Paths of unitary access to exceptional points

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Abstract
With an innovative ideas of acceptability and usefulness of the non-Hermitian representations of Hamiltonians for the description of unitary quantum systems (dating back to the Dyson’s papers), the community of quantum physicists was offered a new and powerful tool for the building of models of quantum phase transitions. In this paper the mechanism of such transitions is discussed from the point of view of mathematics. The emergence of the direct access to the instant of transition (i.e., to the Kato’s exceptional point) is attributed to the underlying split of several roles played by the traditional single Hilbert space of states $L$ into a triplet (viz., in our notation, spaces $K$ and $H$ besides the conventional $L$). Although this explains the abrupt, quantum-catastrophic nature of the change of phase (i.e., the loss of observability) caused by an infinitesimal change of parameters, the explicit description of the unitarity-preserving corridors of access to the phenomenologically relevant exceptional points remained unclear. In the paper some of the recent results in this direction are summarized and critically reviewed.

Keywords
exceptional points; quasi-Hermitian quantum theory; perturbations; quantum catastrophes;

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1 Introduction.

In the context of quantum physics the first signs of appreciation of the phenomenological relevance of exceptional points\cite{1} appeared during the studies of the so called open quantum systems\cite{2}. In these studies the effective Hamiltonians act in a model subspace of the full Hilbert space and are non-Hermitian. Thus, it was not too surprising to reveal that “the positions of the exceptional points” vary “in the same way as the transition point of the corresponding phase transition”\cite{3}. The possibility of a generic connection between exceptional points and phase transitions has been born.

In our present paper we will summarize several aspects of this connection. In order to narrow the subject we will only consider the exceptional-point-related phenomena emerging in the theory of the closed, stable, unitary quantum systems.

1.1 Mathematical concept of exceptional point.

In mathematics the exceptional point (EP) can be defined as the value of an (in general, complex) parameter $g$ at which a linear operator (which is, say, non-Hermitian but analytic in $g$) loses its diagonalizability. For Hamiltonians, one of the possible consequences is schematically depicted in Fig. 1. This picture indicates that near an EP singularity there may exist an $N$–plet of eigenvalues of the operator (i.e., typically, bound state energies specified by a Hamiltonian $H(g)$) which merge in the limit of $g \rightarrow g^{(EP)}$. Simultaneously, in contrast to the non-EP dynamical scenarios, the EP or EPN degeneracy also involves the eigenvectors\cite{1}.

![Figure 1: A schematic sample of the degeneracy of an $N$–plet of energies at an exceptional point of order $N$ (EPN) with $N = 8$ (EP8).](image)

1.2 Early applications of exceptional points in quantum physics of closed systems.

The confluence of eigenvalues as studied by mathematicians and sampled by Fig. 1 did not initially find any immediate applications in quantum physics of closed systems. Among the reasons one can find, first of all, the widespread
habit of keeping all of the realistic phenomenological bound-state Hamiltonians self-adjoint. This also required, for pragmatic reasons, a replacement of the general complex parameter (say, $g \in \mathbb{C}$ in $H(g)$) by a real variable (i.e., by $\lambda \in \mathbb{R}$ in $H(\lambda)$). A combination of the two constraints rendered the mergers impossible. Only after an abstract mathematical operation of analytic continuation of Hamiltonian $H(\lambda)$ it was possible to reveal, in several models [4, 5], the existence of the EPs. Naturally, all of them were manifestly non-real, $\text{Im} \lambda^{(EP)} \neq 0$ [1]. Only an indirect indication of their presence near a real line of $\lambda$ could have been provided by the avoided level crossings, a spectral feature sampled in Fig. 2.

![Figure 2: Avoided crossing of four real (i.e., observable) energy levels (arbitrary units).](image)

In the quantum unitary-evolution setting a dramatic change of the situation only came with the Bender’s and Boettcher’s pioneering letter [6]. The authors revealed that a suitable weakening of the property of the self-adjointness of $H(\lambda)$ could make the EP singularities “visible” and real. What followed the discovery (cf. also the later review paper [7]) was an enormous increase of interest of the physics community in a broad variety of Hamiltonians $H(\lambda)$ possessing the real (i.e., in principle, experimentally accessible) EP singularities with $\text{Im} \lambda^{(EP)} = 0$. In 2010, the conference organized by W. D. Heiss in Stellenbosch [8] was even exclusively dedicated to the role of the EPs in multiple branches of physics.

In our present paper we are going to interpret the EP and EPN degeneracies as sampled by Fig. 1 in a strict unitary-evolution sense. This means that we will only consider the real parameters $\lambda$ lying in a small vicinity of $\lambda^{(EPN)}$. Under this assumption we will require that the whole spectrum of energies remains real and non-degenerate either on both sides of $\lambda^{(EPN)}$ (i.e., at any not too remote $\lambda \neq \lambda^{(EPN)}$) or on one side at least (i.e., for $\lambda < \lambda^{(EPN)}$ or for $\lambda > \lambda^{(EPN)}$). We will, naturally, also admit that the value of $\lambda$ parametrizes a smooth curve passing through a larger, $d$–dimensional space $\mathbb{R}^d$ of the real parameters determining a $d$–parametric Hamiltonian $H(\lambda) = H[a(\lambda), b(\lambda), \ldots, z(\lambda)]$. 

3
1.3 Two-parametric example.

For illustration let us recall the two-parametric real-matrix Hamiltonian of Ref. [9],

\[
H(a, b) = \begin{pmatrix}
-3 & b & 0 & 0 \\
-b & -1 & a & 0 \\
0 & -a & 1 & b \\
0 & 0 & -b & 3
\end{pmatrix}.
\]

(1)

Its eigenvalues

\[
E_{\pm, \pm}(a, b) = \pm \frac{1}{2} \sqrt{20 - 4 b^2 - 2 a^2 \pm 2 \sqrt{64 - 64 b^2 + 16 a^2 + 4 b^2 a^2 + a^4}}
\]

(2)

remain real and non-degenerate inside a two-dimensional unitarity-supporting domain \(D^{(\text{physical})}\) of parameters \(a = a(\lambda)\) and \(b = b(\lambda)\) which is displayed in Fig. 3.

