Crypto-unitary forms of quantum evolution operators

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Abstract

The description of quantum evolution using unitary operator $u(t) = \exp(-i\mathbf{h}t)$ requires that the underlying self-adjoint quantum Hamiltonian $\mathbf{h}$ remains time-independent. In a way extending the so called $\mathcal{PT}$—symmetric quantum mechanics to the models with manifestly time-dependent “charge” $C(t)$ we propose and describe an extension of such an exponential-operator approach to evolution to the manifestly time-dependent self-adjoint quantum Hamiltonians $\mathbf{h}(t)$. 
1 Introduction

It is well known from textbooks that quantum theory describes the unitary evolution of a system in time via its self-adjoint generator called Hamiltonian. Thus, in principle, one prepares a state (i.e., an element of a physical Hilbert space \( \mathcal{H}(P) \)) at time \( t = t_{\text{initial}} = 0 \). Subsequently, one performs a measurement over the system at a positive \( t = t_{\text{final}} > 0 \). Inside the interval, the time-evolution of the state may be reconstructed via Schrödinger equation

\[
    i\partial_t |\varphi(t)\rangle = \hat{h} |\varphi(t)\rangle, \quad |\varphi(t)\rangle \in \mathcal{H}(P).
\]  

(1)

In practice, our attention remains often restricted to the case of the stationary models based on the time-independent \( \hat{h} = \hat{h}(0) \) for which the states are described by the well known operator-exponential formula

\[
    |\varphi(t)\rangle = \exp(-i\hat{h}(0) t) |\varphi(0)\rangle.
\]  

(2)

In such a setting, nontrivial difficulties may only emerge when the Hamiltonian \( \hat{h} \) (which is not allowed to vary with time) proves prohibitively difficult by itself. For an illustrative example one may recall the review paper where several phenomenological, highly instructive illustrations of such a scenario have been analyzed in the context of nuclear physics. A few years later, the similar problem of the practical intractability of an overcomplicated realistic Hamiltonian \( \hat{h} \) re-emerged in the context of field theory and has been solved in similar manner (cf., e.g., the review papers or ).

The essence of the underlying common theoretical idea of the potential simplification of the overcomplicated but still time-independent and self-adjoint Hamiltonian \( \hat{h} \) will be briefly summarized in section below. Its core will be shown to lie in the replacement of \( \hat{h} \) by its isospectral-partner representation

\[
    H = \Omega^{-1} \hat{h} \Omega.
\]  

(3)

Naturally, once one follows such a recipe and tries to replace a complicated operator \( \hat{h} \) by its sufficiently simplified alternative \( H \), a number of problems emerges in connection with the search for the suitable mapping \( \Omega \).
In the literature one finds, in essence, two alternative strategies of avoiding such a trap. Firstly, in a way exemplified in [2] one starts from the knowledge of a prohibitively complicated but still well-defined (i.e., typically, realistic and microscopic) Hamiltonian \( h = h^\dagger \). By the method of trial and error (based, usually, on some additional, physics-based knowledge about the system in question) one then tries to select a suitable operator \( \Omega \). In the third step of the algorithm one finally checks the required gain in simplicity, typically, by checking the amendment of the rate of the practical numerical convergence of the eigenvalues \( E_n \) when calculated from \( H \) [2].

The second methodical alternative is well known under the nickname of \( \mathcal{PT} \)-symmetric quantum mechanics [3] or, in an inessentially more universal formulation, of the pseudo-Hermitian quantum mechanics [4]. In this approach one starts from a suitable and, by assumption, sufficiently elementary second representation \( H \) of the realistic Hamiltonian. Subsequently one reconstructs the bound-state spectrum \( E_n \) and compares it with the experimental or phenomenological data (if any) immediately.

In the latter (let us conventionally call it, for the time being, \( \mathcal{PT} \)-symmetric) approach, the reconstruction of the original, “true” Hamiltonian \( h \) is often being postponed to the very end of all of the considerations. This has, in principle, two rather unpleasant consequences. Firstly, one usually encounters rather serious technical [5] as well as conceptual [6] difficulties with the very physical interpretation of the \( \mathcal{PT} \)-symmetric models. Secondly, the construction of the original self-adjoint version \( h \) of the Hamiltonian itself becomes almost redundant. In the majority of cases, moreover, this construction remains just approximative and, in addition, also remarkably difficult as a rule [7].

