Hybrid form of quantum theory with non-Hermitian Hamiltonians

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Abstract

In Schrödinger picture the unitarity of evolution is usually guaranteed by the Hermiticity of the Hamiltonian operator $\hat{h} = \hat{h}^\dagger$ in a conventional Hilbert space $\mathcal{H}_{\text{textbook}}$. After a Dyson-inspired operator-transformation (OT) non-unitary preconditioning $\Omega : \hat{h} \rightarrow H$ the simplified Hamiltonian $H$ is, in its manifestly unphysical Hilbert space $\mathcal{H}_{\text{auxiliary}}$, non-Hermitian. Besides its natural OT-based physical interpretation it can also be “Hermitized” (i.e., made compatible with the unitarity) via a metric-amendment (MA) change of the Hilbert space, $\mathcal{H}_{\text{auxiliary}} \rightarrow \mathcal{H}_{\text{physical}}$. In our present letter we propose another, third, hybrid form (HF) of the Hermitization of $H$ in which the change involves, simultaneously, both the Hamiltonian and the metric. Formally this means that the original Dyson map is assumed factorizable, $\Omega = \Omega_M \Omega_H$. A key practical advantage of the new HF approach lies in the model-dependent adaptability of such a factorization. The flexibility and possible optimality of the balance between the MA-related (i.e., metric-amending) factor $\Omega_M$ and the OT-related (i.e., Hamiltonian-changing) factor $\Omega_H$ are explicitly illustrated via an elementary two-state quantum model.

Keywords

- non-Hermitian quantum mechanics of unitary systems;
- hiddenly Hermitian quantum Hamiltonians;
- factorized Dyson map;
- Hermitization using a combined amendment of the inner product and Hamiltonian;
1 Introduction

In the Dyson’s paper [1] the author had to deal with a specific realistic quantum Hamiltonian

\[ \mathfrak{h} = \mathfrak{h}^\dagger \]  

which was defined as acting and self-adjoint in a conventional Hilbert space \( \mathcal{H}_{\text{textbook}} \). During calculations such a representation of the system appeared “user-unfriendly” and, for this reason, Schrödinger equation had to be simplified. For the purpose, the author made use of an isospectral preconditioning of the Hamiltonian,

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

A remarkable as well as not quite expected success has been achieved via an insightful choice of an unusual, manifestly non-unitary preconditioning operator

\[ \Omega \neq (\Omega^{-1})^\dagger. \]  

The original Schrödinger equation containing the prohibitively complicated initial Hamiltonian \( \mathfrak{h} = \mathfrak{h}_{(\text{Dyson})} \) appeared converted into a more easily tractable evolution and eigenvalue problem.

In loc. cit., in spite of the related loss of the Hermiticity of \( H \neq H^\dagger \), the invertible operator-transformation (OT) change (2) of the Hamiltonian based on a judicious choice or construction of a suitable Dyson map (3) paid off. The first step towards the innovative use of non-Hermitian Hamiltonians \( H \neq H^\dagger \) with real spectra in the quantum mechanics of unitary systems has been made (see Refs. [2, 3] and also a few more detailed explanatory comments in section 2 below).

Unfortunately, a wider acceptance of the OT idea appeared slowed down by the numerous emerging mathematical obstacles. In a way emphasized, almost simultaneously, by mathematicians [4], the manifest non-Hermiticity of \( H \) may cause a serious conceptual concern because it often implies, among other, the emergence of instabilities of the spectrum caused even by very small perturbations of the Hamiltonian [5].

One of the remedies has been proposed, in 1992, by Scholtz et al [6]. In essence, these authors emphasized another, alternative (viz., “metric-amendment”, MA) aspect of the Dyson’s concept of the Hermitization (see also a concise outline of the MA theory in section 3 below). From the new perspective the above-mentioned mathematical obstacles have been shown “removable” via additional assumptions like, typically, via the purely technically motivated requirement that the admissible non-Hermitian Hamiltonian operators \( H \) have to be bounded.