![Figure 3: The boundary of domain \(D^{(\text{physical})}\) for toy-model (1) with \(d = 2\).](image)

It is worth adding that once one moves to the EP-supporting models with more parameters, \(d > 2\), the illustrative shape of the \(d = 2\) domain in Fig. 3 (viz., a deformed square with protruded vertices) appears to be, in some sense, generic. For a family of solvable models with \(N > 4\) such an intuition-based conjecture has been confirmed in [10, 11]. A more recent, abstract theoretical explanation of the hypothesis may be found in [12, 13]. On this background one can expect that the most interesting smooth curves parametrized by \(\lambda\) would be those which end at one of the EPN vertices with maximal \(N\) (i.e., with \(N = 4\) in Fig. 3).

1.4 Paradox of stability near exceptional points.

In a way inspired by the above example one can expect that the behavior of the closed quantum system with parameters lying deeply inside \(D\) would not be too surprising. In such a dynamical regime, small changes of the parameters leave the spectrum real. The formulation of predictions can be based on a conventional perturbation theory.
Close to the boundary $\partial \mathcal{D}$ the situation is different and much more interesting. Indeed, in a small vicinity of this boundary, a small change of the parameter seems to be able to cause an abrupt loss of the observability of the system. A spontaneous collapse *alias* quantum phase transition caused by a small fluctuation of the interaction seems unavoidable.

Our present paper will be fully devoted to its study. In fact, a major part of the paper will provide a concise explanation that in the specific context of the closed, unitary quantum systems the latter, intuitive expectation of instabilities is incorrect (see section 2 for introduction). We will clarify why such an interpretation of dynamics is incorrect (see section 3), why a deeper clarification of the point is important (cf. section 4), and, finally, what would be a valid conclusion (section 5).

Keeping this purpose in mind, our text will start by a sketchy presentation of a (very non-representative) sample of the current state of applications of the stationary version of the formalism represented, schematically, by Fig. 4. This will be followed by a (partially critical) review of some open questions connected, first of all, with the role of the Kato’s exceptional points in phase transitions. We will clarify the role of parameters in the vicinity of EPs. In this dynamical regime, a few comments will be also added on the correct analysis of stability of the non-Hermitian but unitary quantum systems with respect to small perturbations.

A concise summary of our present message will finally be formulated in section 6.

### 2 Unitary evolution in Schrödinger picture using non-Hermitian Hamiltonians.

#### 2.1 Theoretical background

The above-mentioned paradox of stability near EPs is reminiscent of the old puzzle of the stability of atoms in classical physics. In fact, the resolution of the latter puzzle belongs among the most remarkable successes which accompanied the birth of quantum mechanics. The innovation was based on Schrödinger equation representing bound states by ket-vector elements of a suitable Hilbert space $\mathcal{K}$,

$$ H |\psi_n \rangle = E_n |\psi_n \rangle , \quad |\psi_n \rangle \in \mathcal{K} , \quad n = 0, 1, \ldots . \quad (3) $$

Subsequently, the incessant growth of the number of successful phenomenological applications of quantum theory was accompanied by the emergence of various innovative mathematical subtleties. One of the ideas of the latter type (and of a decisive relevance for the present paper) can be traced back to the papers by Dyson [14] and Dieudonné [15]. Independently, they
introduced the concept of the \( \Theta \)-pseudo-Hermitian Hamiltonians. These operators (with real spectra) are assumed to remain non-Hermitian in \( \mathcal{K} \) but restricted by the quasi-Hermiticity relation

\[
H = \Theta^{-1} H^\dagger \Theta \neq H^\dagger, \quad \Theta = \Theta^\dagger > 0. \tag{4}
\]

For details see the text below, or the older review paper [16], or its more recent upgrades [7, 17, 18, 19, 20, 21].

Briefly, the \( \Theta \)-pseudo-Hermiticity innovation can be characterized as a reclassification of the status of the Hilbert space of states (cf. Fig. 4). Indeed, in conventional textbooks the choice of \( \mathcal{K} \) in Schrödinger Eq. (3) is usually presented as unique. In the textbook cases of stable, unitarily evolving quantum systems, in a way observing Stone theorem [22], also the Hamiltonian itself would necessarily be required self-adjoint in \( \mathcal{K} \). After the reclassification, in contrast, the meaning of symbols \( \mathcal{K} \) and \( H \) is being changed. Firstly, in the Dyson’s spirit one decides to admit that \( H \) can be non-Hermitian in \( \mathcal{K} \). In the light of the Stone theorem this means that the status of \( \mathcal{K} \) must be changed from “physical” to “unphysical”. Secondly, in the Dieudonné’s spirit, the postulate of validity of quasi-Hermiticity relation (4) enables us to interpret operator \( \Theta \) as a metric [16]. Thus, we may amend the inner product in order to convert the unphysical Hilbert space \( \mathcal{K} \) into a new, unitarity non-equivalent physical Hilbert space \( \mathcal{H} \),

\[
\langle \psi_1 | \psi_2 \rangle_\mathcal{H} = \langle \psi_1 | \Theta | \psi_2 \rangle_\mathcal{K}. \tag{5}
\]

Thirdly, the factorization \( \Theta = \Omega^\dagger \Omega \neq I \) of the metric enables us to introduce an operator

\[
\mathfrak{h} = \Omega^{-1} H \Omega \tag{6}
\]
and to interpret is as a hypothetical alternative isospectral Hamiltonian in another, alternative physical Hilbert space $\mathcal{L}$ which is, by the assumption which dates back to Dyson [14, 16], self-adjoint but constructively as well as technically inaccessible.