The former approach starts from the initial knowledge of \( h = h^\dagger \) and its main merit is that the related physical interpretation of the system is without problems. The success of such an approach (let us conventionally call it, for the reasons which will be clarified later, crypto-unitary) is then measured but the success of the trial and error selection of \( \Omega \) leading to a sufficiently friendly (and, in principle, potentially also \( \mathcal{PT} \)-symmetric or, in the language of
mathematics, Krein-space self-adjoint \( [8] \) effective Hamiltonian \( H \) of Eq. (3).

In comparison, the respective merits of these two approaches may be perceived as complementary and application-dependent. In parallel, one of their “shared” weaknesses can be seen, in a way explained and summarized in our paper I \([9]\), in the unnecessary and mathematically rather artificial above-mentioned requirement of the time-independence of the individual operators \( h, H \) and/or \( \Omega \). In this sense, our present paper may be perceived as an immediate continuation of paper I \([9]\) (cf. also its conference-proceeding extension \([10]\)) where we generalized, consequently, the methods of Refs. \([2, 3, 4]\) to the class of quantum models where the initial (i.e., presumably, complicated) Hamiltonian of Eq. (1) becomes allowed \textit{manifestly time-dependent}, i.e., where \( h = h(t) \) for \( t \in (t_{\text{initial}}, t_{\text{final}}) \).

The readers may perceive our present paper as motivated by the difficulties encountered during the attempted solution of Schrödinger Eq. (1) with the Hamiltonian \( h = h(t) \). In other words, we shall offer here a continuation of paper I in which we shall develop further the very pragmatic attitude of Ref. \([2]\) where the key purpose of the whole approach has been emphasized to lie in the perceivable \textit{simplification} of practical calculations. In this sense we may formulate our present aim as the statement of a \textit{possibility of an elimination} of the manifest time-dependence from the properly simplified version of the generator of quantum evolution.

The mathematical motivation of such a project may be traced back to the unexpected emergence of a few rather serious obstacles which have been encountered during attempted implementations of the generalized formalism of paper I. \textit{Pars pro toto}, we found it rather unpleasant that virtually all of these applications appeared to require an additional simplification of technicalities mediated, typically, by the choice of a trivial time-dependence in \( h(t) \) \([11, 12]\) or by the use of various versions of adiabatic-approximation hypothesis \([13, 14]\).

The key technical ingredients of our present proposal will make use of the details explained in paper I. We shall recall also Ref. \([10]\) and, in its spirit, we shall also make use of the notation of this reference. The presentation
of our message will be separated into a concise review of the existing time-independent theory (section 2) and of its time-dependent completion as given in paper I (section 3), followed by the description of the main result (section 4), by the discussion (section 5) and by a brief summary (section 6).

2 Time-independent non-Hermitian quantum Hamiltonians

The current popularity of non-Hermitian Hamiltonians $H \neq H^\dagger$ [15] grew from multifaceted physical origins ranging from relativistic quantum field theory [16] and from cosmology [17,4] to nuclear physics [2,18], optics [19], magnetohydrodynamics [20], thermodynamics [21], scattering theory [6], electromagnetism [22] and quantum chemistry [23]. The mathematical and formal aspects of these innovative applications involve, in the context of the very traditional quantum theory, perturbation analysis [24], analytic continuations [25], the calculus of variations [2], supersymmetry [26] and the Feshbach’s model-space techniques [18,23,27].

The profit provided by these developments is a simplification of constructive analyses. This inspired an unexpected and powerful innovation of the traditional model-building strategies. One of the oldest illustrations of the recipe has been offered via the so called “interacting boson models” [2] where the use of non-Hermitian phenomenological Hamiltonians $H \neq H^\dagger$ shortened the computer-assisted numerical predictions of the energy-level spectra of heavy nuclei. Similarly, several field-theory models appeared tractable solely in specific non-Hermitian (a.k.a. $\mathcal{PT}$–symmetric) versions with $H \neq H^\dagger = \mathcal{P}H\mathcal{P}$ where $\mathcal{P}$ denotes parity [3,7]. Last but not least, analogous models found their innovative applications in cosmology [17].

At the very beginning of model-building considerations we usually assume and test [28] (or prove [29]) that the spectrum of $H \neq H^\dagger$ is real and discrete and bounded below. Under these assumptions we may introduce a family of
isospectral images of the Hamiltonian,
\[ h = \Omega H \Omega^{-1}. \]

We may identify them with the Hamiltonians of section 1 and require that they are self-adjoint (i.e., observable), \( h = h^\dagger \). Formally, this merely imposes a constraint upon the eligible (sometimes called Dyson’s [2]) operators \( \Omega \),
\[ H^\dagger \Theta = \Theta H, \quad \Theta = \Omega^\dagger \Omega. \]

In the light of Ref. [30] we may call such a constraint “Dieudonné’s equation”. It may be perceived as a hidden Hermiticity property or crypto-Hermiticity condition [10].