Naturally, the latter requirement (which proved not too essential, say, for the model-building in nuclear physics [7]) appeared hardly acceptable in a broader quantum-theoretical context. Fortunately, a truly sophisticated way out of the dead end has been found by Bender with Boettcher.
In a way not unknown in the older mathematical literature, these authors shifted emphasis, in effect, from the mathematical, OT-mediated correspondence between $H$ and its isospectral partner $\mathfrak{h}$ to the underlying, MA-mediated physics. In particular, there authors turned attention to the concept of parity-times-time-reversal symmetry of $H$ ($\mathcal{PT}$-symmetry of $H$). As a consequence their study inspired the current enormous popularity of the widespread use of the manifestly non-Hermitian Hamiltonians $H$ in the various areas of physics (see, e.g., the early paper, the standard reviews or the more recent monographs).

In our present letter we intend to complement these developments by an innovative proposal of a certain third, “hybrid-form” (HF) combination of the two standard and apparently distinct OT and MA theory-building strategies. In a way explained in section and illustrated by a schematic application in section we will show that for a unitarily evolving quantum system characterized by a preselected phenomenological Hamiltonian $H$ (with real spectrum) an optimal representation of its unitary evolution might be based on a mere partial (i.e., not too complicated) modification of the Hamiltonian operator accompanied by a mere partial (i.e., not too complicated) amendment of the related correct physical Hilbert-space metric.

### 2 The Dyson-inspired Hermitization $H \to \mathfrak{h}$

In the early nineties Scholtz et al recalled the success of the isospectral simplification by mapping in nuclear physics. In its light they proposed an extension of the theory and a replacement of the de-Hermitizing mapping $\Omega : \mathfrak{h} \to H$ by its Hermitizing inversion,

$$ H \to \mathfrak{h} = \Omega H \Omega^{-1} = \mathfrak{h}^\dagger. \quad (4) $$

This means that one could consider certain less usual quantum models which are controlled by a manifestly non-Hermitian candidate $H$ for the Hamiltonian. The transition to its isospectral self-adjoint partner $\mathfrak{h}$ can be then interpreted as an OT-mediated Hermitization and a guide to the standard probabilistic interpretation of the system in question. The unitarity of the evolution of the underlying quantum system as required by the Stone theorem in Schrödinger picture would then be restored.

In this spirit an innovative model-building process can start from any sufficiently user-friendly non-Hermitian candidate $H$ for the Hamiltonian. Still, a necessary guarantee of the unitarity of the evolution must be provided, but this can be achieved by the mere reference to the isospectrality between $H$ and its self-adjoint partner $\mathfrak{h}$. What is obtained is an apparently non-Hermitian or, in the current mathematical terminology, quasi-Hermitian formulation of quantum mechanics (QHQM). According to its reviews in the newer literature the QHQM theory can be also assigned alternative names of $\mathcal{PT}$-symmetric quantum mechanics, three-Hilbert-space quantum mechanics or pseudo-Hermitian quantum mechanics.
In the latter, quantum-mechanics-representation context let us emphasize that in the three reviews [6, 11] and [12] (as well as in our present forthcoming text, for the sake of brevity) the Dyson map itself is always assumed stationary,

$$\Omega \neq \Omega(t).$$  \hspace{1cm} (5)

Here, such a stationarity assumption is important. I.a., this will enable us to follow, in section 4 below, the methodical guidance as provided by a truly exceptional stationary-model study [9] by Buslaev and Grecchi. Indeed, Buslaev with Grecchi were probably the first authors who opened the question of having the Dyson map factorized. In this sense, their paper can be read as an immediate predecessor and support of our present fundamental factorization ansatz (cf. Eq. (11) in section 4 below). In addition, their paper can also be read as complementing our present illustrative HF model of section 5 by a non-numerical (i.e., rather rare) and constructive exemplification of the preference of the extreme, purely OT, Dyson-map-based Hermitization (1) of a sufficiently realistic and, at the same time, mathematically friendly and analytic ordinary-differential Hamiltonian $H$.

