Quantum catastrophes: a case study

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Abstract
The bound-state spectrum of a Hamiltonian $H$ is assumed real in a non-empty domain $D$ of physical values of parameters. This means that for these parameters, $H$ may be called crypto-Hermitian, i.e. made Hermitian via an \textit{ad hoc} choice of the inner product in the physical Hilbert space of quantum bound states (i.e. via an \textit{ad hoc} construction of the operator $\Theta$ called the metric). The name quantum catastrophe is then assigned to the $N$-tuple-exceptional-point crossing, i.e. to the scenario in which we leave the domain $D$ along such a path that at the boundary of $D$, an $N$-plet of bound-state energies degenerates and, subsequently, complexifies. At any fixed $N \geq 2$, this process is simulated via an $N \times N$ benchmark effective matrix Hamiltonian $H$. It is being assigned such a closed-form metric which is made unique via an $N$-extrapolation-friendliness requirement.

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1. Introduction
The measurement of an $N$-plet of energy levels belongs among the most frequently encountered forms of the experimental verification of theoretical conjectures concerning quantum systems. This is one of the key reasons why people often turn attention from a realistic Hamiltonian $H^{(P)}$ (where $P$ stands for physical) to its ‘friendlier’ version $H^{(F)}$ yielding the same energies. This means that we can write, formally,

$$H^{(P)} = \Omega H^{(F)} \Omega^{-1}. \quad (1)$$

Besides the most common cases in which $\Omega$ is required to be unitary, simplifications $H^{(P)} \rightarrow H^{(F)}$ are accompanied by the loss of the manifest Hermiticity of the effective Hamiltonian, $H^{(F)} \neq [H^{(F)}]^\dagger$. At first sight, this looks like a discouraging paradox. The non-numerical replacements of a complicated $H^{(P)}$ by its simpler avatar $H^{(F)}$ found just a few fully explicit realizations in the literature, therefore (cf, e.g., [1]). In parallel, the pragmatic
numerical recipes of the form of equation (1) were more successful. In nuclear physics, for example, the use of non-unitary (often called Dyson) maps $\Omega$ proved feasible and efficient [2].

Non-numerical theoretical activities in the field have been perceptibly revitalized recently (cf., e.g., reviews [3–6]). People imagined that the friendly, non-Hermitian Hamiltonians $H^{(F)}$ with real spectra may be proposed and studied directly, without any recourse and explicit reference to their partners $H^{(P)}$. For this purpose, it appeared sufficient to translate, via equation (1), the postulate of Hermiticity of $H^{(P)} = \left[H^{(P)}\right]^\dagger$ into the equivalent (sometimes called Dieudonné’s [7] or crypto-Hermiticity [8]) requirement

$$\left[H^{(F)}\right]^\dagger \Theta = \Theta H^{(F)}$$

(2)

involving merely the effective Hamiltonian. This relation also contains just the product of Dyson operators $\Theta = \Omega^\dagger \Omega$ called, conveniently, Hilbert-space metric or, simply, metric [2].

Whenever the spectrum of energies remains real, the use of non-unitary maps $\Omega$ does not lead to any conceptual difficulties (cf appendix A for more details). One simply has to keep in mind that the definition and/or an exhaustive description of a quantum system in question may employ either the manifestly self-adjoint Hamiltonian $H^{(P)}$ or its crypto-Hermitian reincarnation $H^{(F)}$ plus a sophisticated metric $\Theta = \Theta^{(S)} \neq I$.

In our present paper, we intend to study and discuss what happens near Kato’s exceptional points [9], at which the spectrum ceases to be real [10]. In particular, we intend to offer and describe a series of crypto-Hermitian quantitative models simulating the quantum catastrophes (QC) during which an $N$-plet of the bound-state energies degenerates at an exceptional point and, subsequently, complexifies.

2. The domains of hidden Hermiticity

2.1. One-parametric Hamiltonians $H(\lambda)$

The difference between the use of the trivial metric $\Theta^{(P)} = I$ and its more involved form $\Theta^{(S)} \neq I$ might look purely technical. During the first stages of the intensive development of the crypto-Hermitian representations of the operators of observables, this opinion prevailed. People felt addressed by the questions of non-emptiness of the domains of parameters in which the Hamiltonian was diagonalizable, while its bound-state spectrum remained real:

$$\text{all } E_n(\lambda) \in \mathbb{R} \iff \lambda \in D^{(\text{physical})}.$$  

(3)

The subtleties of the correspondence between Hermitian $H^{(P)}$ and simplified $H^{(F)}$ appeared inessential, in the weak-coupling perturbation regime at least (cf., e.g., [11, 12]).

A few years later, the emphasis was shifted to the strong-coupling dynamical regime. People started paying attention to the existence and the role of Kato’s exceptional points $\lambda = \lambda^{(EP)} \in \partial D^{(\text{physical})}$ [12, 13]. Step by step, the studies of this possibility transcended the boundaries of quantum theory. The complexification of the spectrum, i.e. the often encountered fact that

$$\text{some } E_n(\lambda) \notin \mathbb{R} \quad \text{when } \lambda \notin \overline{\mathcal{D}}^{(\text{physical})}$$

(4)

appeared relevant, e.g., in magnetohydrodynamics (where the related instabilities do exist and are measurable [14]) or in classical and experimental optics [15].

