}\kappa_{0,1}, \ldots, M_{1N}\kappa_{0,1}) = (M_{11}^{*}\kappa_{0,1}, M_{21}^{*}\kappa_{0,2}, \ldots, M_{N1}^{*}\kappa_{0,N})$$

where all the matrix elements M_{jk} are known. In the generic case and up to an irrelevant overall factor this relation defines all the parameters $\kappa_{0,n}$ in the metric (A6), therefore. The rest of Eq. (A7) is redundant. This observation may be read either as a proof of the nonexistence of $\Theta^{(QS)}$ for a general "dynamical input" $H_{(1)}$ or, alternatively, as a set of nontrivial compatibility conditions which must be imposed upon the "acceptable" matrices $H_{(1)}$ in Eq. (A3).

We see that even the linear time dependence of the Hamiltonian characterized by the matrix coefficient $H_{(1)}$ is not arbitrary. Moreover, once we choose its most general form we are left with no free parameters which could guarantee the compatibility between our quasistationary metric $\Theta^{(QS)}$ and any higher-order coefficient $H_{(m)}$ at some $m \geq 2$ in Taylor series (A1). We may summarize that in the crypto-Hermitian quantum models restricted to the quasistationary regime the quadratic and higher-power time dependence of its observables can only occur as a very exceptional, fine-tuned phenomenon.

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