3  The Hilbert-space metric-operator-based Hermitization

$\mathcal{H}_{\text{auxiliary}} \rightarrow \mathcal{H}_{\text{physical}}$

The distinguishing feature of the most recent implementations of the QHQM formalism is that the necessary Hermitization of the observables, i.e., the guarantee of the unitarity of the evolution is not provided by a reconstruction of the textbook Hamiltonian $\hat{h}$ defined as acting in a textbook Hilbert space $\mathcal{H}_{\text{textbook}}$ but rather by the replacement of the Hermiticity requirement (1) imposed upon $\hat{h}$ in $\mathcal{H}_{\text{textbook}}$ by its equivalent form imposed directly upon $H$. It is only necessary to imagine that the latter operator is assumed introduced and defined as manifestly non-Hermitian in a manifestly unphysical Hilbert space (say, $\mathcal{H}_{\text{auxiliary}}$). In the light of its definition in terms of self-adjoint $\hat{h}$ [cf. Eq. (2)] it is easy to see that the conventional Hermiticity postulate (1) imposed upon $\hat{h}$ is formally equivalent to relation

$$H^\dagger \Theta = \Theta H, \hspace{1cm} \Theta = \Omega^\dagger \Omega,$$

i.e., to the quasi-Hermiticity requirement imposed upon $H$ in $\mathcal{H}_{\text{auxiliary}}$. Now, what remains to do is to recognize that the quasi-Hermiticity (3) of $H$ in $\mathcal{H}_{\text{auxiliary}}$ is equivalent to the Hermiticity of the same operator in another, non-equivalent Hilbert space (say, $\mathcal{H}_{\text{physical}}$) which only differs from $\mathcal{H}_{\text{auxiliary}}$ by an appropriate ad hoc redefinition of the inner product,

$$\langle \psi_a, \psi_b \rangle_{\text{auxiliary}} = \langle \psi_a | \psi_b \rangle \rightarrow \langle \psi_a, \psi_b \rangle_{\text{physical}} = \langle \psi_a | \Theta | \psi_b \rangle.$$

(7)
In other words, all of the mathematical calculations may stay represented in $\mathcal{H}_{auxiliary}$. For the purposes of physics (i.e., typically, for the evaluation of predictions) the auxiliary bra-vectors $\langle \psi \rangle \in \mathcal{H}_{auxiliary}'$ (where the prime ‘ marks the dual vector space [16]) have only to be replaced by the amended, different bra-vector elements

$$\langle \psi_{physical} \rangle = \langle \psi | \Theta \equiv \langle \psi | \in \mathcal{H}_{physical}'$$

simplifying the correct and physical dual vector space $\mathcal{H}_{physical}'$. The triplet of the relevant Hilbert spaces may be then arranged in a diagram

This diagram shows that the operator-transformation Hermitization (OT Hermitization) of Eq. (4) which changes the Hamiltonian finds its alternative in the Hamiltonian-preserving and metric-amending Hermitization (MA Hermitization) of Eq. (7). In both of these scenarios, all of the ket- and bra-vector elements of the relevant Hilbert spaces can be represented in one, “mathematical” Hilbert space $\mathcal{H}_{auxiliary}$ in a way summarized by the three-Hilbert-space diagrams (9) and

$$\langle \psi_m | \rangle, \langle \psi_n | \rangle \xrightarrow{\text{MA path}} \langle \psi_m | \rangle, \langle \psi_n | \Omega^\dagger \Omega$$

(cf. also review [15]).

4 A hybrid, partial-Dyson-map plus partial-metric-operator Hermitization

In our present paper we intend to complement the latter two forms of alternative Hermitizations by a new, third, hybrid one. A basic motivation of our proposal resulted from the following two observations.

• In the case of the Dyson-inspired Hamiltonian-transformation Hermitization $H \rightarrow \mathfrak{h} = \mathfrak{h}^\dagger$ there exist several important weak points of the strategy. The main one is that whenever one is able to construct $\mathfrak{h}$ in closed form, the major part of the motivation of working with its non-Hermitian partner is lost. In such a case it makes good sense to forget about $H$ and to relocate all of the necessary calculations directly to $\mathcal{H}_{(textbook)}$. In practice, only a few exceptions do exist: Buslaev and Grecchi [9], for example, found a rather exceptional
anharmonic-oscillator quantum system in which the OT strategy and the active use of both of
the formally equivalent representation operators \( H_{(BG)} \) and \( h_{(BG)} \) have been found feasible
and proved equally easy. In such a case, naturally, the ultimate choice between the two
operators may be dictated by some complementary phenomenological criteria [17, 18].