The turn of attention to models based on the use of non-trivial $\Theta^{(S)} \neq I$ changed the paradigm even inside quantum theory. In our present paper, we intend to show that new perspectives are truly opened by the possibility of explicit constructions of the metrics in the strong-coupling regime. This challenging theoretical option is made important by its phenomenological appeal, connected either with the possible abrupt loss of correspondence
(1) at $\lambda = \lambda^{(\text{EP})}$ or with the phase-transition-resembling violation (4) of the spectral reality beyond the EP horizon.

2.2. Crossing the horizons $\partial D^{(\text{physical})}$

In phenomenological applications of equations (1) and (2) the quantum system is often studied in a fragile dynamical regime [16]. In the language of mathematics, this means that the parameter $\lambda$ (typically, a coupling [9]) is located in a close vicinity of one of its EP values.

Naturally, one has to distinguish between the parametric dependence of the complicated Hamiltonian $H^{(P)} = H^{(P)}(\lambda)$ and the combined parametric dependence of the simplified effective Hamiltonian $H^{(F)} = H^{(F)}(\lambda)$ and of the effective metric $\Theta = \Theta^{(S)}(\lambda)$. The main formal reason is that it is virtually impossible to speak about the operator $H^{(P)}(\lambda)$ in any non-trivial vicinity of $\lambda^{(\text{EP})}$. Indeed, its Hermiticity is robust so that it cannot produce any non-real eigenvalues. In other words, this operator ceases to exist at any point $\lambda = \lambda^{(\text{EP})}$ of the horizon.

In contrast, no relevant difficulties in the crypto-Hermitian representation of the systems emerge near a QC. The dynamics using the doublet of operators $[H^{(F)}(\lambda), \Theta(\lambda)]$ is flexible and can be prolonged till the horizon, i.e. up to the limit $\lambda \to \lambda^{(\text{EP})}$. In our recent papers [17–25] on this subject, we solely paid attention to the study of the spectra in this limit. As a consequence, all of our results just concerned the geometry of the domain $D^{(\text{physical})}$. In other words, we were interested in the behavior of the energies and not in the behavior of the wavefunctions and of their inner products. Thus, in spite of our initial optimism [20], we only managed to parallel Thom’s theory of classical catastrophes [26] by a rather formal combinatorial classification of the energy mergers [27].

In our present paper, we intend to broaden our perspective and to fill the gaps. We will make use of the family of $N \times N$ matrix models as reviewed briefly in appendix B. For the sake of definiteness, we shall merely select one of its most friendly one-parametric subfamilies. For these particular toy-model Hamiltonians $H^{(F)}(\lambda)$, the construction of the (up to now, missing) physical metrics $\Theta(\lambda)$ will be shown feasible and outlined in detail.

2.3. The metrics

The simulation of the catastrophe at $\lambda = \lambda^{(\text{EP})}$ must be based on our specification of the Hamiltonian and metric (cf appendix A). The usual, ‘friendly’ inner product $(f, g)^{(F)} = \sum_{n=1}^{N} f^*_{n} g_{n}$ must be replaced by its ‘sophisticated’ double-sum generalization

$$(f, g)^{(S)} = \sum_{m=1}^{N} \sum_{n=1}^{N} f^*_{m} \Theta^{(S)}_{mn} g_{n}$$

defined in terms of a suitable physical Hilbert-space metric $\Theta = \Theta^{\dagger} > 0$. On the level of abstract principles [4], the related amendment of the Hilbert space $\mathcal{H}^{(F)} \to \mathcal{H}^{(S)}$ is of vital theoretical importance since it changes the status of the Hamiltonian $H(\lambda)$ from ‘non-Hermitian’ (i.e. unphysical) to ‘Hermitian’ (i.e. observable). On the level of practical calculations, in contrast, the interpretation of equation (5) as defining another Hilbert space $\mathcal{H}^{(S)}$ is redundant and may be, in the present context, treated as formal. We may always keep working inside $\mathcal{H}^{(F)}$ where every use of the ‘correct’ product (5) may simply be translated, via equation (5), into the friendly space language in which the matrix $\Theta^{(S)}$ is inserted wherever necessary. This will allow us to keep using Dirac’s bra and ket symbols without any danger of misunderstanding. In particular, we may work with the usual Schrödinger equation

$$H(\lambda)\ket{\psi_{j}(\lambda)} = E_{j}(\lambda)\ket{\psi_{j}(\lambda)}$$

(6)
in Dirac’s notation. In a useful additio nal convention of [4] the eigenvectors of the conjugate Hamiltonians may be denoted by the specific, doubled ket symbols
\[ H^\dagger(\lambda)|\psi_k(\lambda)\rangle = E_k(\lambda)|\psi_k(\lambda)\rangle. \] (7)
Such a convention simplifies the spectral representation of the metric (cf [28] for more details),
\[ \Theta(\lambda) = \sum_{n=1}^{N} |\psi_n(\lambda)\rangle \langle \psi_n(\lambda) |. \] (8)

Once we restrict our attention to the QC scenario in which an \( N \)-plet of the bound-state energies \( \{E_n(\lambda)\} \) stays real inside \( D(\text{physical}) \) and complexifies beyond an exceptional point \( \lambda(\text{EP}) \in \partial D(\text{physical}) \), we need not be particularly careful. Enhanced difficulties with the proper physical interpretation of the system should merely be expected due to the increasing sensitivity of both the strongly non-Hermitian matrix \( H = H(\lambda) \) and increasingly ill-conditioned matrix \( \Theta = \Theta(\lambda) \) to perturbations. Hence, in the QC regime, full-precision knowledge of metric \( \Theta(S) \) would be highly desirable. This may be identified as one of our present main constructive targets.