### 2.2 Notation conventions

Further details characterizing such an apparently redundant representation of a single state $\psi$ will be recalled and summarized below. Now, let us only point out that the Dyson’s and Dieudonné’s reformulation of the postulates of quantum theory was deeply motivated. It is only necessary to accept and appreciate both the Dyson’s activity and the Dieudonné’s scepticism. Indeed, Dyson discovered and used, constructively, several positive and truly innovative aspects of the use of quasi-Hermiticity in physics and phenomenology. At the same time, the Dieudonné’s well founded critical analysis of the “hidden dangers” behind the quasi-Hermiticity is still a nontrivial and exciting subject for mathematicians [23, 24].

In the context of physics the latter “hidden dangers” were, fortunately, cleverly circumvented (cf. review [16]). Some of the corresponding technical and mathematical recommendations will be recollected below. Immediately, let us only mention that the amendment of mathematics led to an ultimate compact and explicit three-Hilbert-space (3HS) formulation of the most general non-stationary version of quasi-Hermitian quantum mechanics as first proposed in [25] and as subsequently reviewed in [17].

In what follows, we will employ the most compact notation as introduced in our latter two papers. The reason is twofold. Firstly, along the lines indicated in [17], the choice of such a notation will simplify the separation of our present perception of physics from its alternatives which often share the mathematical terminology while not sharing the phenomenological scope. Secondly, the emphasis put on notation will enable us to review the field of our present interest in a sufficiently compact and concise manner, avoiding potential misunderstandings caused by the variability of the notation used in the literature (cf. Table 1).

| concept                  | symbol |
|--------------------------|--------|
| Hilbert space metric     | $\eta_+$ $\rho$ $T$ $\Theta$ |
| Dyson’s map              | $\rho$ $\eta$ $S$ $\Omega$ |
| state vector             | $|\psi\rangle$ $\Psi$ $|\Psi\rangle$ $|\psi\rangle$ |
| dual state vector        | $|\phi\rangle$ $\rho\Psi$ $T|\Psi\rangle$ $|\psi\rangle$ |
| reference                | [18] [26] [16] here |

Table 1: Sample of confusing differences in notation conventions.
2.3 The concept of hidden Hermiticity.

2.3.1 Motivation.

In an incomplete sample of ambitions of the 3HS reformulation of quantum theory let us mention, first of all, the Dyson’s description of correlations in many-body systems [14] inspired by numerical mathematics (where one would speak simply about a “preconditioning” of the Hamiltonian). Secondly, in combination with the assumption of $\mathcal{PT}$-symmetry [21] the 3HS approach (complemented by the mathematical Krein-space methods [27, 28]) opened new horizons in our understanding of the first-quantized relativistic Klein-Gordon equation [29, 30]. Thirdly, a transfer of the underlying “hidden Hermiticity” ideas to relativistic quantum field theory [31] and/or to the studies of supersymmetry [32] inspired a number of methodical studies of various elementary toy models [6, 33, 34]. Last but not least it is worth mentioning that the applications of the 3HS formalism even touched the field of canonical quantum gravity based on the use of Wheeler-DeWitt equation [35].

2.3.2 Disambiguation.

The solution $\Theta = \Theta(H)$ of Eq. (4) does not exist whenever the spectrum of $H$ ceases to be real. This means that only certain parameters in non-Hermitian $H(\lambda)$ remain unitarity-compatible and “admissible”, $\lambda \in \mathcal{D}$. In the admissible cases, in a way explained in [17], there exists a mapping $\Omega$ which realizes an equivalence of predictions made in $\mathcal{H}$ with those made in a third, hypothetical and, by our assumption, practically inaccessible Hilbert space $\mathcal{L}$. The latter space is precisely the space of states used in conventional textbooks. In the present 3HS context (depicted in Figure 4), its role is purely formal because in this space, operator (6) representing the Hamiltonian and formally self-adjoint in $\mathcal{L}$ is, by assumption, too complicated to be useful or tractable (for example, it may happen to be a highly non-local pseudo-differential operator [18]).

In the literature devoted to applications of unitary quantum theory the authors working in the 3HS version of Schrödinger picture do not always sufficiently clearly emphasize the Hermiticity of the physical Hamiltonian in the physical Hilbert space $\mathcal{H} = \mathcal{H}^{(\text{Standard})}$ (say, by writing $H = H^\dagger$ [17]). Another potential source of confusion lies in the widespread habit (or rather in the abuse of language) of using shorthand phrases (like “non-Hermitian Hamiltonians”) or shorthand formulae (like $H \neq H^\dagger$) without adding that one just temporarily dwells in an irrelevant, auxiliary, unphysical Hilbert space $\mathcal{K}$. The resulting, fairly high probability of misunderstandings is further enhanced by the diversity of conventions as sampled in Table 1.
3 Constructive aspects of the triple Hilbert space formalism.

3.1 Metric and its ambiguity.

Two alternative model-building strategies based on the “generalized Hermiticity” have been used in applications. In the first one one chooses $\mathfrak{h} = \mathfrak{h}^\dagger$ and $\Omega$ and reconstructs $H$ and $\Theta$. In fact, the use of such a strategy remained restricted just to nuclear physics of heavy nuclei in practice [16]. At present, almost exclusively [18], one picks up the Hamiltonian (i.e., a “trial and error” operator $H$ which is non-Hermitian in $\mathcal{K}$) and reconstructs, via Eq. (4), the (necessarily, nontrivial) metric $\Theta > 0$ (i.e., the correct physical Hilbert space of states denoted, here, by dedicated symbol $\mathcal{H}$). The approach based on the reconstruction of metric now forms the mainstream in research. The false but friendly space $\mathcal{K}$ and a non-Hermitian Hamiltonian $H$ are both assumed to be given in advance while a suitable Hermitizing inner-product metric must be reconstructed, in principle at least. The Hermiticity of any other observable $\Lambda$ in $\mathcal{H}$ must also be guaranteed. In the auxiliary space $\mathcal{K}$ this requirement has the form $\Lambda^\dagger \Theta = \Theta \Lambda$.

