Admissible perturbations and false instabilities in $\mathcal{PT}$-symmetric quantum systems

Miloslav Znojil*
Nuclear Physics Institute of the CAS, Hlavní 130, 250 68 Řež, Czech Republic

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One of the most characteristic *mathematical* features of the $\mathcal{PT}$-symmetric quantum mechanics is the explicit Hamiltonian dependence of its physical Hilbert space of states $\mathcal{H} = \mathcal{H}(H)$. Some of the most important *physical* consequences are discussed, with emphasis on the dynamical regime in which the system is close to phase transition. Consistent perturbation treatment of such a regime is proposed. An illustrative application of the innovated perturbation theory to a non-Hermitian but $\mathcal{PT}$-symmetric user-friendly family of J-parametric "discrete anharmonic" quantum Hamiltonians $H = H(\vec{\lambda})$ is provided. The models are shown to admit the standard probabilistic interpretation if and only if the parameters remain compatible with the reality of the spectrum, $\vec{\lambda} \in \mathcal{D}^{(\text{physical})}$. In contradiction to conventional wisdom, the systems are then shown to be stable with respect to admissible perturbations, inside the domain $\mathcal{D}^{(\text{physical})}$, even in the immediate vicinity of the phase-transition boundaries $\partial\mathcal{D}^{(\text{physical})}$.

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I. INTRODUCTION

The conventional textbook formulations of quantum theory [1] were recently complemented by several innovative pictures of the quantum world, which may be characterized as a quasi-Hermitian [2], alias $\mathcal{PT}$-symmetric [3], alias pseudo-Hermitian, representation of quantum mechanics [4]. Except for a few technical differences (cf. several more mathematical updates of the reviews in [5]), all of these methodical innovations were originally aimed at an amendment of the description of the stable bound states in a closed (i.e., unitary) quantum system, be it a ferromagnet [6], an atomic nucleus [7], or a toy-model field [8,9]. All of these innovative, sophisticated treatments of quantum reality remained compatible with the quantum theory of textbooks. Still, the mere rearrangement of mathematical ingredients helped to resolve several old theoretical problems, say, in relativistic quantum mechanics [10] or in our understanding of the mechanisms of the quantum phase transitions [11,12].

The not-quite-expected user friendliness of the new formalism [let us call it here, for the sake of definiteness, $\mathcal{PT}$-symmetric quantum mechanics (PTQM)] inspired huge parallel progress in multiple neighboring branches of physics. It ranged from the more traditional quantum theory of resonances in atoms, molecules, and nuclei (and, in general, in any open quantum system; cf. [13,14]) up to the very successful modern developments in experimental phenomenology within classical physics and, first of all, in optics [15]. In the present paper, we will return to the narrower, old-fashioned versions of the PTQM philosophy, the basic ideas of which may be traced back, in retrospective, to the Dyson's [6] replacement of a given, "realistic" Hamiltonian $\mathfrak{h} = \mathfrak{h}^\dagger$ by its manifestly non-Hermitian isospectral partner,

$$H = \Omega^{-1}\mathfrak{h}\Omega \neq H^\dagger, \quad \Omega^\dagger\Omega \neq I. \tag{1}$$

The Dyson's key idea was that whenever we manage to choose the invertible nonunitary mapping Ω as carrying a nontrivial information about the system, we may make the "preconditioned" quasi-Hermitian Hamiltonian (1) computation friendlier. The price to pay seemed reasonable. In place of staying in the conventional picture (where the prediction of the measurements is given by the overlaps $\prec\psi|\mathfrak{q}|\psi\succ$, where $|\psi\succ$ is the wave function while symbol $\mathfrak{q}$ denotes the observable of interest [16]), one merely changes the Hilbert space (cf., e.g., [17] for the more detailed explanations) and one evaluates the analogous overlaps,

$$\langle\psi|\Theta\, Q|\psi\rangle, \quad Q = \Omega^{-1}\mathfrak{q}\Omega. \tag{2}$$

Here, the symbol $\Theta = \Omega^\dagger\Omega = \Theta^\dagger > 0$ denotes the physical Hilbert-space metric [2], while the time evolution of the wave functions is assumed to be generated by the non-Hermitian Hamiltonian (1) with a real spectrum,

$$i\frac{d}{dt}|\psi\rangle = H\,|\psi\rangle. \tag{3}$$

In applications, the Dyson's trick proved extremely successful, e.g., in the computational nuclear physics of heavy nuclei [7]. Still, it did not inspire any immediate developments in the abstract quantum theory itself. One of the reasons can be seen in the manifest non-Hermiticity of the Hamiltonian,

$$H^\dagger = \Theta\, H\, \Theta^{-1}. \tag{4}$$

Indeed, the naive use of such a "quasi-Hermitian" generalization of the conventional Hermiticity opened the Pandora's box of mathematical difficulties [18,19]. Most of these questions are open or remain only partially answered at present [20].

In the context of physics, fortunately, people managed to circumvent the danger along two alternative lines. In one of these directions, it was Bender and Boettcher [11] who noticed that for a family of benchmark toy-model ordinary differential

*znojil@ujf.cas.cz

operator examples,

$$H^{(BB)} = -\frac{d^2}{dx^2} + x^2(ix)^\delta, \ \ \delta > 0, \tag{5}$$

the spectrum is real. On this ground, it has been conjectured that the Dyson's mapping $\mathfrak{h} \to H^{(BB)}$ of Eq. (1) could have been inverted, returning us, in principle at least, to the safe waters of the traditional unitary quantum mechanics. An alternative, mathematically safer approach to the problem has been accepted in the context of nuclear physics. The authors of Ref. [2] noticed that the major part of the formal difficulties disappears whenever all of the eligible operators of observables are required to be bounded, i.e., $H \in \mathcal{B}(\mathcal{H})$, etc.

Here we shall follow the latter strategy, leaving the mathematically more complete treatment of unbounded models to mathematicians [21]. Our decision will keep the necessary mathematical manipulations on an elementary level, facilitating our study of the question of the stability of a generic $\mathcal{PT}$-symmetric quantum system with respect to its small perturbations. Our assumptions will be shown to be satisfied, in Sec. II, by a family of illustrative $\mathcal{PT}$-symmetric finite-dimensional Hamiltonians $H = H(\vec{\lambda}) \in \mathcal{B}(\mathcal{H})$ taken from Refs. [22,23]. The variability of the physical parameters of the models is confined to domain $\mathcal{D}^{(\text{physical})} \subset \mathbb{R}^J$ which is, at any integer parameter $J = \dim \mathcal{D}$, *bounded*. The bound-state energies are real and observable inside, and only inside, this domain.

The discrete anharmonic form endows our benchmark oscillators with a remarkable phenomenological as well as formal appeal. On the formal side, every Hamiltonian of the class will be real, asymmetric, tridiagonal, and particularly suitable for an exhaustive discussion of stability with respect to perturbations. On the side of phenomenology, our higher-dimensional matrices $H^{(N)}$ will be shown to be interesting as an interpolation between the two extreme scenarios, viz., between the weak- and strong-anharmonicity dynamical regimes. In the former case, one can split $H = H^{(HO)} + H^{(\text{perturbation})}$ and use the routine methods, appreciating an equidistant spectrum in the diagonal unperturbed harmonic-oscillator-like matrix $H^{(HO)}$. The much more complicated analysis of the latter case is our present interest.