3. Solvable crypto-Hermitian toy models in the strong-coupling QC regime

As long as \( N < \infty \) is finite, formulae (7) + (8) represent one of the most natural recipes for the practical construction of the metric. In this sense our present results may be formulated, briefly, as a successful application of this recipe to the sequence of matrix models as sampled, at even \( N \), by equation (B.1) in appendix B.

For our present purposes we decided to study just a one-parametric subset of this family. Having skipped the \( N = 2 \) model as trivial, let us pick up, for illustration, the next, \( N = 4 \) example [19]. Once we reparametrize the Hamiltonian \( H^{(4)}_{(a,b)} \) in terms of a distance \( \lambda \) from the exceptional-point value \( \lambda(\text{EP}) = 0 \),
\[ H^{(4)}(\lambda) = \begin{bmatrix} -3 & \sqrt{3}\sqrt{1-\lambda} & 0 & 0 \\ -\sqrt{3}\sqrt{1-\lambda} & -1 & 2\sqrt{1-\lambda} & 0 \\ 0 & -2\sqrt{1-\lambda} & 1 & \sqrt{3}\sqrt{1-\lambda} \\ 0 & 0 & -\sqrt{3}\sqrt{1-\lambda} & 3 \end{bmatrix}, \] (9)
we reveal that the new parametrization simplifies the spectrum,
\[ E_0 = -3\sqrt{\lambda}, \quad E_1 = -\sqrt{\lambda}, \quad E_2 = \sqrt{\lambda}, \quad E_3 = 3\sqrt{\lambda}. \]
It remains real at any \( \lambda \in (0, \infty) \equiv D(\text{physical}) \). The comparison of this result with its trivial \( N = 2 \) predecessor [17] opened in fact the way towards its extrapolation to all \( N \), even or odd, as given, in appendix B, by equation (B.2).

3.1. The simplest metrics and observables: \( N = 2 \)

Any two-by-two real-matrix candidate \( H^{(2)} \) could play the role of a toy model for which we would be able to specify the subdomain \( D(\text{physical}) \) of free real parameters leaving the spectrum real. Equally easily we would even construct the related metrics \( \Theta^{(2)} \) and determine the Hilbert space(s) \( H^{(S)} \) in which the matrix \( H^{(S)} \) would become, constructively, tractable as a self-adjoint Hamiltonian [17].

The weak point of such an approach would lie in a vast ambiguity of the transition to any larger \( N \times N \) matrix \( H^{(N)} \). That is why our present selection of the class of Hamiltonians started at large \( N \). Once we specified the general structure of \( H^{(N)} \) we were able to study its consequences in more detail.

Let us now return to the first non-trivial dimension \( N = 2 \) at which our toy-model Hamiltonian reads
$$H^{(2)}(\lambda) = \begin{bmatrix} -1 & \sqrt{1-\lambda} \\ -\sqrt{1-\lambda} & 1 \end{bmatrix}.$$  

This is precisely the matrix which also appeared, in a slightly different notation and in an entirely different physical context, in our preceding paper [25]. Still, the mathematics remains the same, including the recommended replacement of $r$ by $r = r(\lambda) = \sqrt{\lambda}$. This has been shown to facilitate the solution of the conjugate Schrödinger equation (7), i.e. equivalently, via equation (8), the construction of the necessary Hermitizing metric in closed form. Secondly, the introduction of the further two apparently redundant abbreviations $\sqrt{1-r} := u = u(\lambda)$ and $\sqrt{1+r} := v = v(\lambda)$ enabled us to write down the resulting ketkets $|\psi_1\rangle = \{u, -v\}^T$ and $|\psi_0\rangle = \{-v, u\}^T$ in a particularly compact and symmetric manner (note that the superscripted $T$ means transposition while the ordering of the ketkets is, for some inessential reasons, reversed).

Once we return to the $N = 2$ case (and to the construction of the metric), another abbreviation appears also useful, $z = uv = \sqrt{1-\lambda}$. This in fact makes the sum (8) for the matrix of metric most compact,

$$\Theta = \Theta^{(2)}(\lambda) = \begin{bmatrix} 1 & -\sqrt{1-\lambda} \\ -\sqrt{1-\lambda} & 1 \end{bmatrix} = \begin{bmatrix} 1 & -z \\ -z & 1 \end{bmatrix}.$$  

One might also note that this matrix becomes diagonal in the far-from-QC limit $\lambda \to 1$. In the opposite direction, any other observable quantity must be guaranteed to be crypto-Hermitian, i.e. compatible with Dieudonné's [7] constraint $G^\dagger \Theta = \Theta G$. Thus, our knowledge of the metric is vital. It implies that any $N = 2$ candidate for an operator of an observable represented, say, by the ansatz

$$G = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

must be restricted by Dieudonné's constraint yielding the single rule $c - b = z(a - d)$. Optionally, we may make the new observable $G$ independent of $\lambda$ (i.e. of $z$). For this purpose, it suffices to satisfy the two separate constraints $a = d$ and $c = b$. In the latter case, the ultimate condition of the reality of the eigenvalues of $G$ is trivially satisfied for any real $d$ and $b$.