In an elementary illustration the Wheeler-DeWitt-like equation

$$H = H^{(W DW)}(\tau) = \begin{bmatrix} 0 & \exp 2\tau \\ 1 & 0 \end{bmatrix} \neq H^\dagger \quad \text{in} \quad \mathcal{K} = \mathbb{R}^2$$

yields the two real closed-form eigenvalues $E = E_\pm = \pm \exp \tau$ so that it can serve as a sample of the Dyson-Dieudonné definition of quasi-Hermiticity [11]. A decisive advantage of the use of such a highly schematic one-parametric two-by-two real-matrix example is that one can easily solve Eq. (4) and construct all of the eligible physical inner-product-metric operators

$$\Theta = \Theta^{(W DW)}(\tau, \beta) = \begin{bmatrix} \exp(-\tau) & \beta \\ \beta & \exp \tau \end{bmatrix} = \Theta^\dagger, \quad |\beta| < 1.$$  

These solutions form a complete set of candidates for the (Hermitian and positive definite) eligible metric [16]. In this example one notices that parameter $\beta$ is an independent variable. This observation is, indeed, compatible with the well known fact that the assignment $\Theta = \Theta(H)$ of the metric to a preselected Hamiltonian is not unique [16, 18, 36].

3.2 False instabilities and open systems in disguise

In the literature devoted to applications the authors interested in non-Hermiticity often do not sufficiently clearly separate the quantum and non-quantum theories. Here, we are not going to deal with the latter branch of physics.
Nevertheless, even within the range of quantum mechanics the authors often intermingle the results concerning the open and closed quantum systems. Here, almost no attention will be paid to the former family of models, either. An exception should be made in connection with the papers dealing with certain non-Hermitian but $\mathcal{PT}$-symmetric quantum systems where, typically, the authors claim that “complex eigenvalues may appear very far from the unperturbed real ones despite the norm of the perturbation is arbitrarily small” [37].

As long as the latter claims (of a top mathematical quality) are accompanied by certain fairly vague quantum-theoretical considerations (which could certainly prove misleading), we feel forced to point out that recently, the study of the parametric domains of unitarity near EPs [38] clarified the point (cf. also the less formal explanation in [9]). The essence of the misunderstanding can be traced back to the fact that the loss of stability was deduced, in [37], from the properties of the pseudospectrum [23]. Unfortunately, the construction was only performed using the trivial form of the inner-product metric defining just the manifestly unphysical Hilbert space $\mathcal{K}$ where $\Theta = I$. For this reason the mathematical results about pseudospectra in $\mathcal{K}$ make sense in, and only in, the open quantum systems. In these systems the predicted instabilities really do occur because the space $\mathcal{K}$ itself still keeps there the status of the physical space.

We may summarize that in the 3HS models of closed systems the Hamiltonians are in fact self-adjoint in $\mathcal{H}$. This means that the evaluation of their pseudospectra would necessarily require the work with norms which would be expressed in terms of the physical metric $\Theta$. Thus, once the existence of such a metric is guaranteed (which is, naturally, a nontrivial task!), the proofs of stability based on the pseudospectra will apply.

We should also add that the smallness of perturbations is a concept which crucially depends on the metric $\Theta$ defining the physical Hilbert space $\mathcal{H}$. From this point of view it is obvious that as long as the metric itself becomes necessarily strongly anisotropic in the vicinity of EPs [36], also some of the perturbations which might look small in $\mathcal{K}$ become, in such a regime, large in $\mathcal{H}$, and vice versa [39].

### 3.3 EP (hyper)surfaces and their geometry.

For the lovers of closed formulae the existence as well as the geometry of access to EPs was made very explicit in paper [13]. An advertisement of the contents of this paper can be brief: a list of transmutations is given there between various versions of a special Bose-Hubbard (BH) system (represented by certain complex finite matrices) and of a discrete and truncated anharmonic oscillator (AO). It is sufficient to recall here just the ultimate message of the paper: at an EP singularity of order $N$ it is possible to match, via a phase transition, many entirely different quantum systems. Represented in
their respective Hilbert spaces $\mathcal{K}$ and sharing just their dimension $N < \infty$.

In [13] the idea is illustrated via its several closed-form realizations. Incidentally, all of these models happened to be unitary in a domain $\mathcal{D}$ of a shape resembling a (hyper)cube with protruded vertices. In a broader perspective one can say that by definition [1], the latter vertices are precisely the EP extremes of our present interest. In this light, our present paper could be briefly characterized as a study of the geometry of the generic unitarity-supporting domains of parameters, with particular emphasis on understanding of the sharply spiked shapes of their surfaces $\partial \mathcal{D}$ in a small vicinity of their EP vertices and edges. Indeed, we found such phenomenologically relevant features of the geometry mathematically remarkable and worth a dedicated study.

4 Real-world models and predictions.

4.1 Mathematics: Amended inner products and exceptional points.

The main purpose of the introductory recollection of the 3HS formalism was to prepare a turn of attention to the key role played, in the 3HS applications, by the concept of exceptional points (EPs). Although their original rigorous definition may be already found in the old Kato’s monograph on perturbation theory [1], their usefulness for quantum physics of unitary systems only started emerging after Bender with Boettcher pointed out, in their pioneering letter [6], that the EPs (also known as Bender-Wu singularities [4, 5]) could also acquire an immediate phenomenological interpretation of the points of quantum phase transition. Alternatively, their properties appeared relevant in the more speculative contexts of Calogero models and/or of supersymmetry [40].