The latter conclusion makes the core of the whole methodical message more or less trivial. One merely replaces the standard textbook Schrödinger Eq. (1) by its, by assumption, “friendlier” crypto-Hermitian re-arrangement
\[ i \partial_t |\Phi(t)\rangle = H |\Phi(t)\rangle, \quad |\Phi(t)\rangle = \Omega^{-1} |\varphi(t)\rangle \in \mathcal{H}^{(F)} \]
yielding the elementary evolution operator whenever \( H \neq H(t) \). The time-evolution of the friendlier solutions \( |\Phi(t)\rangle = \exp(-iHt)|\Phi(0)\rangle \) appears non-unitary (unless \( H = H^\dagger \) of course),
\[ \langle \Phi_1(t)|\Phi_2(t)\rangle = \langle \Phi_1(0)|e^{i(H^\dagger - H)t}|\Phi_2(0)\rangle \neq \langle \Phi_1(0)|\Phi_2(0)\rangle. \]

Under certain subtle mathematical assumptions, fortunately, the representation of the system may be changed in such a manner that its evolution in time is made unitary again. In essence, one must just abandon the traditional (i.e., the so called Dirac’s “transposition plus complex conjugation”) special Hermitian-conjugation operation
\[ \mathcal{T}^{(\text{Dirac})} : |\Phi(t)\rangle \rightarrow \langle \Phi(t)| \]
and replace it by the fully general, arbitrary-metric-dependent version
\[ \mathcal{T}^{(\Theta)} : |\Phi(t)\rangle \rightarrow \langle \Phi(t)| \Theta. \]

The details may be found in Ref. [10].
The related replacement of the (by assumption, prohibitively complicated) Eq. (1) by its (by assumption, computationally friendly) alternative Eq. (6) is rendered consistent by the time-independence assumptions $\hbar \neq \hbar(t)$ and $H \neq H(t)$. In what follows we shall pay attention to the more general, time-dependent crypto-Hermitian-Hamiltonian scenario which has been described in paper I and in which $\hbar = \hbar(t)$, $H = H(t)$ and $\Omega = \Omega(t)$.

3 Manifestly time-dependent non-Hermitian quantum Hamiltonians

The method of simplification $\hbar \rightarrow H$ of the Hamiltonians as mediated by Eq. (4) using non-unitary $\Omega \neq 1/\Omega^\dagger$ cannot be transferred to the case of manifestly time-dependent Hamiltonians. Still, the very idea itself remains applicable. In a way described in our preceding paper I [9] one only has to rewrite Eq. (4) accordingly,

$$\hbar(t) = \Omega(t) H(t) \Omega^{-1}(t) .$$  (10)

It is necessary to start from the time-dependent-Hamiltonian version of the standard textbook Schrödinger Eq. (11) without any elementary solution,

$$i \partial_t |\varphi(t)\rangle = \hbar(t) |\varphi(t)\rangle , \quad |\varphi(t)\rangle \in \mathcal{H}^{(P)} .$$  (11)

Next, we set

$$|\varphi(t)\rangle = \Omega(t) |\Phi(t)\rangle , \quad \langle \varphi(t)| = \langle \Phi(t)| \Omega^\dagger(t) .$$  (12)

and, in the notation of Ref. [10], define the auxiliary ketkets and brabras,

$$|\Phi(t)\rangle \rangle = \Omega^\dagger(t) |\varphi(t)\rangle , \quad \langle \langle \Phi(t)| = \langle \langle \varphi(t)| \Omega(t) .$$  (13)

This notation enables us to replace Schrödinger Eq. (11) with hermitian $\hbar(t)$ by the following pair of its equivalent non-Hermitian descendants

$$i \partial_t |\Phi(t)\rangle = G(t) |\Phi(t)\rangle , \quad |\Phi(t)\rangle \in \mathcal{H}^{(F)} ,$$  (14)

$$i \partial_t |\Phi(t)\rangle \rangle = G^\dagger(t) |\Phi(t)\rangle \rangle , \quad |\Phi(t)\rangle \rangle \in \mathcal{H}^{(F)} .$$  (15)
where we abbreviated \( G(t) = H(t) - \Sigma(t) \) with

\[
\Sigma(t) = i\Omega^{-1}(t) [\partial_t \Omega(t)] = i\Omega^{-1}(t) \dot{\Omega}(t) \equiv \Omega^{-1}(t) \sigma(t) \Omega(t).
\]  

(16)

A few further relevant remarks may be found in paper I.