### 3.2. The metric at $\mathbf{N = 3}$

At first sight the use of the doublet of ad hoc functions $u = u(\lambda)$ and $v = v(\lambda)$ of $\lambda$ seems artificial. Recently, we imagined that their appeal need not necessarily be restricted to $N = 2$. We rewrote the triple-level Hamiltonian in the same variables:

$$H^{(3)}(u, v) = \begin{bmatrix} -2 & \sqrt{2uv} & 0 \\ -\sqrt{2uv} & 0 & \sqrt{2uv} \\ 0 & -\sqrt{2uv} & 2 \end{bmatrix}.$$  

We felt that this introduces a new symmetry in our present problem. In a backward perspective, this idea will truly play a key role in our forthcoming considerations.

On the level of energies, the idea looks trivial. Indeed, after transition from $N = 2$ to $N = 3$ we merely obtain a robust, coupling-independent new level $E = 0$. From the qualitative point of view, no new insight into the QC mechanism of spectral complexifications is gained. The situation only becomes more interesting when we recall formula (8) and try to define the metric. This must be preceded by the construction of the left eigenketkets of the Hamiltonian $H^{(3)}(u, v)$. After some elementary calculations one obtains the formula

$$|\psi_2\rangle = \{u^2, -\sqrt{2uv}, v^2\}^T, \quad |\psi_1\rangle = \{-\sqrt{2uv}, 2, -\sqrt{2uv}\}^T, \quad |\psi_0\rangle = \{v^2, -\sqrt{2uv}, u^2\}^T.$$
The comparison with its $N = 2$ predecessor does not offer any hint for extrapolation to $N > 3$. In a search for some new symmetries, the latter result must be further amended.

By the trial-and-error technique we succeeded in verifying that the key to a successful amendment should be sought in the homogenization of the individual ketkets, treated exclusively as functions of $u$ and $v$. At $N = 3$, the only item which violates such an overall principle is the second element of $|\psi_1\rangle$, which is equal to 2. Thus, in place of this digit we will insert the expression $u^2 + v^2$ which is identically equal to 2. This seems to be the trick. After we insert the amended vectors in equation (8), we obtain the metric in its highly indicative form of the matrix sum:

$$\Theta^{(3)} = I - z \begin{bmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix} + \sqrt{2} \mathcal{J}, \quad z = uv,$$

where the symbol $\mathcal{J}$ denotes the matrix with units along the second diagonal. This matrix–polynomial version of the metric at $N = 3$ seems to exhibit all of the expected symmetries. The presence of these ‘hidden’ symmetries may also be expected to simplify the matrix structure of the metric at higher dimensions $N$.

3.3. Crypto-Hermitian observables at $N = 3$

Every unique specification of the metric determines the complete family of eligible observables $G$. The only constraint is that these matrices must be crypto-Hermitian, i.e. compatible with Dieudonné’s crypto-Hermiticity condition $G^\dagger \Theta = \Theta G$. From the ansatz

$$\Theta = \begin{bmatrix} 1 & -\sqrt{2}z & z^2 \\ -\sqrt{2}z & 1 + z^2 & -\sqrt{2}z \\ z^2 & -\sqrt{2}z & 1 \end{bmatrix}, \quad G = \begin{bmatrix} a & b & c \\ d & f & g \\ h & k & m \end{bmatrix},$$

this enables us to deduce the triplet of explicit crypto-Hermiticity conditions imposed upon the general candidate matrix $G$:

$$z^2a - \sqrt{2}zd + h - c + \sqrt{2}zg - z^2m = 0,$$
$$-\sqrt{2}za + d + dz^2 - \sqrt{2}zh - b + \sqrt{2}zf - z^2k = 0,$$
$$z^2b - \sqrt{2}zf + k + \sqrt{2}zk - g - gz^2 + \sqrt{2}zm = 0.$$

The general solution may be written in the following form:

$$b = -\sqrt{2}za + d + dz^2 - \sqrt{2}zh + \sqrt{2}zf - z^2k,$$
$$c = z^2a - \sqrt{2}zd + h + z^2m + 2z^2h - 2z^2f - \sqrt{2}z^3d + \sqrt{2}z^2k + \sqrt{2}zk,$$
$$g = \sqrt{2}zm + \sqrt{2}zh - \sqrt{2}zf - dz^2 + z^2k + k.$$

Whenever needed, our observables may even be required to be $z$-independent (i.e. independent of the $\lambda$-controlled changes of the Hamiltonian). The explicit form of the latter observables is, naturally, less flexible. Still, they may be shown to possess the following three-parametric general form:

$$F = \begin{bmatrix} a & d & h \\ d & a + h & d \\ h & d & a \end{bmatrix}.$$

The three related eigenvalues

$$\{a - h, a + h + \sqrt{2}d, a + h - \sqrt{2}d\}$$

should be required to be real of course. Thus, it is important to conclude that the latter subfamily of specific observables $F$ remains conserved and uninvfluenced by the occurrence of the global QC in the QC limit $z \to 1$. 6
4. The extrapolation pattern

The technical core of our present message lies in the description of merits of a rather counterintuitive replacement of the single parameter \( \lambda \) by an apparently redundant pair of functions \( u = u(\lambda) \) and \( v = v(\lambda) \). This trick enables us to make use of the symmetries hidden in the problem. As a consequence, an efficient extrapolation strategy may be developed, simplifying decisively the use of the spectral formula (8) for the metric via the decisive clarification of the structure of the necessary set of the left eigenvectors of our conjugate Hamiltonians \( H^{(b)}(\lambda) \) at any matrix dimension \( N \).