From all of the similar 3HS-applicability points of view it is necessary to start the model-building processes from a preselected candidate for the Hamiltonian which is parameter-dependent, $H = H(\lambda)$. Moreover, it must be non-Hermitian in the auxiliary Hilbert space $\mathcal{K}$ and, at the same time, properly Hermitian and self-adjoint in an “amended” Hilbert space of states $\mathcal{H}$. Now, the key point is that in the light of assumption (4), the latter space can be represented via a mere amendment (5) of the inner product in $\mathcal{K}$.

In other words, any solution $\Theta = \Theta(H)$ of Eq. (4) defines the necessary physical space $\mathcal{H} = \mathcal{H}(H)$. In opposite direction, many of the eligible and Hamiltonian-dependent metrics and spaces may and will cease to exist before the variable, path-specifying parameter $\lambda$ reaches the ultimate EP value $\lambda^{(EP)} \in \partial \mathcal{D}$. For the parameters lying inside the physical domain $\mathcal{D}$, the Hamiltonian must still be assigned such a specific metric $\Theta$ and space $\mathcal{H}$ which would exist up to the required limit of $\lambda \to \lambda^{(EPN)}$. In this sense, for any preselected quasi-
Hermitian quantum system, our knowledge and specification of the boundary \( \partial \mathcal{D} \) near EPNs are of an uttermost importance.

### 4.2 Realistic many-body systems.

In the latter setting we should return, once more, to Fig. 3 illustrating the sharply spiked, fragile, parameter-fine-tuning nature of the shape of the sample domain near its EPN extremes. Due to their potential phase-transition interpretation, these extremes seem to be the best targets of a realistic experimental search.

#### 4.2.1 Realistic systems inclined to support an approximate decomposition into clusters.

The manifestly non-unitary mapping \( \Omega \) as mentioned in Fig. 4 connects the ket-vector elements of two non-equivalent Hilbert spaces: In the notation of Ref. [17] we have

\[
|\psi\rangle = \Omega |\psi\rangle, \quad |\psi\rangle \in \mathcal{L}, \quad |\psi\rangle \in \mathcal{K}.
\]

(9)

Recently it has been revealed that precisely the same mapping (attributed to Dyson [16]) also forms a mathematical background of the so called coupled cluster method (CCM, [41]). In fact, the implementation aspects of the latter, CCM interpretation of formula (9) were already used in calculations and tested, say, in quantum chemistry. What was particularly successful are the variational (or, more precisely, bi-variational) realizations of the CCM philosophy, with emphasis put upon the construction of ground states, and with a well-founded preference of mappings (9) in the exponential form \( \Omega = \exp S \) where \( S \) is represented in a suitable operator basis.

The latter, apparently purely technical restriction seems to be responsible for the success of the method which is currently “one of the most versatile and most accurate of all available formulations of quantum many-body theory” [42]. In paper [42], extensive 3HS-CCM parallels have been found. The respective strengths and weaknesses of the two approaches look mutually complementary. Currently [43], their further analysis is being concentrated upon the strengths. One may expect that the consequent, mathematically consistent 3HS quantum theory might enhance the range of applicability of the more pragmatic but very precise CCM ground-state constructions. Along these lines, in particular, the new theoretical predictions may be expected to concern the EP-related many-body quantum phase transitions which could be also, in parallel, experimentally detected.
4.2.2 Bose-Hubbard model and its open- and closed-system interpretations.

The Bose-Hubbard Hamiltonian

\[ H = \varepsilon (a_1^\dagger a_1 - a_2^\dagger a_2) + v (a_1^\dagger a_2 + a_2^\dagger a_1) + \frac{c}{2} (a_1^\dagger a_1 - a_2^\dagger a_2)^2 \]  

(10)

of Graefe et al [44] has been developed to describe an \((N-1)\)-particle Bose-Einstein condensate in a double well potential containing a sink and a source of equal strengths. Besides the usual annihilation and creation operators the definition contains the purely imaginary on-site energy difference \(2\varepsilon = 2i\gamma\). In the fixed-\(N\) representation the Hamiltonian is a matrix: At \(N = 6\) we have, for example,

\[ H^{(6)}(\gamma, c, v) = \begin{pmatrix} 
-5i\gamma + \frac{25c}{2} & \sqrt{5}v & 0 & 0 & 0 & 0 \\
\sqrt{5}v & -3i\gamma + \frac{9c}{2} & 2\sqrt{2}v & 0 & 0 & 0 \\
0 & 2\sqrt{2}v & -i\gamma + \frac{3c}{2} & 3v & 0 & 0 \\
0 & 0 & 3v & i\gamma + \frac{1c}{2} & 2\sqrt{2}v & 0 \\
0 & 0 & 0 & 2\sqrt{2}v & 3i\gamma + \frac{9c}{2} & \sqrt{5}v \\
0 & 0 & 0 & 0 & \sqrt{5}v & 5i\gamma + \frac{25c}{2} 
\end{pmatrix} \]  

(11)

Once we fix the inessential single particle tunneling constant \(v = 1\) and once we localize the EPN singularity at \(\gamma = 1\) and at the vanishing strength of the interaction between particles \(c = 0\), we reveal, at any \(N\), that after an arbitrarily small \(c \neq 0\) perturbation, the spectrum abruptly ceases to be real (see loc. cit.). This means that the metric \(\Theta\) and space \(H\) cease to exist, either. The perturbed system admits, exclusively, the non-unitary, open-system interpretation in \(K\).

In our present framework restricted to closed systems, only the parameters contained inside the suitable physical domain \(D = \{\gamma, c \mid \gamma \in (-1, 1), c \in (c_{\text{min}}(\gamma), c_{\text{max}}(\gamma))\}\) (with the shape resembling, locally, Fig. 3 near its spikes) would be compatible with the reality of the energies. Interested readers may find an extensive study and detailed constructive description of the shape of such a unitarity compatible domain in our rather lengthy recent paper [45].