For our stability-investigation purposes, the choice of the illustrative toy models initially seemed to be far from optimal. The main reason was explained in [24]. Fortunately, the removal of the obstacle (which lies in the necessity of construction of the so-called transition matrices) appeared feasible. The point will be presented and explained in Sec. III. Another formal merit of the model lies in the boundedness of its parametric domains $\mathcal{D}^{(\text{physical})}$. This feature (proven in [22]) is welcome as it makes the phase-transition boundaries $\partial\mathcal{D}^{(\text{physical})}$ of the stability of the system experimentally as well as theoretically accessible. It is worth adding that in mathematics, the elements of the boundary $\partial\mathcal{D}$ were given the name of "exceptional points" (EP) [19]. The original motivation of the introduction of the concept of EPs appeared in perturbation theory, where the domains $\mathcal{D}$ of parameters were usually considered complex and, in general, unbounded [19]. In the prevalent Taylor-series form of perturbation expansions, the knowledge of the (usually, isolated) EP singularities in the complex domains of couplings then offered a key to the rigorous determination of the radius of the convergence of the series.

In the applied perturbation-expansion considerations, the relevant EPs were almost never real. This reflected the virtually exclusive interest in self-adjoint Hamiltonians (see, e.g., the dedicated special issue [25] from 1982 for illustration). In the broader context of physics it soon became clear that the use of EPs, real or complex, may go far beyond their auxiliary role in perturbation theory. One of the best summaries of the situation was provided during the 2010 international conference "The Physics of Exceptional Points" in Stellenbosch [26]. All of the titles of the invited talks shared the generic clause "Exceptional points and ...." The list of the samples and reviews of *different* physical applications of the EP concept proved impressive. It involved atoms and molecules in external fields, light-matter interactions, and the processes of photodissociation, quantum phase transitions, and the many-particle models, the questions of stability with illustrations in magnetohydrodynamics, the results of the experiments with the microwave billiards and microdisk cavities, plus, last but not least, the study of the Bose-Einstein condensates and of the generic quantum phenomena related to the spontaneous breakdown of $\mathcal{PT}$ symmetry.

Such a diversity enhances the importance of the EPs in physics [27]. At the same time, the necessary *ad hoc* adaptations of the related mathematics could lead to misunderstandings. We shall restrict attention, therefore, to the specific subset of applications in which a closed quantum system exhibits a spontaneously unbroken $\mathcal{PT}$ symmetry. We shall assume that the domain $\mathcal{D}$ of variable parameters as well as its EP boundaries are real and bounded. This will enable us to construct a strong-coupling perturbation recipe in which

$$H(\vec{\lambda}) = H(\vec{\lambda}^{(EP)}) + V_{(\text{perturbation})}. \tag{6}$$

This means that the unperturbed Hamiltonian will already be manifestly unphysical and nondiagonalizable, with its parameters $\vec{\lambda}^{(EP)} \in \partial\mathcal{D}^{(\text{physical})}$ not lying inside the domain of applicability of quantum theory. In Sec. IV, we shall clarify the apparent contradiction by studying, in detail, the most characteristic case of the unperturbed Hamiltonian containing just the single Jordan block of a finite dimension. Admitting just the finite values $K < \infty$ of this dimension, we will simplify the technicalities and we will explain the main specific features of the resulting singular perturbation theory. We will show that even when the unperturbed Hamiltonian has the nondiagonal, unphysical, Jordan-block form, the evaluation of perturbation corrections themselves remains feasible, comparatively user friendly, and fully analogous to the more conventional degenerate versions of the textbook Rayleigh-Schrödinger perturbation theory.

The presentation of these methodical results will be complemented, in Sec. V, by the explicit description of perturbation approximations for a few low-dimensional models. After an exhaustive analysis of these toy models living in finite-dimensional Hilbert spaces, we will be able to conclude that the quantum unitary-evolution physics, which is "hidden" behind the non-Hermitian operators of observables, is sound and acceptable. In subsequent Sec. VI, devoted to discussion, we shall point out, in particular, that the problem of the sensitivity of the results to perturbations is highly nontrivial and that the key role is played by a self-consistently determined, interaction-dependent measure ϵ of the smallness of the perturbation.

The last Sec. VII is the summary. We will reemphasize there that one of the most important consequences of the constructive use of the perturbation-approximation strategy near the EP singularities should be seen in the resolution of many puzzles caused by the non-Hermiticity of the operators and matrices [28]. In the PTQM setting, the situation is still rather specific because the new factor which enters the game is the metric Θ. Whenever it exists, i.e., whenever the evolution remains unitary and whenever $\mathcal{PT}$ symmetry remains unbroken, the nontriviality of the metric induces an anisotropy in the physical Hilbert space $\mathcal{H}$. In other words, in the PTQM setting, the physical quasi-Hermiticity constraints upon perturbations are counterintuitive. Still, from the point of view of the control of stability, these "hidden Hermiticity" constraints remain fully analogous to the more traditional Hermiticity constraints encountered in conventional quantum mechanics.

II. BENCHMARK MODEL

In Ref. [28], one finds a number of persuasive examples in which the knowledge of the spectrum $\sigma(H)$ offers extremely poor and unreliable information about the results of the evolution which is controlled by a manifestly non-Hermitian (i.e., in general, non-normal) generator H in Eq. (3). In these examples, the key role is played by the so-called pseudospectra $\sigma_\epsilon(H)$. They are recommended as the main mathematical tool of an amendment of the information. In a broad variety of applications, this tool proved able to characterize the consequences of the generic small perturbations, i.e., the consequences of the replacement of H by the set of its perturbed versions $H + V$ such that V is small, $||V|| < \epsilon$.

The main weakness of this approach is that it is not applicable to the PTQM models in which the Hilbert-space metric is Hamiltonian dependent, i.e., not only nontrivial [i.e., such that $\Theta = \Theta(H) \neq I$], but also anisotropic [i.e., such that its spectrum $\sigma(\Theta)$ is nondegenerate]. Moreover, the construction of the metric appears prohibitively complicated in the prevailing majority of the examples with nontrivial pseudospectra. This implies that the only feasible studies of the influence of perturbations seem to be restricted to the matrix (i.e., finite-dimensional) models. Indeed, they trivially satisfy the above-discussed physical (i.e., bounded-operator) constraints. In addition, the use of the finite, parameter-dependent matrices $H^{(N)}(\lambda)$ will also make the fundamental linear algebraic time-independent Schrödinger equation

$$H^{(N)}(\lambda)\,|\psi_n^{(N)}(\lambda)\rangle = E_n^{(N)}(\lambda)\,|\psi_n^{(N)}(\lambda)\rangle,\quad n = 0,1,\ldots,N-1, \tag{7}$$

exactly solvable (cf., e.g., [29]). In what follows, we shall therefore accept such a strategy of circumventing the functional-analytic subtleties.