4.1. The first non-trivial case—the confluence of the two complexifications at \( N = 2J \) with \( J = 2 \)

At \( N = 4 \), our toy model (9) experiences its QC collapse at the boundary of the acceptability interval, i.e. at \( z = \zeta^{(\text{EP})} \approx \pm 1 \) where the quadruplet of the energies completely degenerates, \( E^{(\text{EP})}_n = 0 \). The parallel QC degeneracy also involves the wavefunctions. They collapse into the same eigenvector in the QC limit as well. The same degeneracy rule applies, finally, also to the left eigenvectors of \( H \), i.e. the right eigenvectors of \( H^\dagger \).

The latter statement is not so easily checked at \( N = 4 \). Indeed, the direct calculations using symbolic manipulations (e.g., in MAPLE) offer just the quadruplet of the eigenvectors of \( [H^{(d)}(z)]^\dagger \) in a rather complicated closed form:

\[
\begin{pmatrix}
|\psi_3\rangle_1 \\
|\psi_3\rangle_2 \\
|\psi_3\rangle_3 \\
|\psi_3\rangle_4 \\
|\psi_2\rangle_1 \\
|\psi_2\rangle_2 \\
|\psi_2\rangle_3 \\
|\psi_2\rangle_4 \\
|\psi_1\rangle_1 \\
|\psi_1\rangle_2 \\
|\psi_1\rangle_3 \\
|\psi_1\rangle_4 \\
|\psi_0\rangle_1 \\
|\psi_0\rangle_2 \\
|\psi_0\rangle_3 \\
|\psi_0\rangle_4 \\
\end{pmatrix} = \begin{pmatrix}
3\sqrt{1-z^2}z^2 + 9z^2 - 12\sqrt{1-z^2} - 12 \\
3z(-z^2 + 2 + 2\sqrt{1-z^2})\sqrt{3} \\
-3z^2\sqrt{3}(\sqrt{1-z^2} + 1) \\
3z^3 \\
-3z^2(\sqrt{1-z^2} + 1) \\
z\sqrt{3}(2\sqrt{1-z^2} + z^2 + 2) \\
-z^2\sqrt{3}(\sqrt{1-z^2} + 3) \\
3z^3 \\
3z^2(\sqrt{1-z^2} - 1) \\
-z\sqrt{3}(2\sqrt{1-z^2} - z^2 - 2) \\
z^2\sqrt{3}(\sqrt{1-z^2} - 3) \\
3z^3 \\
-3\sqrt{1-z^2}z^2 + 9z^2 + 12\sqrt{1-z^2} + 12 \\
-3z(-z^2 - 2 + 2\sqrt{1-z^2})\sqrt{3} \\
3z^2\sqrt{3}(\sqrt{1-z^2} - 1) \\
3z^3
\end{pmatrix}.
\]

The apparently complicated structure of this result is deceptive, and a perceiveable compactification of these formulae is possible. In [25], we only managed to obtain a partial answer, namely a solution in a hard-to-extrapolate form

\[
|\psi_3\rangle = [u^3, -\sqrt{3}uv^2, \sqrt{3}uv^2, -v^3]^T,
\]

\[
|\psi_2\rangle = [\sqrt{3}uv^2, -(3+r)u, (3-r)v, -\sqrt{3}uv^2]^T, \ldots
\]

A more extrapolation-friendly structure of these formulae is needed. The trial-and-error method led us to success when we applied the identities \( 3 + r \rightarrow u^2 + 2v^2 \) and \( 3 - r \rightarrow 2u^2 + v^2 \).
This finally produced an extrapolation-friendly result. On this basis, we may now conjecture the following general formula:

\[
\begin{pmatrix}
|\psi_{N-1}\rangle \\
|\psi_{N-2}\rangle \\
\vdots \\
|\psi_0\rangle
\end{pmatrix} = \sum_{j=1}^{N} u^{N-j}(-v)^{j-1}M^{(N)}(j).
\]

(10)

The individual matrix coefficients are assumed diagonal \((M^{(N)}(1) = I)\), bidiagonal \((M^{(N)}(2))\), tridiagonal and ‘rhomboidal’ \((M^{(N)}(3))\) etc, ending up with the same antidiagonal \(M^{(N)}(N) = J = \sqrt{I}\) as above.

At \(N = 4\), the validity of this conjecture may be confirmed by the brute-force solution of equation (7). The explicit version of the formula for the left eigenvectors is obtained as follows:

\[
\begin{pmatrix}
|\psi_3\rangle \\
|\psi_2\rangle \\
|\psi_1\rangle \\
|\psi_0\rangle
\end{pmatrix} = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix}
\begin{bmatrix}
0 & 0 & \sqrt{3} & 0 \\
0 & 0 & 0 & \sqrt{3} \\
\sqrt{3} & 0 & 2 & 0 \\
0 & \sqrt{3} & 0 & 0
\end{bmatrix}
\begin{bmatrix}
u^3 \\
\sqrt{3} \\
u \\
\sqrt{3}
\end{bmatrix}
\begin{bmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0
\end{bmatrix}
v^3.
\]

(11)

This result exhibits the expected symmetries as well as the extrapolation-friendly sparse-matrix structure of the individual expansion matrices. At any dimension \(N\), the knowledge of this pattern will decisively facilitate the concrete determination of the numerical values of the matrix elements as well as the ultimate use of equation (8).