- In the case of the strategy based on the reconstruction of the necessary amended physical
Hilbert-space metric \( \Theta \) one can encounter multiple non-trivial and not always expected
technical obstacles. Their source is that whenever one decides to treat Eq. (6) as an implicit
definition of \( \Theta = \Theta(H) \), one reveals that such a definition is not only ambiguous [19] but
also, mostly, yielding just an approximate form of the metric: A fairly long list of these
technical MA-related obstacles may be found presented, e.g., in review paper [12].

The main idea of our present methodical innovation can be traced back to the Dyson’s physics-
rooted papers [1] in which the essence of the success (i.e., the sufficiently persuasive reason for the
preference of the use of the non-Hermitian Hamiltonian model \( H_{(Dyson)} \)) lied in the access to some
additional information about the properties (i.e., typically, correlations [7] or clusterings [20]) of
the system in question. Naturally, such a supplementary knowledge facilitated the specification
of the “good” forms of the mapping \( \Omega \).

Without the latter advantage the probability of success (i.e., of the simplifications achieved as
a compensation of the loss of the Hermiticity) would be lower. Still, we believe that the “user-
friendliness” of the mapping \( \Omega \) and/or of the metric \( \Theta(H) \) (which is, for the success, crucial) could
be also enhanced, in the generic situation, by a tentative factorization of the operator \( \Omega \) itself. In
particular, we propose the use of the two-term ansatz

\[
\Omega = \Omega_M \Omega_H. \tag{11}
\]

Under this assumption, the generic Dyson map can be reinterpreted as a sequence of the two sub-
maps. Subsequently, also the operator-transformation of the Hamiltonian can be made sequential.
In such a setting the emerging “interpolative” step

\[
H \rightarrow H_H = \Omega_H H \Omega_H^{-1} \neq H_H^\dagger
\]

might precede the ultimate OT Hermitization

\[
H_H \rightarrow h = \Omega_M H_H \Omega_M^{-1} = \Omega H \Omega^{-1} = h^\dagger. \tag{13}
\]

This is, in nuce, the main message of our present paper.

One can almost immediately deduce that the “last step” (13) is in fact not unavoidable. Alter-
natively one may finalize the Hermitization in the MA and Hilbert-space-amendment spirit. Tech-
nically, such a methodical alternative would simply mean that one keeps the new non-Hermitian
Hamiltonian $H_H$ unchanged. Thus, one recalls only the Hermiticity of $h$ and re-expresses this property as the quasi-Hermiticity property of $H_H$. In this manner, the Hermiticity rule $h = h^\dagger$ becomes replaced by the formally equivalent relation

$$H_H^\dagger \Theta_M = \Theta_M H_H, \quad \Theta_M = \Omega_M^\dagger \Omega_M$$

in which one just has to confirm that the definition

$$\Theta_M = \Omega_M^\dagger \Omega_M$$

of the new metric operator is correct and consistent with all of the formal QHQM postulates.

Fortunately, the latter confirmation requires just an elementary algebra so that it may be left to the readers. What one obtains is a hybrid-form Hermitization (HF Hermitization) of $H$. What is, at the same time, most important is the question about the potential usefulness of the new HF-type Hermitization (12) + (15) in applications. In the next section, we will try to persuade the readers about the existence of the specific merits of the HF strategy via an implementation of the recipe to a schematic illustrative two-level quantum system.

5 Illustration

For an explicit illustration of our abstract HF representation of the hiddenly unitary quantum evolution let us pick up just a maximally schematic two-by-two real-matrix model. For the sake of simplicity let us also assume that the Hermitian textbook Hamiltonian (with the real and non-degenerate spectrum, say, $E_0 = 1$ and $E_1 = 2$) is, for our methodical purposes, diagonalized,

$$h = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix}.$$  

Also, let us choose, in (11), the two Dyson-map factors (and their product) as follows,

$$\Omega_H = \begin{bmatrix} 1 & t \\ 0 & 1 \end{bmatrix}, \quad \Omega = \begin{bmatrix} 1 & t \\ s & st + 1 \end{bmatrix}.\tag{17}$$

In the light of Eq. (2) we may replace our $h$ of Eq. (16) by its manifestly non-Hermitian isospectral alternative

$$H = \begin{bmatrix} -st + 1 & - (st + 1) t \\ s & st + 2 \end{bmatrix}.\tag{18}$$

Obviously, in a sharp contrast to trivial Eq. (16), the new Hamiltonian-sampling matrix $H$ looks “complicated”. For our present methodical purposes it is important that the latter observation
can be also reinterpreted as a statement that the contrast of complexities will survive in any other basis, with an optimal representation relocated, including the opposite extreme case in which the matrix form of $H$ would look decisively simpler than the matrix form of $\mathfrak{h}$.