A. Weakly non-Hermitian dynamical regime

For illustrative purposes, we shall use the family

$$H^{(2)}(a) = \begin{bmatrix} 1 & a \\ -a & -1 \end{bmatrix},\quad H^{(3)}(a) = \begin{bmatrix} 2 & a & 0 \\ -a & 0 & a \\ 0 & -a & -2 \end{bmatrix},$$

$$H^{(4)}(a,b) = \begin{bmatrix} 3 & b & 0 & 0 \\ -b & 1 & a & 0 \\ 0 & -a & -1 & b \\ 0 & 0 & -b & -3 \end{bmatrix},$$

$$H^{(5)}(a,b) = \begin{bmatrix} 4 & b & 0 & 0 & 0 \\ -b & 2 & a & 0 & 0 \\ 0 & -a & 0 & a & 0 \\ 0 & 0 & -a & -2 & b \\ 0 & 0 & 0 & -b & -4 \end{bmatrix},\ldots, \tag{8}$$

of the real and finite-dimensional tridiagonal matrices. This set was introduced in Ref. [22]. Besides the user-friendly nature of these non-Hermitian but $\mathcal{PT}$-symmetric real toy-model Hamiltonians, their other merits lie in an enormous phenomenological flexibility (i.e., multiparametric variability) and in their sparse-matrix tridiagonality with an intuitive nearest-neighbor-interaction appeal. An additional benefit is that the set $\partial\mathcal{D}$ of all of the relevant phase-transition points of these models has a smooth and topologically trivial shape of surface of a certain deformed hypercube with protruded vertices at any matrix dimension $N < \infty$ (cf. the proof in [23]).

From the conventional point of view, all of the weakly non-Hermitian forms of Hamiltonians (8), i.e., of the multiparametric illustrative tridiagonal matrices

$$H^{(2J)} = \left[\begin{array}{cccc|cccc} 2J-1 & z & 0 & \ldots & & & & \\ -z & \ddots & \ddots & \ddots & \vdots & & & \\ 0 & \ddots & 3 & b & 0 & \ldots & & \\ \vdots & \ddots & -b & 1 & a & 0 & \ldots & \\ \hline & \ldots & 0 & -a & -1 & b & 0 & \ldots \\ & & \ldots & 0 & -b & -3 & \ddots & \\ & & & \vdots & \ddots & \ddots & \ddots & z \\ & & & & \ldots & 0 & -z & 1-2J \end{array}\right] \tag{9}$$

and

$$H^{(2J+1)} = \left[\begin{array}{ccc|c|ccc} 2J & z & 0 & 0 & 0 & 0 & 0 \\ -z & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & \ddots & 2 & a & 0 & 0 & 0 \\ \hline 0 & 0 & -a & 0 & a & 0 & 0 \\ \hline 0 & 0 & 0 & -a & -2 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & z \\ 0 & 0 & 0 & 0 & 0 & -z & -2J \end{array}\right], \tag{10}$$

can be perceived as small and fully regular perturbations of certain shifted and truncated toy-model harmonic oscillators having the strictly equidistant spectrum. All of these multiparametric toy models are eligible as the generators of the standard unitary quantum evolution.

B. Strongly non-Hermitian regime

The energy spectra of models (9) and (10) were proven real and nondegenerate (i.e., in principle, observable) if and only if the parameters lie inside a compact physical stability domain $\mathcal{D}^{(J)}$ [22]. The boundary of this domain of stability (i.e., the hypersurface $\partial\mathcal{D}$) has been shown to be compact. Its extreme points of maximal non-Hermiticity were localized, non-numerically, as lying on a circumscribed hypersphere (at odd $N = 2J + 1$) or on a prolate hyperellipsoid (at even $N = 2J$).

In the more detailed study [23], it has been found that the separation of the Hamiltonians into two special cases (9) and (10) by the parity of their dimension N is not needed. After a renumbering $z \to g_1$, ..., $b \to g_{J-1}$ and $a \to g_J$ of the couplings, we introduced a redundant parameter $t \in (0,1)$ (meaning "time" or "strength of perturbation") and we admitted a "slow" (presumably, adiabatic) variability of the couplings,

$$g_n = g_n(t) = g_n(0)\sqrt{[1-\xi_n(t)]},$$
$$\xi_n(t) = t + t^2 + \cdots + t^{J-1} + G_n t^J \in (0,1), \tag{11}$$

$$g_n(0) = \sqrt{n\,(N-n)}, \quad n = 1,2,\ldots,J. \tag{12}$$

This enabled us to specify the shape of the boundary using the computer-assisted algebra.

During all of our considerations concerning the *small, regular* non-Hermitian, alias quasi-Hermitian, perturbations in Eqs. (9) and (10), we have to keep in mind that our $\mathcal{PT}$-symmetric Hamiltonian H just provides one of the user-friendliest representations of some hypothetical, prohibitively complicated, but entirely traditional self-adjoint operator $\mathfrak{h}$ (cf. Eq. (1) or Ref. [2]). Thus, our present non-Hermitian but $\mathcal{PT}$-symmetric time-evolution Schrödinger equation (3) must be perceived as strictly equivalent to its hypothetical and presumably untractable textbook alternatives, with the equivalence between the two pictures determined by their mutual "Dyson's" mapping (1). The difference between the use of H and $\mathfrak{h}$ is, in some sense, purely technical. Still, a strong preference of the use of non-Hermitian H may be recommended whenever the non-Hermiticities become large, i.e., typically when the parameters get close to the EP phase-transition boundary of quantum stability.

The strong-coupling version of models (9) and (10) has been found to be unitary (i.e., the reality of the spectrum was guaranteed) if and only if the parameters lie inside a physical domain $\mathcal{D}^{(J)} \subset \mathbb{R}^J$ [22]. All of the exceptional points forming the quantum phase-transition boundary $\partial\mathcal{D}^{(J)}$ could have been classified by the number K of the energy levels which merge at them and, subsequently, complexify. Thus, at $J = 1$, the domain $\mathcal{D}^{(J)}$ is an interval (with the two energies merging at its two ends); at $J = 2$, the domain $\mathcal{D}^{(J)}$ is a deformed square with the pairs of energies merging at its edges and with all four energies merging at its four vertices; and at $J = 3$, we deal with a deformed cube with protruded edges and protruded vertices, etc.

In such a visualization of the guarantee of unitarity, the maximally non-Hermitian extreme taking place at a vertex represents the merger of the set of energy levels degenerating to a single real value, gauged, for simplicity, to zero. This is paralleled by the convergence of every Hamiltonian in the list (8) to the respective Jordan-block-equivalent matrix,

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

$$H^{(4)}_{(EP)} = \begin{bmatrix} 3 & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & 1 & 2 & 0 \\ 0 & -2 & -1 & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & -3 \end{bmatrix},$$
$$H^{(5)}_{(EP)} = \begin{bmatrix} 4 & 2 & 0 & 0 & 0 \\ -2 & 2 & \sqrt{6} & 0 & 0 \\ 0 & -\sqrt{6} & 0 & \sqrt{6} & 0 \\ 0 & 0 & -\sqrt{6} & -2 & 2 \\ 0 & 0 & 0 & -2 & -4 \end{bmatrix}, \tag{13}$$

etc. Now, we will ask what happens in the vicinity of these strong-coupling limiting extremes under perturbations, provided that we stay inside the physical domain $\mathcal{D}$ of parameters.

III. PERTURBATION-INDEPENDENT TRANSITION MATRICES

Let us first recall the definition

$$HQ = QS \tag{14}$$

of the Jordan-block representative S of a given non-Hermitian matrix H. In this relation, the intertwiner Q is called the transition matrix.