4 Simplification: constructive guarantee of the time-independence of \( G(t) = G(0) \)

The implementation costs of the generalization \( \mathfrak{h} \rightarrow \mathfrak{h}(t) \rightarrow G(t) \neq G^\dagger(t) \) as reviewed in preceding section were most thoroughly discussed in Refs. [13]. The author suggested that from a purely pragmatic perspective, our main attention should be paid to the applications in which one is allowed to work in an adiabatic approximation where the influence of \( \Sigma(t) \) may be neglected. One of such applications (viz., in cosmology) has subsequently been outlined in Ref. [14].

In our present text we do not intend to propose any approximations. Rather, we shall follow the methodical guidance offered by Ref. [2]. In this setting one assumes, first of all, that the operator \( \mathfrak{h}(t) \) is, for virtually any purpose, prohibitively complicated. This is accompanied by the second assumption that there exists a non-unitary Dyson’s map \( \Omega = \Omega(t) \) such that the solution of the mutually adjoint Schrödinger Eqs. (14) or (15) becomes \textit{perceivably simpler} than the solution of their self-adjoint predecessor Eq. (11).

Next, we shall accept the most natural assumption that our choice of \( \Omega(t) \) is such that the new crypto-Hermitian generator \( G(t) \) of time evolution becomes time-independent. Thus, we must show that such an arrangement is possible and consistent and that it can lead to the sufficiently persuasive simplification of the description of the quantum system in question.

The latter requirement means that \( G(t) = G(0) \) at all of the relevant times. This would immediately imply the validity of the explicit and compact exponential-operator formula for wave functions. Thus, for \( |\Phi(t)\rangle \in \mathcal{H}^{(F)} \) and \( |\Phi(t)\rangle \rangle \in \mathcal{H}^{(F)} \) we would have

\[
|\Phi(t)\rangle = \exp(-iG(0) t) |\Phi(0)\rangle, \quad |\Phi(t)\rangle \rangle = \exp(-iG^\dagger(0) t) |\Phi(0)\rangle \rangle.
\]

(17)
The manifestly guaranteed unitarity of the time evolution follows in both the old (i.e., trivial-metric) and new (i.e., ad hoc-metric) pictures. Indeed, having any product $\langle \varphi_1(t)|\varphi_2(t) \rangle \equiv \langle \Phi_1(t)|\Theta(t)|\Phi_2(t) \rangle$ we may rewrite it, in the light of Eq. (17), in the equivalent form

$$\langle \langle \Phi_1(t)|\Phi_2(t) \rangle = \langle \langle \Phi_1(0)|\Phi_2(0) \rangle = \langle \varphi_1(0)|\varphi_2(0) \rangle.$$  (18)

Our task is reduced to the analysis of the existence of the necessary time-dependent Dyson mapping $\Omega(t)$ such that it satisfies our simplification requirements. In other words, we must postulate the existence of the suitable time-dependent mapping mediated by a not yet specified operator $\Omega(t)$ and by Eq. (10) such that the Dyson-type time-dependent transformation of the Hamiltonian operator $h(t) \rightarrow H(t)$ is a simplification.

In the preparatory step it is sufficient to guarantee (or assume) such a simplification property at an initial instant $t = 0$ and at an infinitesimally shifted time $t = 0 + dt = \Delta > 0$. This will enable us to

- select and fix one of many eligible [2] time-independent operators $\Omega(0)$;
- evaluate the transformed, simplified operator $H(0) = \Omega^{-1}(0) h(0) \Omega(0)$;
- select and fix one of the operators $\Omega(\Delta)$;
- evaluate, with any predetermined precision, the time-independent auxiliary operator $\dot{\Omega}(0) \approx \left[\Omega(\Delta) - \Omega(0)\right]/\Delta + O(\Delta^2)$;
- recall the appropriate definitions and specify operators $\Sigma(0)$ and

$$G(t) = G(0) = \Omega^{-1}(0) h(0) \Omega(0) - i\Omega^{-1}(0) \dot{\Omega}(0) ;$$  (19)

- construct, ultimately, the time-evolving states in closed form (17).

Our task is completed. Naturally, what is still missing here is a constructive return to the original Hilbert space $\mathcal{H}^{(P)}$ which remains complicated. Whenever asked for, this step would require the explicit reconstruction of the Dyson’s operator $\Omega(t)$ at all times. The necessary recipe will be outlined in the next section.