4.2. A confirmation of the pattern: \(N = 5\)

At \(N = 5\) our Hamiltonian matrix still fits on the printed page, especially if we abbreviate \(z = uv\),

\[
H^{(5)}(u, v) = \begin{bmatrix}
-4 & 2z & 0 & 0 & 0 \\
-2z & -2 & \sqrt{6}z & 0 & 0 \\
0 & -\sqrt{6}z & 0 & \sqrt{6}z & 0 \\
0 & 0 & -\sqrt{6}z & 2 & 2z \\
0 & 0 & 0 & -2z & 4
\end{bmatrix}.
\]

After all of the symbolic manipulations needed we get the expected extrapolations of the coefficient matrices in (10) at \(N = 5\); accompanied by the ‘missing’, not yet predicted two items

\[
M^{(5)}(2) = \begin{bmatrix}
0 & 2 & 0 & 0 & 0 \\
2 & \sqrt{6} & 0 & 0 & 0 \\
0 & \sqrt{6} & 0 & \sqrt{6} & 0 \\
0 & 0 & \sqrt{6} & 0 & 2 \\
0 & 0 & 0 & 2 & 0
\end{bmatrix},
M^{(5)}(3) = \begin{bmatrix}
0 & 0 & \sqrt{6} & 0 & 0 \\
0 & 3 & 0 & 3 & 0 \\
\sqrt{6} & 0 & 4 & 0 & \sqrt{6} \\
0 & 3 & 0 & 3 & 0 \\
0 & 0 & \sqrt{6} & 0 & 0
\end{bmatrix}.
\]

This observation demonstrates that the move to any higher dimension \(N\) becomes easily implemented via the sparse-matrix ansatz (10). In the same spirit, also the construction of the metric becomes just a matter of very routine linear algebra. The only obstacle emerges due
to the growth of the size of the resulting matrices. As long as they do not fit the printed page anymore, their elements must be displayed, whenever needed, in a suitably compressed form (in a different context, interested readers may find a sample of such a compression in [29]).

5. Summary

In contrast to the classical Thom’s theory of catastrophes [26], it seems rather difficult to formulate the very purpose of its sufficiently satisfactory quantum counterpart, not even speaking about its mathematics itself. In this context, we described here just one of many possible approaches to the problem.

During the preparatory and purely formal considerations we imagined that from the pragmatic, phenomenological point of view, a smooth change of a suitable parameter may lead, in many models, to an abrupt complexification of some energy level or levels, i.e. to an abrupt loss of their observability status. This is what we decided to call here a QC.

In our text, we simulated the QC process (during which the parameter crosses its exceptional-point value $\lambda(\text{EP}) \in \partial D(\text{physical})$) via suitable toy models. Our motivation was obvious; as long as the textbooks on quantum theory rarely cover the QC phenomena in a systematic manner, the field may be perceived as open to new theoretical developments. In parallel, the recent reformulations of the representation theory characterized by the use of a non-trivial inner product in the physical Hilbert space appeared suitable for the purpose. Last but not the least, we felt encouraged by the recent growth of activity in experimental physics where the question of relevance of Kato’s exceptional points in quantum phenomenology and measurements has been revitalized in several directions [10].

An overall mathematical difficulty of the problem (and, in particular, of its more sophisticated, fine-tuned $N = 2J \geq 4$ versions) exposed us to the necessity of choice between a phenomenological numerical study of some realistic models (this is the way we choose in our recent papers [25]) and an instructive non-numerical description of some carefully selected toy models.

In this paper, we opted for the latter. During our lucky choice of the family of models we felt attracted by the unexpectedly friendly nature of their spectra and of their geometry in the space of the dynamics-determining parameters (this is an older result recollected in appendix B). In this text, we complemented these observations by the discovery of an equally unexpected friendliness of these models from the point of view of the systematic construction and extrapolation of their metrics to all dimensions.

In summary, we believe that our toy models will offer useful guidance for continued research in the field of QC, not only due to the feasibility of our present constructions but also due to the transparency of the matrix structure of their metrics $\Theta^{(N)}$. Indeed, as long as these matrices specify the inner products in the physical Hilbert spaces of states $\mathcal{H}^{(S)}$, their compact form opens the way not only towards a facilitated physical probabilistic interpretation of the quantum systems in question but also, as we demonstrated, to an unexpectedly transparent matrix structure of other, generic crypto-Hermitian observables.

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Appendix A. Crypto-Hermitian Hamiltonians

In [4], we introduced the notation in which the same state $\psi$ of a quantum system in question is represented by three alternative ket-vector elements $|\psi^{(j)}\rangle$ of the respective different Hilbert spaces $\mathcal{H}^{(j)}$ with superscripts $j = P, F, S$. The meaning of these superscripts [7] is given by the following scheme:

$$
\text{[P] - primitive physical space} \quad \xrightarrow{\text{simplification}} \quad \text{[F] - false space} \quad \xrightarrow{\text{Hermitization}} \quad \text{[S] - standard physical space} \quad \xleftarrow{\text{unitary equivalence}}
$$

The role of the arrows is the following. Firstly, the ‘simplification’ arrow means that the presumably complicated ket $|\psi^{(P)}\rangle$ is redefined as the so-called Dyson’s map of a simpler ket $|\psi^{(F)}\rangle$, namely $|\psi^{(P)}\rangle = \Omega |\psi^{(F)}\rangle$. Secondly, the bidirectional ‘unitary-equivalence’ relationship requirement implies that for non-unitary $\Omega$s the Hilbert space $\mathcal{H}^{(S)}$ must be endowed with a non-trivial metric $\Theta = \Omega^\dagger \Omega$ [2]. Thirdly, the ‘Hermitization’ arrow should be read as a replacement of the conventional Hermitian conjugation $H \rightarrow H^\dagger$ using trivial $\Theta^{(F)} = I$ by the crypto-Hermitian conjugation $H \rightarrow H^{\dagger} := \Theta^{-1} H^\dagger \Theta$ using unconventional, non-trivial $\Theta = \Theta^{(S)} \neq I$.