A. Solvable model in two dimensions

In the limit $a \to 1$, the first item in the sequence of real matrices (8) acquires, after an auxiliary shift of spectrum s, the most elementary tilded form,

$$H^{(2)}(a) + sI \to \widetilde{H}_0 = \begin{bmatrix} -1+s & 1 \\ -1 & 1+s \end{bmatrix}. \tag{15}$$

The tilde gets removed when we use prescription (14) and move to the Jordan-block representative $S = Q^{-1}\widetilde{H}_0 Q = H_0$ of the unperturbed Hamiltonian, with

$$Q = Q^{(2)}_{(EP)} = \begin{bmatrix} 1 & 1 \\ -1 & 0 \end{bmatrix}, \quad H_0 = H^{(2)}_0 = \begin{bmatrix} s & 1 \\ 0 & s \end{bmatrix}. \tag{16}$$

In time-independent Schrödinger equation (7), we now abbreviate $|\psi_1\rangle = x$ and $|\psi_2\rangle = y$. For any $H = H_0 + W$, i.e., in *any* vicinity of the Jordan block $H^{(2)}_0$, we can now assume that there exists a measure $\lambda \ll 1$ of the smallness of the perturbation, $W_{m,n} = O(\lambda)$. Then, the entirely general real form of the perturbation,

$$W = \begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix}, \tag{17}$$

can be inserted in Schrödinger equation (7). This makes it equivalent to the two linear relations

$$(\alpha - \epsilon)x + (1+\beta)y = 0,$$
$$\gamma\, x + (\delta - \epsilon)y = 0.$$

We eliminate $y = -(\alpha - \epsilon)x/(1+\beta)$ from the first line, insert it in the second line, and solve for the *exact* energy,

$$\epsilon_\pm = 1/2\,\delta + 1/2\,\alpha \pm 1/2\sqrt{\delta^2 - 2\,\delta\,\alpha + \alpha^2 + 4\,\gamma + 4\,\gamma\,\beta}$$
$$= \pm\sqrt{\gamma} + O(\lambda).$$

The following conclusions are imminent.

(i) Models with vanishing $\gamma = 0$ are less interesting and not to be discussed immediately.

(ii) For the *negative* parameters $\gamma < 0$ in the perturbation, we get the *manifestly complex* energies. The unitarity and stability will be lost. This is true for an arbitrarily small size of the perturbation when measured in an usual manner, i.e., in terms of any conventional norm.

(iii) For *positive* $\gamma > 0$, the first-order corrections are real, $\epsilon_\pm = \pm\lambda^{1/2} + O(\lambda)$. Thus, the parameter lies inside $\mathcal{D}$ and the quantum system itself remains stable, in the leading-order approximation at least.

(iv) In the higher-order computations, it will be sufficient to replace the standard Taylor-series perturbation-series ansatz by the Puiseux series expansion in the powers of $\lambda^{1/2}$ (cf. also Ref. [30]).

B. Tridiagonal nondiagonalizable EP Hamiltonians

The passage through a phase-transition interface is equivalent to the coincidence of parameter λ with its exceptional-point value $\lambda^{(EP)}$. In this limit, one observes a confluence of eigenenergies *and also* of the related eigenvectors. The diagonalizability of the Hamiltonian is lost. A number of illustrative examples may be found in Kato's book [19]. Let us recall that for a Hermitian Hamiltonian $H(\lambda)$, the EP singularities $\lambda^{(EP)}$ will be complex. They will lie out of the range of variability of the real parameter λ. From an opposite perspective, whenever we ask for the existence of the quantum phase transitions, i.e., for the *real* EP values $\lambda = \lambda^{(EP)}$, the non-Hermiticity of the Hamiltonian matrix in its vicinity becomes necessary.

The phenomenon of the EP-generated phase transition becomes particulary interesting when the merger of the observable discrete eigenvalues involves more than two items, i.e., say, $K \geqslant 2$ energy levels at once. Without the inessential spectral shift (i.e., with $s = 0$), we may now rewrite Eq. (14) as an explicit definition of the "unperturbed" Jordan block $S = H_0$,

$$H_0 = \left[Q^{(K)}_{(EP)}\right]^{-1} H^{(K)}_{(EP)}\, Q^{(K)}_{(EP)}. \tag{18}$$

This formula can be perceived as an introduction of the Jordan-block-related unperturbed basis. By construction, it will be composed of the columns of the respective transition matrices. The construction of these matrices was formulated as an open problem in Ref. [24]. Now, the solution can be sampled at $K = 3$,

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

as well as at $K = 4$ and $K = 5$,

$$Q^{(4)}_{(EP)} = \begin{bmatrix} 6 & 6 & 3 & 1\\ -6\sqrt{3} & -4\sqrt{3} & -\sqrt{3} & 0\\ 6\sqrt{3} & 2\sqrt{3} & 0 & 0\\ -6 & 0 & 0 & 0 \end{bmatrix},$$

$$Q^{(5)}_{(EP)} = \begin{bmatrix} 24 & 24 & 12 & 4 & 1\\ -48 & -36 & -12 & -2 & 0\\ 24\sqrt{6} & 12\sqrt{6} & 2\sqrt{6} & 0 & 0\\ -48 & -12 & 0 & 0 & 0\\ 24 & 0 & 0 & 0 & 0 \end{bmatrix}, \ldots. \tag{19}$$

It is also not too difficult to extend this construction using computer-assisted algebra. We shall need some of these matrices in what follows.

C. Exact solution for $K = N = 3$

In a way inspired by the second item in (8), let us consider

$$\widetilde{H}_0 = \begin{bmatrix} -2+s & \sqrt{2} & 0\\ -\sqrt{2} & s & \sqrt{2}\\ 0 & -\sqrt{2} & 2+s \end{bmatrix} \tag{20}$$

as well as its Jordan-block transform

$$H_0 = \begin{bmatrix} s & 1 & 0\\ 0 & s & 1\\ 0 & 0 & s \end{bmatrix}. \tag{21}$$

With an additional abbreviation of $|\psi_3\rangle = z$, we will again take into consideration, along the same lines as above, an arbitrary real-matrix perturbation,

$$W = \begin{bmatrix} \alpha & \nu & \delta\\ \mu & \beta & \sigma\\ \tau & \rho & \gamma \end{bmatrix}. \tag{22}$$

We shall assume that this perturbation is not too large, $W_{m,n} = O(\lambda)$. The Schrödinger equation then evaluates to the three linear relations,

$$(\alpha - \epsilon)x + (1+\nu)y + \delta\,z = 0,$$
$$\mu\,x + (\beta - \epsilon)y + (1+\sigma)z = 0,$$
$$\tau\,x + \rho\,y + (\gamma - \epsilon)z = 0,$$

where we eliminate

$$y = -\frac{x\alpha - x\epsilon + \delta\,z}{1+\nu}$$

from the first line, insert it in the second and the third lines, eliminate

$$z = \frac{x(-\mu - \mu\,\nu + \beta\,\alpha - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2)}{-\delta\,\beta + \delta\,\epsilon + 1 + \nu + \sigma + \sigma\,\nu}$$

from the second line, insert it in the third line, and, in the normalization with $x = 1$, we obtain the ultimate secular equation

$$\tau - \rho\left[\alpha - \epsilon + \frac{\delta(-\mu - \mu\,\nu + \beta\,\alpha - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2)}{-\delta\,\beta + \delta\,\epsilon + 1 + \nu + \sigma + \sigma\,\nu}\right](1+\nu)^{-1}$$
$$+ \frac{(\gamma - \epsilon)(-\mu - \mu\,\nu + \beta\,\alpha - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2)}{-\delta\,\beta + \delta\,\epsilon + 1 + \nu + \sigma + \sigma\,\nu} = 0.$$

This equation defines the energies exactly. In the small-perturbation regime, such an equation can be reduced to its simplified form,

$$\tau - \rho\,[\alpha - \epsilon + \delta\,(-\mu - \mu\,\nu + \beta\,\alpha - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2)] + (\gamma - \epsilon)(-\mu - \mu\,\nu + \beta\,\alpha - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2) = 0,$$

and, after further reduction,

$$\tau - \rho\,[\alpha - \epsilon + \delta\,(-\mu - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2)] + (\gamma - \epsilon)(-\mu - \beta\,\epsilon - \epsilon\,\alpha + \epsilon^2) = 0.$$

Assuming that $1 \gg |\epsilon| \gg |\lambda|$, we get the final formula $\tau - \epsilon^3 = 0$. We have a choice between three eligible small-perturbation roots of the same size. Once we select the real one,

$$\epsilon = \sqrt[3]{\tau}, \tag{23}$$

our perturbative bound-state solution remains compatible with the unitary-evolution requirement. The previous conclusions need not be modified too much.