4.3 Generalized Bose Hubbard models

Up to now we paid attention to the models (sampled by the Bose Hubbard Hamiltonian (10)) with the EPN singularities possessing the trivial geometric multiplicity \(K = 1\) [1]. Interested readers may find, in paper [46], an introduction into a more general category of the EPs characterized by a clustered, \(K\)-centered degeneracy of the wave functions with \(K > 1\). In these cases the EP-related quantum catastrophes (i.e., the generalized \(\mathcal{PT}\)-symmetry breakdowns) appeared to be of the form of confluence of several independent
EPs with $K = 1$. The paper illustrated the advanced mathematics of the degeneracy of degeneracies via low-dimensional matrix models. The emergence of unusual horizons found its mathematical formulation in the language of geometry of Riemann surfaces, accompanied by the phenomenological predictions of certain anomalous phase transitions.

A model-independent analysis of these anomalies in the dynamical EP-unfolding scenarios was based, in subsequent paper \[47\], on their parametrization by the matrix elements of admissible (i.e., properly scaled and unitarity-compatible) perturbations. A consistency of algebra with the EP-related deformations of the Hilbert-space geometry has been confirmed. The new degenerate perturbation techniques were developed and their implementation has been found feasible. Via a class of schematic models, a constructive analysis of the vicinity of the simplest nontrivial EPN with $K = 2$ was performed.

An implementation of the schematic recipe to the Bose-Hubbard-type generalized models may finally be found described in \[45\]. It was shown that there always exists a non-empty unitarity domain $\mathcal{D}$ comprising a multiplet of variable matrix elements of the admissible perturbations for which the spectrum is all real and non-degenerate. The intuitive expectations were confirmed: the physical parametric domains near EPs were found sharply spiked.

A richer structure was revealed to characterize the admissibility of the perturbations. Two categories of the models were considered. In the first one the number of bosons was assumed conserved (leading to the matrix Hamiltonians of the form (11)). The alternative assumption of the particle-number non-conservation led to the realistic $K > 1$ scenarios in which the spectra also remain real and non-degenerate. The quantum evolution controlled by the Hamiltonians of larger (or even infinite) dimensions still remains unitary.

In all of these cases, in spite of a rapid increase of the complexity of the formulae with the number of particles, the existence as well as a sharply spiked structure of $\mathcal{D}$ near EPN has again been reconfirmed. The first steps of the explicit constructive analysis of the structure of $\mathcal{D}$ were performed in the simplest case with $N = 5$ where the access to EP5 appeared mediated by eight independently variable parameters.

### 4.4 Further phenomenological challenges.

The early abstract words of warning against the deceptive nature of the concept of quasi-Hermiticity \[15, 23\] were recently reconfirmed by the authors of paper \[18\]. After a detailed analysis of the popular non-Hermitian but $\mathcal{PT}$-symmetric imaginary cubic anharmonic oscillator these authors came to the conclusion that such a “fons et origo” of the theory can be characterized by the singular behavior attributed to an “intrinsic” EP. Such a discovery contributed to the motivation of our present study since it enhanced the
importance of the knowledge of the behavior of the 3HS models at parameters lying close to their EP limits.

Another, independent source of interest in the study and explicit description of the domains $\mathcal{D}$ of the unitarity-compatible “admissible” parameters in the close vicinity of EPs may be seen in the frequently experimentally observed phenomenon of the avoided level crossings. In a way sampled by Figure 3 this phenomenon occurs even in the spectra of finite-dimensional Hermitian matrices.

The related, highly desirable analytic continuation of the spectra towards their EP degeneracies is by far not an easy task. The task is intimately connected with the 3HS-inspired turn of attention to the description of quantum dynamics using non-Hermitian Hamiltonians. This opens multiple technical questions. One of them is that after one perturbs a quasi-Hermitian Hamiltonian or even only its parameter, $H(\lambda) \rightarrow H(\lambda')$, one immediately encounters the re-emergence of the well known ambiguity of the Hilbert-space inner product in Eq. (5) \cite{18,36,49}. As a byproduct of this observation there appeared a need of a deep and thorough reformulation of perturbation theory itself \cite{39}, with nontrivial consequences concerning, in particular, the systems lying close to the boundary $\partial\mathcal{D}$.

Besides the technical open questions there also exists a number of the strong parallel challenges emerging in the context of quantum phenomenology. Their truly prominent samples emerged in the context of quantum cosmology and, in particular, in the attempted descriptions of the evolution of the Universe shortly after its initial Big Bang singularity. The key point is that the classical-theory-supported existence of Big Bang seems to contradict the conventional quantum-theoretical paradigm of Hermitian theory. By the latter theory the Big-Bang-type phase transitions cannot exist, being “smeared” and reduced to the mere avoided crossing behavior of the spatial coordinates called Big Bounce of the Universe \cite{50}.

A disentanglement of the puzzle could be, in principle, offered by the 3HS models in which the Big Bang would correspond to a real EP-related

Figure 5: Schematic 3HS picture of the Universe evolving through a sequence of Eons separated by EPs. Sampled by “breathing” one-dimensional $N-$point grids with $N_1 = 2$, $N_2 = 4$, etc.
spectral singularity of a suitable non-Hermitian operator (cf., e.g., [51]). Such a hypothesis would admit even a highly speculative “evolutionary cosmology” pattern of Fig. 5 in which a sequence of penrosian Eons separated by the Big-Crunch/Big-Bang singularities would render the structure of the “younger” Universes richer and more sophisticated.

5 Exceptional-point-mediated quantum phase transitions.

5.1 EPs as quantum crossroads.

In paper [13] we emphasized that a classification of passages of closed quantum systems through their EP singularities could be perceived as a quantum analogue of the classical catastrophe theory [52]. In this context let us only add that the EP-mediated phase transitions could acquire the form of a quantum process of bifurcation,

\[
\begin{align*}
\text{initial phase, } t < 0, & & \text{Hamiltonian } H^{(-)}(t) \\
\downarrow & & \\
\text{process of degeneracy} & & \\
\downarrow & & \\
\text{option A} & & \text{option B} \\
\begin{cases}
\text{branch A, } t > 0, \\
\text{Hamiltonian } H^{(+)}_{(A)}(t), \\
\text{indeterminacy at } t = 0
\end{cases} & & \begin{cases}
\text{branch B, } t > 0, \\
\text{Hamiltonian } H^{(+)}_{(B)}(t)
\end{cases}
\end{align*}
\]

Thus, in principle, the future extensions of our present models might even incorporate a multiverse-resembling branching of evolutions at \( t = 0 \).