One tacitly assumes that the given Hamiltonian $H = H(\lambda)$ has a real spectrum (i.e. that $\lambda \in D^{(\text{physical})}$) and that the selected metric $\Theta$ is a bounded, invertible and positive-definite operator. In such a dynamical regime, there is no real reason for calling our Hamiltonian (defined as acting in both of the spaces $\mathcal{H}^{(F, S)}$) non-Hermitian. It is more natural to declare $\mathcal{H}^{(F)}$ a false or manifestly unphysical space. Unfortunately, this space $\mathcal{H}^{(F)}$ is precisely the space in which we make all calculations. Often, it is chosen in the most common form $L^2(\mathbb{R})$ in which the kets $|\psi\rangle$ are represented by the quadratically integrable functions $\psi(x)$, where the real variable $x$ does not represent the observable position [30].

The latter conventions often become the source of misunderstandings. For this reason, the Hamiltonian $H$ (which is, in full compatibility with the first principles of quantum theory, Hermitian in its proper and manifestly physical Hilbert space $\mathcal{H}^{(S)}$) should better be called crypto-Hermitian (this emphasizes the not too frequently encountered fact that the correct physical metric is chosen non-trivial, $\Theta^{(S)} \neq I$).

In the literature, the crypto-Hermitian operators $H$ are also known as quasi-Hermitian. In this case one should have in mind the newer definition used in [2] and not the older, more abstract one which was introduced, by Dieudonné [7], in the context of pure mathematics.

The majority of physicists who write about the subject think that one should put the main emphasis upon the practical aspects of the quantum model in question. One of these aspects is that the concrete physical predictions (e.g., the spectra of bound-state energies) may still be based on the calculations performed in the friendly space representation of $\psi$ (and then just transferred to physical $\mathcal{H}^{(S)}$ for interpretation purposes). This explains why one finds the crypto-Hermitian (i.e. in their proper space $\mathcal{H}^{(S)}$, Hermitian) operators $H(\lambda)$ with real spectra still called, in a large number of truly serious and influential papers, ‘non-Hermitian’.

Naturally, the situation changes when the parameter $\lambda$ leaves the physical domain $D^{(\text{physical})}$ and when at least some of the energies become complex. Then, the name ‘non-Hermitian $H(\lambda)$’ becomes fully deserved. Indeed, in our three Hilbert-space scheme of [4], two out of the three Hilbert spaces (namely $\mathcal{H}^{(P)}$ and $\mathcal{H}^{(S)}$) simply cease to exist. One must find another, open- or sub-system [5] or resonance theory [6] physical interpretation of the quantum system in question.
At \( \lambda = \lambda^{(EP)}(\partial D^{(\text{physical})}) \), i.e. at the exceptional, QC values of the parameters there also does not exist any reasonable physical interpretation of the physical system under consideration. In particular, the metric ceases to exist so that the system does not possess any standard quantum interpretation. The measurability status of the energies survives (they are still all real), but some vital dynamical information is missing. The mechanism of the QC is unspecified. If asked for, it must be added via an appropriate enrichment of the model. Typically, such enrichments are in active use in magnetohydrodynamics [14] or in laser physics [31].

### Appendix B. Solvable \( N \times N \) models

The study of properties of the general \( N \times N \) Hamiltonians \( H^{(N)} \) remains non-numerical up to the dimension \( N = 4 \), i.e. up to the secular polynomials of the fourth order (cf [19]). At higher \( N \), the spectra are usually studied by numerical or perturbation methods. In the latter context, the most popular models are the so-called anharmonic oscillators

\[
H^{(\text{AHO})}(g) = \begin{bmatrix}
1 & 0 & 0 & \ldots \\
0 & 3 & 0 & \ldots \\
0 & 0 & 5 & \ldots \\
\vdots & \vdots & \vdots & \ddots
\end{bmatrix} + \mathcal{O}(g),
\]

which were chosen, in [22], as a starting point of a simplification intended to lead to non-numerically tractable toy models.

We restricted our attention to the tridiagonal and antisymmetric perturbations. We also truncated our Hamiltonians to \( N \times N \) matrices. With even \( N = 2J \) this yielded the sequence

\[
\tilde{H}^{(2)}_{(a)} = \begin{bmatrix} 1 & a \\ -a & 3 \end{bmatrix}, \quad \tilde{H}^{(4)}_{(a,b,c)} = \begin{bmatrix}
1 & b & 0 & 0 \\
-b & 3 & a & 0 \\
0 & -a & 5 & c \\
0 & 0 & -c & 7
\end{bmatrix}, \ldots.
\]

Finally, we shifted the energy scale and imposed an additional symmetry on perturbations. For the resulting set of toy-model Hamiltonians

\[
H^{(2)} = \begin{bmatrix} -1 & a \\ -a & 1 \end{bmatrix}, \quad H^{(4)} = \begin{bmatrix}
-3 & b & 0 & 0 \\
-b & -1 & a & 0 \\
0 & -a & 1 & b \\
0 & 0 & -b & 3
\end{bmatrix}, \ldots. \quad (B.1)
\]

the secular equations simplified so that the bound of feasibility of constructive considerations grew up to \( N = 11 \) [24]. Still, the comparatively large number \( J = \lfloor N/2 \rfloor \) of variable matrix elements kept the model sufficiently flexible and well adapted to many phenomenological needs [17, 18, 20].