(1) The discussion of the models with vanishing $\tau = 0$ will be skipped again. They might have been discussed, if asked for, easily.

(2) For a real $\tau \neq 0$, there always exists a unique real leading-order solution. The other two roots are complex and have to be discarded as incompatible with the unitarity and with the stability of the evolution.

(3) The generic corrections are proportional to $\epsilon = \lambda^{1/3}$ so that, again, the standard Taylor-series perturbation-series ansatz must be replaced by the Puiseux series.

We have to add that both of the spurious solutions of the perturbative Schrödinger equation reflect the action of an inadmissible perturbation under which the system would lose its operational meaning. Along this line of evolution, the given Hamiltonian as well as the related physical Hilbert space would cease to exist. There will also be no operator of metric Θ. Consequently, the metric-dependent norm of the perturbation will be undefined. The related perturbation itself can only be characterized as unacceptable, mathematically divergent, and carrying no physical meaning anymore.

IV. GENERAL SINGULAR PERTURBATION THEORY

One of the most characteristic properties of the anomalous limits $H(\lambda^{(EP)})$ of a generic perturbed Hamiltonian (6), with the EP parameter $\lambda^{(EP)}$ being real or not, is that these operators cannot be diagonalized. This is a key difference from the diagonalizable operators H used in the conventional perturbation calculations. A bridge connecting the two areas is to be sought in relation (14). It characterizes the action of H in both of the diagonalizable and nondiagonalizable cases. In the former scenario, the array Q of the eigenvector columns is complete and the spectrum-representing matrix S is diagonal plus, in all of the Hermitian and quasi-Hermitian cases, real. In the latter scenario, a key to the search for parallels will now be sought in the low-dimensional examples.

A. Unitarity-compatible perturbations

The general pattern of the behavior of our toy models near their EP extremes with any $K \geqslant 2$ is now obvious. We can expect that in the PTQM setting, the perturbation-correction strategy will therefore prove as productive as in the various conventional Hermitian theories. We also believe that its PTQM versions will be able to clarify the essence of numerous phenomena. In the literature devoted to the mathematics of non-Hermitian Hamiltonians, one can find a number of attempts in this direction [31]. *Pars pro toto*, let us recall the widespread, above-mentioned conjecture that for non-Hermitian Hamiltonians, the concept of spectrum is much less relevant and that its use should be replaced by the more or less purely numerical constructions of the pseudospectra [28]. We believe that in the very specific PTQM setting, such a type of scepticism is not entirely acceptable, and that our present perturbation-approximation concept could be more useful.

Originally, the EPs only served as an insightful tool in the conventional Hermitian perturbation theory. Recently, the massive turn of attention of physicists to the simulations of the quantum phase transitions by the classical-physics means in the laboratory [32] was also followed by the growth of interest in the EP-related mathematics [30,33]. For this reason, we believe that the implementation of the basic ideas of perturbation theory will prove efficient especially near the boundaries of stability of the quantum systems exhibiting the spontaneously unbroken $\mathcal{PT}$ symmetry.

B. Jordan block H_0 of any finite dimension

With the vector indices running from 1 to K, let us normalize $x = |\psi_1\rangle = 1$, abbreviate $|\psi_j\rangle = y_{j-1}$, $j = 2,3,\ldots,K$, and introduce an artificial quantity $y_K = 0$. The $K \times K$ matrix Schrödinger equation,

$$(H_0 + W)|\vec{\psi}\rangle = \epsilon\,|\vec{\psi}\rangle,$$

for the K-dimensional ket vector $|\vec{\psi}\rangle$ with Jordan block H_0 (and $s = 0$) may then be re-arranged into the $K \times K$ matrix-inversion form,

$$(L + Z)\vec{y} = \vec{r},\;\; \vec{r} = \begin{pmatrix} \epsilon - W_{1,1} \\ -W_{2,1} \\ \vdots \\ -W_{K,1} \end{pmatrix},\quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_K \end{pmatrix}, \tag{24}$$

with

$$L = L(\epsilon) = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ -\epsilon & 1 & 0 & \ddots & \vdots \\ 0 & -\epsilon & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 & 0 \\ 0 & \ldots & 0 & -\epsilon & 1 \end{pmatrix},$$

$$L^{-1} = L^{-1}(\epsilon) = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ \epsilon & 1 & 0 & \ddots & \vdots \\ \epsilon^2 & \epsilon & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & 1 & 0 \\ \epsilon^{K-1} & \ldots & \epsilon^2 & \epsilon & 1 \end{pmatrix}, \tag{25}$$

and with the *ad hoc* "shifted" interaction matrix

$$Z = \begin{pmatrix} W_{1,2} & W_{1,3} & \dots & W_{1,K+1} \\ W_{2,2} & W_{2,3} & \dots & \dots \\ \dots & \dots & \dots & \dots \\ W_{K,2} & W_{K,3} & \dots & W_{K,K+1} \end{pmatrix} \qquad (26)$$

representing a small $O(\lambda)$ perturbation such that the "artificially added" matrix elements are trivial, $W_{j,K+1} = 0$ at all j.

We may easily solve Eq. (24) in closed form,

$$\vec{y} = L^{-1}(\epsilon)\vec{r} - L^{-1}(\epsilon) Z L^{-1}(\epsilon)\vec{r} + \cdots . \qquad (27)$$

In a way inspired by the illustrative examples with $K \leqslant 4$, it also makes sense to assume that the size of the first-order energy correction ϵ is small, but still larger than the measure λ of the smallness of the individual elements of the perturbation matrix W or Z.

In the first-order approximation, it is sufficient to keep just the first term of the right-hand side of Eq. (27). As a test, it is instructive to check that such a solution reproduces all of the special-case results of the preceding sections.

In both of the exact and approximate settings, our vector $\vec{y}$ contains a not-yet-specified free parameter ϵ. In fact, the value of this parameter is not free because it is to be determined from the last, "artificial quantity" constraint,

$$y_K(\epsilon) = 0. \qquad (28)$$

Precisely such a condition was imposed, at the very beginning of our considerations, upon the lowermost, redundant auxiliary component of $\vec{y}$. This is a self-consistency condition which now plays the role of a secular equation determining all of the real or complex eligible energies ϵ_j, with $j = 1,2,\dots,K$.