5 Discussion

The successful nuclear-physics tradeoff between the fermionic Fock-space antisymmetrizations and the bosonic non-Hermiticity complications has been described in Ref. [2]. Similarly, the manifest non-Hermiticity of certain toy-models in field theory has been found a good price for the resulting feasibility of the search for their discrete spectra [3].

These results should be perceived as a strong methodical support of our present proposal of tradeoff between the loss of the elementary time-evolution formula for the time-dependent Hermitian quantum systems and the apparently non-unitary form of the simplified crypto-Hermitian prescription (17). In order to make such a tradeoff mathematically complete, we must return now to the underlying postulate

\[ \partial_t G(t) = 0 \]  \hspace{1cm} (20)

which may be given the form \( \dot{H}(t) = \dot{\Sigma}(t) \) or, equivalently,

\[ i \dot{\sigma}(t) = \dot{h}(t) + h(t) \sigma(t) - \sigma(t) h(t) \].  \hspace{1cm} (21)

In the light of the above-mentioned definitions we may also write down the second first-order differential equation

\[ i \dot{\Omega}(t) = \sigma(t) \Omega(t) \].  \hspace{1cm} (22)

At \( t = 0 \) the latter relation specifies, first of all, the initial value \( \sigma(0) \) of the (not yet known) auxiliary operator function \( \sigma(t) \). This initial value just combines the above-specified zero-time operators \( \Omega(0) \) and \( \dot{\Omega}(0) \). Subsequently, the full reconstruction of the time-dependent operator \( \sigma(t) \) must be performed via the linear differential Eq. (21).

In the final step, the resulting solution \( \sigma(t) \) must be inserted in Eq. (22). The solution of the latter equation will ultimately resolve the puzzle leading, at all the times \( t \), to the explicit form of the “missing” Dyson operator \( \Omega(t) \).
6 Summary

In the majority of the existing practical applications of the crypto-Hermitian representations of the operators of quantum observables, the most difficult part of the constructions, viz., the explicit determination of the Dyson mappings $\Omega$ is either being declared redundant (and not performed at all) or found not too essential (in such a case one only proceeds approximatively). Thus, we are very rarely interested in the exact knowledge of operator $\Omega$ or of its Hilbert-space-metric descendant $\Theta = \Omega^\dagger \Omega$. For an illustration of this slightly unexpected convention, it is sufficient to recollect that even for one of the most popular crypto-Hermitian and $\mathcal{PT}$-symmetric toy models using the imaginary cubic $H = -\frac{d^2}{dx^2} + i\epsilon x^3$, only the first three terms in the perturbation series for $\Theta$ are known (cf. Ref. [7]). We may summarize that generically, the crypto-Hermitian-representation approach to quantum theory just works with an incomplete, reduced information about the system in question. This feature of the method is one of its key characteristics, concerning the majority of the applications of the crypto-Hermitian quantum models, manifestly time-dependent or not.

There exist several ways towards the concrete implementations of such an approach to quantum theory. For illustration let us just recall the variational-method pattern used in the interacting boson models of nuclear spectra (where one is not interested in the construction of the wave functions or of any other observables [2]), or the recipe applied to the most popular imaginary cubic oscillator (where one selects just a very particular and, in fact, unique mapping $\Omega$ which remains compatible with an additional requirement of the observability of a charge $\mathcal{C}$ [3]).

In our present text our considerations proceeded along the similar lines. They were aimed at the maximal fructification and at an explicit demonstration of the calculations-simplifying role of the generic, time-dependent non-unitary Dyson’s mappings $\Omega(t)$. In a way complementing paper I we emphasized that in the time-dependent cases such a mapping leads not only to the replacement of a given phenomenological Hamiltonian $\mathfrak{h}(t)$ by its “in-
stantaneous”, isospectral friendlier partner \( H(t) = \Omega^{-1}(t)\mathfrak{h}(t)\Omega(t) \) but also to the possibility of the transfer of the evolution-generating role of \( \mathfrak{h}(t) \) to a pair of different and, incidentally, particularly simple and, first of all, manifestly time-independent operators \( G \) and \( G^\dagger \). These operators were shown to appear in the respective partner Schrödinger equations (14) and (15). Both these operators may be characterized by the hidden form of their Hermiticity as well as by their time-independence. Leading to the (perhaps, surprising?) closed exponential-operator form of the evolution operators as well as to the hidden but, naturally, necessary unitarity (or, if you wish, crypto-unitarity) of the resulting quantum evolution law (17).

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