In the language of mathematics, the main results concerned the conditions of the reality of the energy roots. The proofs have been rendered possible by the computer-assisted symbolic manipulations. A brief summary of some technical aspects of these manipulations may be found in [32]. In the second stage of developments, we reanalyzed the secular equations and sought for the strong-coupling extremes of the \( J = \lfloor N/2 \rfloor \)-dimensional real domain \( D^{(\text{physical})} \).
As a result, we obtained the series of matrices representing the degenerate Hamiltonians at the QC instant:

\[
H_{QC}^{(2)} = \begin{bmatrix}
1 & 1 \\
-1 & -1
\end{bmatrix}, \quad H_{QC}^{(4)} = \begin{bmatrix}
3 & \sqrt{3} & 0 & 0 \\
-\sqrt{3} & 1 & 2 & 0 \\
0 & -2 & -1 & \sqrt{3} \\
0 & 0 & -\sqrt{3} & -3
\end{bmatrix}, \ldots
\]

Elements \(a^{(QC)}, b^{(QC)}, \ldots\) were determined, within the Gröbner-basis elimination method, as roots of a polynomial. Although the degree of this polynomial was quickly growing with \(J\) (e.g., it was already 17 at \(J = 4\) [32]), we still managed to find and prove the general extrapolation pattern. The closed-formula version of \(a^{(QC)}, b^{(QC)}, \ldots\) was found for all \(N\), even and odd (cf [22]).

Although the physical meaning of the model is, naturally, completely lost in its fully degenerate QC limit, we specified our next task as the reconstruction of the standard probabilistic interpretation of the system in the close vicinity of this singularity. We revealed that for such a purpose it makes sense to reparametrize our original family of Hamiltonians in terms of a distance \(\lambda > 0\) of the Hamiltonian from its exceptional-point extreme at \(\lambda^{\text{ep}} = 0\). At \(N = 2\) this was easy. We merely replaced the above-mentioned one-parametric matrix \(H_{(\omega)}^{(2)}\) by its reparametrized alternative

\[
H_{(\omega)}^{(2)}(\lambda) = \begin{bmatrix}
1 & \sqrt{1-\lambda A} \\
-\sqrt{1-\lambda A} & -1
\end{bmatrix}
\]

depending just on the product \(A \lambda\). At \(N = 4\), one easily arrives at the less trivial Hamiltonian

\[
H_{(\omega)}^{(4)}(\lambda) = \begin{bmatrix}
3 & \sqrt{3}\sqrt{1-\lambda - B\lambda^2} & 0 & 0 \\
-\sqrt{3}\sqrt{1-\lambda - B\lambda^2} & 1 & 2\sqrt{1-\lambda - A\lambda^2} & 0 \\
0 & -2\sqrt{1-\lambda - A\lambda^2} & -1 & 0 \\
0 & 0 & -\sqrt{3}\sqrt{1-\lambda - B\lambda^2} & -3
\end{bmatrix},
\]

etc.

In [23], we managed to prolong the series of these reparametrizations to all \(N = 2J\) or \(N = 2J + 1\). We revealed that in the new parametrization of the vicinity of the QC extreme, the geometry of the interior of the domain \(D_{\text{physical}}^{(\text{physical})}\) becomes trivial, namely flat and layer-shaped. This means that in the QC regime, our \(J\)-dimensional domain \(D_{\text{physical}}^{(\text{physical})}\) becomes characterized by the mere single inequality at any \(J\). Thus, excluding the first, slightly anomalous \(N = 2\) case we obtained the sequence of inequalities

\[-\mu_2^2 \leq 2A/2 - B \leq +\nu_2^2, \quad N = 4,\]

\[-\mu_4^2 \leq 6A/2 - 4B + C \leq +\nu_6^2, \quad N = 6,\]

\[-\mu_8^2 \leq 20A/2 - 15B + 6C - D \leq +\nu_8^2, \quad N = 8,\]

etc, with \(\mu_4 = 1/2\) and \(\nu_4 = 2/3\), etc. It is worth noting that the coefficients in these layer-specifying inequalities are just the combinatorial numbers \((N-2)\).

In our very recent application-oriented paper [25] we decided to choose just the simplest, one-parametric subset of the \(J\)-parametric Hamiltonian-matrix series \(H_{(\omega)}^{(N)}(\lambda)\) of [23]. For the sake of simplicity, we selected \(A = 1\) at \(J = [N/2] = 1\) and \(A = B = \cdots = 0\) at \(J \geq 2\). Under these assumptions, we were able to complete the task and construct the metrics \(\Theta\), in a ‘brute-force’ manner, up to \(N = 8\).
A strong motivation for our present return to the underlying mathematics may be seen in the fact that the corresponding energy eigenvalues were found to form the equidistant set at any positive \( N \) and \( \lambda \):

\[
E_n = (2n + 1 - N)\sqrt{\lambda}, \quad n = 0, 1, \ldots, N - 1.
\]  

(B.2)

Such an unexpected and important merit of the model appeared to be in a sharp contrast with the feasibility limitations to \( N \lesssim 8 \) as encountered in [25]. In this sense, our present paper just solves this puzzle and outlines the pattern of extension of the construction of the metric to any dimension \( N \).

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