C. Wave functions

In the $K \leqslant 4$ illustrations of the present constructive recipe, we saw that in the scale given by λ, the magnitude of the roots ϵ_j can vary with the disappearance of certain elements in the matrix of perturbations W or Z. Still, in all of these special cases, we only have to replace the conventional Taylor-type ansatz by its Puiseux (i.e., fractional-power-series) generalization, keeping in mind that the selection between the roots of the secular equation is the selection between the branches of the solution which are required to be compatible with the reality (i.e., observability) of the energies.

In Sec. III, we replaced the standard diagonalizable unperturbed Hamiltonian by its singular Jordan-block generalization H_0. Although this made the conventional Rayleigh-Schrödinger perturbation expansions inapplicable, their judicious replacement by the Puiseux power series has been shown to work properly. From the point of view of quantum physics, the feasibility of such a generalization is fortunate.

Details were displayed for the single occurrence of a K-dimensional Jordan block H_0. The perturbations were assumed, for the sake of simplicity, real and bounded, $W = O(\lambda)$. An important byproduct of our analysis was the observation that the generic formal measure

$$\epsilon_{(K)} = \lambda^{1/K} \qquad (29)$$

of the influence of W has to be replaced often by one of its alternative versions. The reason is that formula (29) only holds when the lower leftmost matrix element of the perturbation matrix does not vanish, $W_{K,1} \neq 0$. Otherwise, another, larger parameter $\epsilon_{(K)} = O(\lambda^{1/(K-1)})$ will arise from the formalism in a way which will be sampled below. This means that even if we guarantee that the matrix elements $W_{m,n} = O(\lambda)$ are all "sufficiently small" at all of the subscripts, we come to the conclusion that the extent of influence of perturbation W is *never* sufficiently reliably characterized by the single parameter. Such an observation extrapolates the above low-dimensional experience to any K. Its general validity finds its rigorous proof in the language of Sec. III: The leading-order truncated version of Eq. (27) implies that at any Jordan-block dimension K,

$$|\psi_j\rangle = \epsilon^{j-1} + O(\epsilon^j), \quad j = 1,2,\dots,K. \qquad (30)$$

The insertion of this estimate in secular Eq. (28) reconfirms the generic validity of formula (29). The result leading to formula (30) contributes to a deeper understanding of the failure of the naive, norm-determined perception and estimates of the influence of perturbations. This result indicates that with the growth of the strength λ of the perturbation, the "unfolding" of the wave function components proceeds step by step, in a hierarchical ordering, but in a way which depends on the detailed matrix structure of the perturbation.

D. Four-by-four matrix illustration

The singular EP nature of our toy-model choices of H_0 having the Jordan-block form will be felt by the system even if we regularize the unperturbed Hamiltonian by its very small change and shift inside $\mathcal{D}$. For all of the sufficiently strongly non-Hermitian $\mathcal{PT}$-symmetric Hamiltonians $H(\lambda)$, we can expect a survival of the necessity of an appropriate reinterpretation of the notion of the "sufficient smallness" of perturbations, reflecting the generic component-suppression pattern (30). For this reason, the insight provided by the low-dimensional special cases is still useful.

In the direct continuation of the $K \leqslant 3$ studies, let us now turn our attention to the next, unperturbed nondiagonalizable matrix with $K = 4$,

$$\widetilde{H}_0 = \begin{bmatrix} -3+s & \sqrt{3} & 0 & 0 \\ -\sqrt{3} & -1+s & 2 & 0 \\ 0 & -2 & 1+s & \sqrt{3} \\ 0 & 0 & -\sqrt{3} & 3+s \end{bmatrix}. \qquad (31)$$

Once it gets replaced by its two-diagonal Jordan-block alternative,

$$H_0 = \begin{bmatrix} s & 1 & 0 & 0 \\ 0 & s & 1 & 0 \\ 0 & 0 & s & 1 \\ 0 & 0 & 0 & s \end{bmatrix}, \qquad (32)$$

the stability and unitarity can be studied and guaranteed via the specification of the admissible, nondivergent perturbations, along the same lines as above. Still, in order to deepen our insight in the general tendencies, let us now contemplate the next entirely general real perturbation matrix with 16 free parameters,

$$W = \begin{bmatrix} \alpha_1 & \mu_2 & \nu_3 & \delta \\ \beta_1 & \alpha_2 & \mu_3 & \nu_4 \\ \gamma_1 & \beta_2 & \alpha_3 & \mu_4 \\ \tau & \gamma_2 & \beta_3 & \alpha_4 \end{bmatrix}.$$

Having added the fourth abbreviation $|\psi_4\rangle = w$, we can reduce the Schrödinger equation to the linear algebraic quadruplet,

$$(\alpha_1 - \epsilon)x + (1 + \mu_2)y + \nu_3 z + \delta\, w = 0,$$
$$\beta_1 x + (\alpha_2 - \epsilon)y + (1 + \mu_3)z + \nu_4 w = 0,$$
$$\gamma_1 x + \beta_2 y + (\alpha_3 - \epsilon)z + (1 + \mu_4)w = 0,$$
$$\tau\, x + \gamma_2 y + \beta_3 z + (\alpha_4 - \epsilon)w = 0.$$

In the normalization such that $|\psi_1\rangle = x = 1$, we eliminate

$$y = \epsilon - \nu_3 z - \delta\, w + \text{higher-order corrections},$$
$$z = \epsilon^2 - \nu_4 w + \text{higher-order corrections},$$

and

$$w = \epsilon^3 - \gamma_1 + \text{higher-order corrections},$$

and obtain the secular equation which is rather long but, in the leading order, degenerates to the quartic polynomial in ϵ,

$$\tau + \gamma_1\epsilon + \gamma_2\epsilon - \epsilon^4 = 0.$$

This yields the two eligible real roots of the same size,

$$\epsilon_\pm = \pm\sqrt[4]{\tau}. \tag{33}$$

The spirt of the previous conclusions survives.

(1) The $K = 4$ case is suitable for an illustration of what happens when $\tau = 0$. Such a choice yields the single "undecided" option $\epsilon = 0$ and the modified leading-order relation,

$$\epsilon^3 = \gamma_1 + \gamma_2. \tag{34}$$

The unitarity will survive when one of the three leading-order roots remains real.

(2) For $\tau \neq 0$, there exist two real leading-order energy corrections. The other two solutions are complex and they have to be discarded. The corrections prove proportional to $\epsilon_\pm \approx \lambda^{1/4}$ so that the Puiseux-series ansatz should be employed [33].

In the less restrictive context of open quantum systems, one only needs the construction of the energies and wave functions. In the more restrictive framework of the study of the stable quantum systems considered in the unitary $\mathcal{PT}$-symmetric setting, it is also necessary to select or construct a suitable metric operator Θ. Only such an additional construction makes the theory complete and testable. In the next section, a few comments will be made in this spirit.

V. ACCEPTABLE, OPERATIONALLY DEFINED PERTURBATIONS

The hierarchy (30) of the smallness of the wave-function corrections is an important innovative result of our singular perturbation considerations. Still, new open questions are evoked by our tacit assumption that the tilded-to-untilded simplification of H_0 [cf. the transformation of Eq. (15) into Eq. (16), etc.] does not really change the way of our gauging the size of the perturbation. With an ambition of giving all of these concepts a meaningful operational interpretation, we will now return to the illustrative family (8) of multiparametric non-Hermitian anharmonic-oscillator-resembling $N \times N$ tridiagonal-matrix Hamiltonians $H(\vec{\lambda})$ which remain quasi-Hermitian in a certain well-defined $J = [N/2]$-dimensional domain $\mathcal{D}$ of their free real parameters.