Marginally, let us add that in such a branched-evolution setting one could find applications even for some results on non-unitary, spectral-reality-violating evolutions. An illustration may be found in papers (sampled by [53]) where just the search for the EP degeneracies has been performed without any efforts of guaranteeing the reality of the spectrum.

5.2 Perturbation theory near EPs using nonstandard unperturbed Hamiltonians.

At the above-mentioned “cross-road” EP instant \( t = 0 \) the Hamiltonian ceases to be diagonalizable. This means that such an instant can be perceived as a genuine quantum analogue of the classical Thom’s bifurcation singularity alias catastrophe [52]. The distinguishing feature of the phenomenon in its quantum form is that it is “instantaneously” incompatible with the postulates of quantum theory. Fortunately, the theory returns in full force at any, arbitrarily small time before or after the catastrophe.
In [13], several explicit and strictly algebraic, solvable-model illustrations of such a passage through the EPN singularity may be found described in full detail. Alternatively, the phenomenon can be also described in a model-independent manner. Indeed, a return to the diagonalizability can be characterized as a perturbation of the non-diagonalizable $t = 0$ Hamiltonian $H_{(EP)}$. Thus, any multiplet of states $|\tilde{\psi}(t)\rangle$ can be constructed, before or after $t = 0$, as the solution of a properly perturbed Schrödinger equation

$$(H_{(EP)} + \lambda W)|\tilde{\psi}\rangle = \epsilon |\tilde{\psi}\rangle .$$

(12)

One has to keep in mind that the unperturbed Hamiltonian itself is an anomalous operator, the conventional diagonalization (or, more generally, spectral representation) of which does not exist. Once we have to consider here just its finite-dimensional matrix forms, the constructive approach to Eq. (12) can be based on the evaluation of the so called transition matrices $Q_{(EP)}$, defined as solutions of the Schrödinger-like linear algebraic equation

$$H_{(EP)}Q_{(EP)} = Q_{(EP)}J_{(JB)}(E_{(EP)}) .$$

The symbol $J_{(JB)}(E_{(EP)})$ denotes here the canonical representation of $H_{(EP)}$. Once we decide to choose it in the most common Jordan-matrix form, the related transition matrices $Q_{(EP)}$ can be reinterpreted as an analogue of the unperturbed basis. In this basis, the perturbed Schrödinger equation (12) acquires the canonical form

$$[J_{(JB)}(E_{(EP)}) + \lambda V]|\tilde{\phi}\rangle = \epsilon |\tilde{\phi}\rangle .$$

(13)

Interested readers are recommended to consult Refs. [38] and [45] for the further details of the solution of such an equation.

For our present purposes the essence of the latter technicalities may be explained using the elementary unperturbed real-matrix Hamiltonians of Ref. [13],

$$H_{(EP)}^{(2)} = \begin{bmatrix} 1 & 1 & -1 \\ -1 & -1 & -1 \end{bmatrix} , \quad H_{(EP)}^{(3)} = \begin{bmatrix} 2 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & -2 \end{bmatrix} , \ldots .$$

For this series of examples all of the transition matrices are non-unitary but known in closed form. At $N = 3$ one gets

$$Q_{(EP)}^{(3)} = \begin{bmatrix} 2 & 2 & 1 \\ -2\sqrt{2} & -\sqrt{2} & 0 \\ 2 & 0 & 0 \end{bmatrix} ,$$

etc. As long as the lack of space does not allow us to reproduce here the further details, let us redirect the readers to paper [39] (in which some overall
conceptual features of the EP-related perturbation approximation construction are described) and to paper [47] (in which the more complicated EPs with geometric multiplicity greater than one are taken into consideration).

Out of the most essential conclusions of the latter two studies let us pick up the single and apparently obvious fact (still not observed, say, in Refs. [23, 37]) that the class of admissible, operationally meaningful perturbations must not violate the self-adjointness of the Hamiltonian in the correctly reconstructed physical Hilbert space \( \mathcal{H} \).

5.3 Constructions based on the differential Schrödinger equations.

In the year 1998 Bender with Boettcher discovered the existence of the real (i.e., in principle, experimentally accessible) EPs generated by certain local and non-Hermitian but parity-time symmetric (\( \mathcal{PT} \)-symmetric) potentials [6]. The EPs were interpreted as instants of the spontaneous breakdown of \( \mathcal{PT} \)-symmetry. Their reality was unexpected because for the conventional local potentials the EPs are never real [4].

Among the specific studies of the non-Hermitian but \( \mathcal{PT} \)-symmetric differential Schrödinger equations \( H \psi = E \psi \) a distinguished position belongs to paper [54] by Dorey et al who considered the angular-momentum-spiked oscillator Hamiltonians

\[
H(M, L, A) = -\frac{d^2}{dx^2} + \frac{L(L+1)}{x^2} - (ix)^{2M} - A(ix)^{M-1}, \quad M = 1, 2, \ldots, \quad L, A \in \mathbb{R}
\]

in which the “coordinate” \( x \) lied on a suitable \textit{ad hoc} complex contour. They showed that inside a suitable domain \( \mathcal{D} \) of parameters these Hamiltonians generate the strictly real bound-state-like spectra. These authors were the first to describe the shape and role of the boundaries \( \partial \mathcal{D} \) formed by the EPs. Unfortunately, they did not make the picture complete because they did not construct the corresponding physical inner products.