For the sake of simplicity let us just keep in mind the latter methodical argument while using the illustrative matrices, due to their maximal pedagogical appeal, in their fixed and given form. This means that we may still speak about a generic nature of the sharp contrast between the triviality of the secular equation for one of the models (here, for $\mathfrak{h}$) and an apparently more complicated form of its Dyson-mapping-mediated analogue.

In our particular example, therefore, one is able to estimate the complexity of the matrix model only after some explicit algebraic manipulations. These manipulations also enable us to reveal and demonstrate that the apparently complicated and $s$– and $t$–dependent secular polynomial $\det(H - E)$ associated with $H$ is in fact also elementary and $s$– and $t$–independent and easily factorizable, $\det(H - E) = E^2 - 3E + 2 = (E - 1)(E - 2)$.

Another apparent contrast in complexity between $\mathfrak{h}$ and $H$ emerges during the verification of the validity of the MA-related quasi-Hermiticity relation (6). Indeed, after insertion we obtain the most complicated matrix result

$$H^\dagger \Theta = \Theta H = \begin{pmatrix} 1 + 2s^2 & t + 2ts^2 + 2s \\ t + 2ts^2 + 2s & t^2 + 2t^2s^2 + 4ts + 2 \end{pmatrix}. \tag{19}$$

Indeed, it takes time to see that this matrix is Hermitian and positive definite at any positive values of the real parameters $s$ a $t$: Incidentally, in our recent paper [21] the operator products $H^\dagger \Theta = \Theta H$ were denoted by a dedicated symbol $Y$ and studied per se. Incidentally, such a study was well motivated since these products prove highly relevant in the context of the random matrix theories [22]. Naturally, in such an applied physics context their complexity or simplicity would be an important characteristics, indeed.

In any physical and QHQM context, after all, one finally has to turn attention to the explicit form of the MA-mediating Hermitizing metric. In our model we have

$$\Theta = \begin{pmatrix} 1 + s^2 & (1 + s^2)t + s \\ t + (ts + 1)s & (t + (ts + 1)s)t + ts + 1 \end{pmatrix}. \tag{20}$$

Indeed, one might think that the necessary (and, quite often, difficult [23]) proofs of its positive definiteness can still be done, quite routinely, via the computer-assisted symbolic manipulations. In this sense we encountered a technical surprise because in spite of a virtual triviality of the underlying two-by-two-matrix algebra the explicit evaluation of the spectrum $\{\theta_\pm\}$ of the metric as provided by the routines of MAPLE [24] appeared complicated,

$$\theta_\pm = 1/2 t^2 + 1/2 t^2 s^2 + ts + 1 + 1/2 s^2 \pm 1/2 \sqrt{D} \tag{21}$$
containing, in addition, an unexpectedly long polynomial

\[ D = 2t^4s^2 + 4t^3s + 4t^3s^3 + t^4s^4 + s^4 + t^4 + 4s^2 + 8ts + 4t^2 + 10t^2s^2 + 2t^2s^4 + 4ts^3. \]  \hspace{1cm} (22)

Still, one arrives at a nice result.

**Lemma 1** The matrix of metric (20) is positive definite.

**Proof.** The proof of the positivity of the metric remained, fortunately, easy and straightforward because after the check of the calculation which was still feasible to perform by hand the helpful key simplification

\[ D = (4 + t^2s^2 + (s + t)^2) \left( t^2s^2 + (s + t)^2 \right) \]  \hspace{1cm} (23)

of the long expression (22) by factorization was immediately visible. □

We believe that the latter set of formulae persuaded the readers that the technical obstacles encountered during the pure-form OT or MA Hermitizations need not be inessential. We believe that the hybrid approach offering, via Eq. (12), the next-to elementary Hamiltonian