One of the most relevant questions concerning the perturbed $\mathcal{PT}$-symmetric systems now reads as follows: How should we understand the notion of "small" perturbation? We already know that the answer will depend on whether we insist on the reality of spectrum (in the unitary quantum theory) or not (everywhere else). The analysis is perceivably easier in the latter case because once we follow the Kato's book and once we interpret energies as certain analytic functions of the parameter, we reveal that the reality of the energies (i.e., the unitarity of the quantum evolution) is lost in *any*, arbitrarily small, *complex* vicinity of a typical (e.g., square-root) EP singularity.

The emergence of such a paradox is not surprising because, even near the simplest (viz., square-root) EP singularity, the pair of energies $E_\pm \sim \pm\sqrt{\lambda - \lambda^{(EP)}}$ lives on a two-sheeted Riemann surface. For the real parameters, only the values of $\lambda > \lambda^{(EP)}$ can lie inside $\mathcal{D}$ and keep the energies real. We can say that *no* perturbation with λ leaving the interior of $\mathcal{D}$ can be considered small. The elementary reason is that for $\lambda \notin \mathcal{D}$, the necessary physical Hilbert space $\mathcal{H}(H)$ in which the physics is defined *does not exist* at all.

For $\lambda \in \mathcal{D}$, the construction of $\mathcal{H}(H)$ need not be unique [2]. This ambiguity will be reflected by the ambiguity of the norm of a given perturbation, leading to the relevant differences, especially from the point of view of an experimentalist. We can only conclude that in contrast to the Hermitian interaction Hamiltonians, their non-Hermitian analogues need not admit a clear and reliable separation of perturbations into their "sufficiently small" and "too large" subcategories.

A. $N = 2$

For our present toy models, fortunately, the specification of the interior of $\mathcal{D}$ is feasible, sometimes even by purely non-numerical means [23]. This enables us to pay constructive attention even to the extreme dynamical scenarios in which the parameters coincide with, or lie close to, one of the vertices of the EP boundary $\partial\mathcal{D}$. In its vicinity, naturally, the impact of the non-Hermiticity of perturbation V is maximal [22]. For illustration, the first, one-parametric Hamiltonian-operator element of sequence (8) can be reparametrized in light of Eq. (13) and of Eq. (11) with optional $G_1 = 1$,

$$H^{(2)}[a(t)] = \begin{bmatrix} 1 & \sqrt{1-t} \\ -\sqrt{1-t} & -1 \end{bmatrix} = H^{(2)}_{(EP)} + V^{(2)}_{(\text{perturbation})}(t). \tag{35}$$

The Schrödinger equation (7) with $\lambda = O(t)$, $N = 2J$, normalization $|\psi_1^{(2)}(t)\rangle = 1$, and single unknown wave-function component $y = |\psi_1^{(2)}(t)\rangle$ leads to the two exact bound-state solutions,

$$E_\pm = \pm\sqrt{t}, \quad y_\pm = \frac{-1 \pm \sqrt{t}}{\sqrt{1-t}}. \tag{36}$$

This result confirms the validity of the singular perturbation theory of Sec. III A. What is now new is the choice of the special perturbation regime based on the use of single parameter $t \in (0,1)$ measuring the strength of the perturbation. This choice guarantees the reality of the spectrum. Inside $\mathcal{D}$, it interpolates between the strong-coupling limit of the nondiagonalizable Hamiltonian H_0 at $t = 0$ and the weak-coupling diagonal-Hamiltonian limit at $t = 1$. This choice also determines the perturbation matrix,

$$V^{(2)}_{(\text{perturbation})}(t) = \begin{bmatrix} \sqrt{1-t}-1 & \sqrt{1-t}-1 \\ 2-2\sqrt{1-t} & 1-\sqrt{1-t} \end{bmatrix} = \frac{t}{2}\begin{bmatrix} -1 & -1 \\ 2 & 1 \end{bmatrix} + O(t^2). \quad (37)$$

It is rather counterintuitive that the eigenvalues $\pm\sqrt{2\sqrt{1-t}-2+t}$ of this unitarity-compatible interaction term are purely imaginary. This is a peculiarity which also extends to the higher matrix dimensions.

B. $N = 3$

The second one-parametric Hamiltonian in sequence (8) can be reparametrized in the same manner as above,

$$H^{(3)}[a(t)] = \begin{bmatrix} 2 & \sqrt{2}\sqrt{1-t} & 0 \\ -\sqrt{2}\sqrt{1-t} & 0 & \sqrt{2}\sqrt{1-t} \\ 0 & -\sqrt{2}\sqrt{1-t} & -2 \end{bmatrix} = H^{(3)}_{(EP)} + V^{(3)}_{(\text{perturbation})}(t). \quad (38)$$

In the domain of small $t \approx 0$, the three exact bound-state energies,

$$E_0 = 0, \;\; E_\pm = \pm 2\sqrt{t}, \quad (39)$$

remain small as expected. A similar expectation is also fulfilled by the order of smallness of the partner of Eq. (22), i.e., by the $N = 3$ analog of Eq. (37),

$$V^{(3)}_{(\text{perturbation})}(t) = \frac{t}{2}\begin{bmatrix} -2 & -1 & 0 \\ 4 & 0 & -1 \\ 0 & 4 & 2 \end{bmatrix} + O(t^2). \quad (40)$$

What we detect here is the disappearance of the leftmost lowest matrix element. This means that we have $\gamma = 0$ in Eq. (23) so that we have to use $\epsilon \sim t^{1/2}$ rather than the generic $\epsilon_{(3)} \sim t^{1/3}$. Otherwise, nothing really new is observed at $N = 3$ since one of the energies is a t-independent spectator. At the higher J's, for similar reasons, one could therefore restrict attention to the matrices of even dimensions $N = 2J$.

C. $N = 4$

In the leading-order approximation, it is sufficient to work with the two trivial parameters $G_n = 0$ in Eq. (11). Along the same lines as above, we obtain the exact secular equation $9\,t^2 - 10\,\epsilon^2 t + \epsilon^4 = 0$ which is solvable in closed form,

$$E_{\pm,\pm} = \pm(2 \pm 1)\sqrt{t}. \quad (41)$$

Similarly, the routine evaluation of the product

$$\left[Q^{(4)}_{(EP)}\right]^{-1} H^{(4)}[a(t),b(t)]\,Q^{(4)}_{(EP)}$$

yields the $N = 4$ analog of formula (40),

$$V^{(4)}_{(\text{perturbation})}(t) = \frac{t}{2}\begin{bmatrix} -3 & -1 & 0 & 0 \\ 6 & -1 & -1 & 0 \\ 0 & 8 & 1 & -1 \\ 0 & 0 & 6 & 3 \end{bmatrix} + O(t^2). \quad (42)$$

Several consequences can be formulated. First, in the manner which extends to all of the matrix dimensions $N < \infty$, the perturbation expansions will merely contain the integer and half-integer powers of t. This is connected with the fact that after the transitions to the Jordan block H_0, the leading-order form of perturbation matrix W remains tridiagonal.

Our choice of the illustrative anharmonic oscillators has been fortunate in the sense that they all admit the construction of a smooth path connecting the common, Rayleigh-Schrödinger-tractable weak-coupling dynamical regime where $g_n(t) \approx 0$, i.e., $\xi_n(t) \to 1^-$, with the extremely non-Hermitian but still safely physical strong-coupling dynamical regime. Unambiguously, the smallness of the unitarity-compatible perturbations was then measurable by the smallness of our "redundant" parameter, $t \approx \xi_n(t) \gtrapprox 0$.