5.4 Harmonic oscillator.

Once one restricts attention to the most elementary choice of \( M = 1 \) yielding the one-parametric harmonic-oscillator Hamiltonian \( H(1, L, A) = H^{(HO)}(L) \), the model becomes exactly solvable at all real \( L \in \mathbb{R} \) [55]. For this reason the HO domain of unitarity \( \mathcal{D}^{(HO)} \) has an elementary, multiply connected form of a “punched” interval with EPs (i.e., with elements \( L^{(EP)} \) of boundary \( \partial \mathcal{D}^{(HO)} \)) excluded,

\[
\mathcal{D}^{(HO)} = \left( -\frac{1}{2}, \frac{1}{2} \right) \cup \left( \frac{1}{2}, \frac{3}{2} \right) \cup \left( \frac{3}{2}, \frac{5}{2} \right) \cup \ldots.
\]

This property (cf. Fig. [6]) enabled us to pay more attention, in paper [56],
to one of the key challenges connected with the theory, viz., to the constructive analysis of the practical consequences of the nontriviality and of the ambiguity of the related angular-momentum-dependent metrics $\Theta = \Theta(L)$. Our main result was the construction of a complete menu of the infinite-parametric assignments $H \rightarrow \Theta(H)$ of an eligible metric to the Hamiltonian.

The very possibility of doing so makes the HO model truly unique. For technical as well as phenomenological reasons we restricted our attention just to the parameters $L$ which lied close to the points of the boundary of the domain of the unitarity, i.e., not far from the set of EPs

$$\partial D = \left\{ -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots \right\}. \quad (15)$$

The basic technical ingredient in the construction of the metrics (see its details as well as the rather long explicit formulae in [56]) was twofold. Firstly, the availability of the closed-form diagonalization of $H^{(HO)}(L)$ enabled us to replace the Hamiltonian, at any one of its EP limits, by an equivalent matrix called canonical or Jordan-block representation. Thus, at $L^{(EP)} = -1/2$, for example, such a representation has the elementary block-diagonal form

$$J_{(EP)}^{(-1/2)} = \left( \begin{array}{cccccc} 2 & 1 & 0 & 0 & 0 & \ldots \\ 0 & 2 & 0 & 0 & 0 & \ldots \\ 0 & 0 & 6 & 1 & 0 & \ldots \\ 0 & 0 & 0 & 6 & 0 & \ldots \\ 0 & 0 & 0 & 0 & 10 & \ldots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots \end{array} \right) + \text{corrections}. $$

Secondly, the highly nontrivial fact that all of the unavoidable energy-level crossings occurred pairwise and simultaneously led to the decomposition of the metric-determining relation $H^\dagger(L)\Theta(L) = \Theta(L) H(L)$ (cf. Eq. [14]) to a set of its finite-dimensional (in fact, two-by-two) matrix components numbered by the separate degenerate energies $E^{(EP)} = 2, 6, 10, \ldots$.

Figure 6: Spectrum of Hamiltonian $[14]$ at $M = 1$. 


In such a setup, every value \( L^{(EP)} = -1/2, 1/2, 3/2, \ldots \) may be perceived as an instant of a quantum phase transition which involves all levels at once. In a way accounting, in an exhaustive manner, for the non-uniqueness, the one-parametric ambiguity of every two-by-two submatrix of \( \Theta(L) \) (once more, recall Eq. (8) for illustration) contributes, independently, to the ultimate infinite-parametric ambiguity of selection of the physics-determining inner product in the infinite-dimensional physical Hilbert space \( \mathcal{H}^{(HO)} \).

6 Summary.

At present the Dyson’s traditional 3HS recipe (4) based on the de-Hermitization interpretation \( h \rightarrow H \) of Eq. (6) is usually inverted to yield the flowchart

\[
\begin{array}{ccc}
\text{input:} & \text{non-Hermitian } H \text{ with real spectrum,} & \text{output:} \\
\text{user-friendly Hilbert space } \mathcal{K} & \rightarrow & \text{metric } \Theta = \Omega \Omega^\dagger \text{ (s. t. } H^\dagger \Theta = \Theta H), \\
\text{physical Hilbert space } \mathcal{H} & \text{equivalent predictions} & \text{inaccessible Hilbert space } \mathcal{L}
\end{array}
\]

The model-building process is initiated by the choice of a \textit{bona fide} Hamiltonian \( H \) which is defined and non-Hermitian in auxiliary space \( \mathcal{K} \). The theory is then based on an exact or approximate re-Hermitization of \( H \) via \( \Theta \), with a very rare or marginal explicit subsequent reference to the lower-case Hamiltonian \( h \) or to the map of Eq. (6). Finally, the variability of parameters in \( H = H(\lambda) \) is taken into account, and the physical domain \( \mathcal{D} \) of the admissible values of these parameters is determined.

In applications the 3HS formalism is to be kept user-friendly, with reasonably calculable predictions. Besides the expected enhancement of technical friendliness, an equally important merit of the 3HS formalism should be seen in an emerging access to new and unusual phenomena. By our present selection, all of the phenomena under consideration were characterized by the proximity of EPs, treated as forming the boundary \( \partial \mathcal{D} \) of the domains of “acceptable” \textit{alias} “physical” (i.e., unitarity-compatible) parameters of the model in question. We reviewed and slightly extended several recent related results.

From the abstract methodical point of view we put emphasis upon the suitability and amendments of the necessary (although, sometimes, less usual) perturbation-type construction techniques. This enabled us to clarify several counterintuitive facts characterizing the behavior of the closed quantum systems in the small vicinities of EPs of higher orders. As a main conclusion the readers should remember the fact that in these vicinities, the technique
of perturbations offered one of the most efficient tools of the parametrization and classification of the “admissible” (i.e., unitarity-preserving) multiparametric Hamiltonians $H(\lambda) = H[a(\lambda), b(\lambda), \ldots, z(\lambda)]$. 
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