\[ H_H = \begin{bmatrix} 1 & 0 \\ s & 2 \end{bmatrix} \]  \hspace{1cm} (24)

in combination with the next-to elementary inner-product metric of Eqs. (14) and (15), viz.,

\[ \Theta_M = \begin{bmatrix} 1 + s^2 & s \\ s & 1 \end{bmatrix} \]  \hspace{1cm} (25)

delivers a fairly persuasive argument in favor of the optimality of our newly proposed third, HF Hermitization strategy. *Pars pro toto* it is worth noting that in contrast to the MA-related Lemma 1 the analogous HF-validating proof of the positive definiteness of metric (25) at all \( s \) proceeds via the positivity of its much more elementary eigenvalues \( \sim 2 + s^2 \pm \sqrt{(2 + s^2)^2 - 4} \).

In our final argument supporting the innovative HF Hermitization strategy we may say that the single-parameter dependence of the HF-representing pair of operators \( H_H \) and \( \Theta_M \) symbolizes and underlines a half-way formal character of the HF approach. We see that also by the criteria of complexity of formulae it lies in between the two (viz., OT and MA) extremes, one of which is always, in our schematic illustration, two-parametric.

### 6 Conclusions

We may summarize our present proposal of an innovative HF reformulation of quantum mechanics as a composition of the partial OT mapping \( H \to H_H \) of Eq. (12) with the partial MA
quasi-Hermiticity constraint (14) which is formulated in terms of the reduced HF metric $\Theta_M$. In conclusion let us now add a few complementary comments on such a form of the model-building strategy.

First of all, let us underline the importance of the stationarity assumption (5). It represents a key to the practical applicability and feasibility of the present HF Hermitization. In the language of mathematics the stationarity is really the constraint which enabled us to make the full use of our fundamental Dyson-map-factorization ansatz (11). Now, we just have to add that in the nearest future we plan to generalize and develop the HF theory also towards its non-stationary extensions. In fact, the first steps in this direction were already made, in 2008, in our three-Hilbert-space description of the unitary quantum evolution as proposed in paper [25] and as reviewed, later, in [15]. On these grounds we were able to formulate a non-Hermitian (or, better, hiddenly Hermitian) generalization of the standard unitary quantum mechanics in interaction picture [26] (see also [27]) and, in the special cases, not only in Heisenberg picture [28] (see also the parallel developments in [29]) but also in the generalized Heisenberg picture (see [30] and also [27, 31]).

In all of the latter papers the Dyson maps were assumed manifestly non-stationary, $\Omega = \Omega(t)$. Interested readers should certainly consult the most recent forms of the non-stationary QHQM theory, say, in the comprehensive reviews [32, 33]. Naturally, due to the non-stationarity of these innovations there exists no direct comparison with our present, stationary version of the HF approach. Nevertheless, it is worth adding that the authors of review [33] proposed to call the non-stationary Dyson maps “generalized vielbeins”. This is a truly remarkable detail because it combines the apparently purely terminological decision with a truly deep insight in the possible applicability of the non-stationary Dyson maps in quantum cosmology. Unfortunately, such an observation and remark already go fairly beyond the scope of our present letter. Still, interested readers are recommended to have a look at the corresponding newest considerations in [34] or in the very recent preprint [35].

In our second, independent and last concluding comment on our present HF method let us point out that it is, in some sense, surprising that in the newest literature on the non-Hermitian quantum Hamiltonians (cf., e.g., [13, 36]) the “mainstream” attention is slowly moving from the closed-system theory to the studies of the open and nonlinear quantum systems. In this case, naturally, the unitarity ceases to be an issue. One of the possible explanations of the shift could be sought in the fact that in spite of the initially enthusiastic acceptance of the Hermitization ideas, their subsequent more detailed analysis and implementations encountered multiple (and also not quite expected) conceptual as well as technical complications [3, 37, 38]. Not enough attention has been paid to the quantum systems (sampled, e.g., by the Buslaev’s and Grecchi’s paper [29]) in which a way out of the difficulties could be sought in a decomposition of the Dyson map into a sequence of its simpler factors. In this sense, our present paper on Hermitizations based on the composite Dyson map ansatz (11) can be read as an encouragement of a renewal
of interest in unitarity and of a start of a new active research in the apparently old-fashioned closed-system direction.
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