VI. DISCUSSION

One of the most exciting features of any non-Hermitian but $\mathcal{PT}$-symmetric model, quantum [3] or nonquantum [15], should be seen in its capability of living near, or passing through, an instability. The description of these processes is controlled by Schrödinger equation (3) where the non-Hermiticity of the (say, single-parameter-dependent) Hamiltonian $H = H(t)$ enables us to modify the dynamics by a small change of t. In particular, a sudden jump can occur from the unitary-evolution scenario with the real-energy spectrum to a broken-symmetry dynamical regime [11]. A complexification of the energies then implies a sudden loss of the unitarity of the evolution. One of the possible phase transitions, alias "quantum catastrophes," [34] is encountered.

In our present paper, we addressed precisely the problem of suppression and control of the latter type of sensitivity to perturbations. In a natural continuation of such a study, one might imagine a further continuation of this development of the theory in two directions. In one of them, the constructions would be extended to the systems with several Jordan blocks in the Hamiltonian. This would closely parallel our present approach and the resulting picture would not leave the textbook framework of unitary quantum theory of bound states. The admissible generalized, non-Hermitian but diagonalizable Hamiltonians $H(t)$ would still be required to be quasi-Hermitian in the sense of Ref. [2]. After an appropriate amendment of Hilbert space, the evolution of the quasi-Hermitian system would still be correctly reinterpreted as unitary. The necessary innovations would be purely technical.

In the second possible branch of future developments, one might admit that the sophisticated physical Hilbert space ceased to exist. Besides the solution of Schrödinger equation (3), the new tasks for the theoreticians will be twofold. First, whenever the energies remain real even *after* the phase transition, a new Hamiltonian-dependent physical Hilbert space must be constructed (cf., e.g., Refs. [12] for some comments). Second, in the case of the loss of the reality of the energies, the picture of reality cannot be based on the safe and unitary PTQM theory. Still, the more general, nonunitary interpretations of the evolution may enter the game as an inspiration of such a type of future research.

The latter direction of developments will certainly be less restrictive because the spectra as well as the parameters would be allowed to be complex. The non-Hermitian and non-quasi-Hermitian quantum Hamiltonians may then describe the realistic resonant and/or open systems. Still, such a nonquantum type of physics will use the same mathematics. Non-Hermitian systems with nonreal spectra will exhibit various nonunitary analogues of the EP-related phase transitions. Even the nonconservative open quantum systems will feel the presence of the EPs, and even at a distance, without a direct passage through the singularity, but still with the influence reconstructed by perturbative as well as nonperturbative techniques (cf., e.g., Refs. [35–37] for further details and references).

In the laboratory, the manifestations of the latter types of non-Hermiticities may be demonstrated using, e.g., the framework of classical optics [38]. Thanks to the growing number of experiment-oriented simulations, multiple deeply counterintuitive EP-related phenomena may be studied. *Pars pro toto*, for a pair of wave modes with the loss and gain (simulating $\mathcal{PT}$ symmetry in the medium), the authors of Ref. [36] studied the dynamics of a system which is forced to move along a small circle circumscribing an EP singularity. They discovered and proved that the adiabatic approximation must necessarily fail. In their own words, "in contrast to Hermitian systems, the dynamics cannot be obtained by perturbative corrections to the adiabatic prediction" [36]. In light of the formalism developed in our present paper, such a conclusion might have been modified in the near future. We believe that in similar situations, the standard or modified perturbation techniques should be admitted and used as well. Their implementation might certainly provide a specific insight into the structures and the dynamics of the system. At the same time, the choices of the more sophisticated forms and features of the Hamiltonians will certainly open multiple technical as well as conceptual questions.

A. Towards the unbounded-operator models

In retrospect, several discoveries and rediscoveries [39] of the unexpected robust reality of the bound-state energy spectrum were obtained by the study of the non-Hermitian ordinary-differential Schrödinger equations. Unfortunately, the results were treated, for a long time, as a mere mathematical curiosity [8,40]. The opinions only changed after Bender and Boettcher [11] noticed that such an anomaly characterizing the manifestly non-Hermitian quantum Hamiltonian is valid for the whole class of the next-to-elementary Schrödinger equations,

$$-\frac{d^2}{dx^2}\psi_n(x,\delta) + x^2(ix)^\delta\,\psi_n(x,\delta) = E_n(\delta)\,\psi_n(x,\delta), \quad \psi_n(x,\delta) \in L^2(\mathbb{S}_\delta), \quad n = 0,1,\ldots. \tag{43}$$

A few years later, it was proved that whenever the exponent remains non-negative, $\delta \geqslant 0$, the reality of the spectrum survives [41]. One must only choose $\mathbb{S}_\delta$ as a suitable δ-dependent, $\cap$-shaped complex contour. At the not-too-large exponents, $\delta < 2$, one can even return to the straight real line and choose $\mathbb{S}_\delta = \mathbb{R}$ again.

1. *Phenomenological perspective*

Naturally, the reality of the energies at the non-negative exponents $\delta \geqslant 0$ seemed puzzling. It found its intuitive explanation in the $\mathcal{P}$-pseudo-Hermiticity property $H^\dagger\mathcal{P} = \mathcal{P}H$ of the Hamiltonian, with symbol $\mathcal{P}$ denoting the operator of parity. For mathematicians, this means that $\mathcal{P}$ is the pseudometric in an associated Krein space [42]. In the context of physics, the $\mathcal{P}$-pseudo-Hermiticity of manifestly non-Hermitian Hamiltonians can be reinterpreted as the property of $\mathcal{PT}$ symmetry reflecting the mathematically equivalent relation $H\,\mathcal{PT} = \mathcal{PT}\,H$, in which $\mathcal{T}$ is an (antilinear) operator of time reversal [11].

The $\mathcal{PT}$-symmetric quantum Hamiltonians in Eq. (43) with $\delta \geqslant 0$ were widely accepted as eligible generators of unitary evolution in quantum theory [5]. For a correct probabilistic interpretation of this process, the fundamental requirement of the observability of the energies $E_n(\delta) \in \mathbb{R}$ was only complemented by a phenomenologically well-motivated assignment of the observability status to a charge (cf. [3] and also the general discussion of such a strategy in [2]). The introduction of the operator of charge $\mathcal{C}$ led, ultimately, to a quantum-theoretical picture in which the Hamiltonians $H = H(\delta)$ with $\delta \geqslant 0$ are made quasi-Hermitian [2,18], alias $\mathcal{PCT}$ symmetric, $H^\dagger\mathcal{PC} = \mathcal{PC}H$ [3]. In this sense, the time evolution associated with Eq. (43) was made, formally at least, unitary.

2. *Quantum physics perspective*

The unitarity is lost at $\delta < 0$. The "Hilbert-space-metric" operator $\Theta = \mathcal{PC}$ would cease to exist. In applications, one then has to speak about one of the best known samples of the phase transition at $\delta = 0$, better known as a spontaneous breakdown of $\mathcal{PT}$ symmetry [3]. From such a point of view, the conventional quantum harmonic oscillator with $\delta = 0$ may be interpreted as unstable with respect to the perturbations which would deform the exponent. At $\delta = 0$, the quantum system described by Eq. (43) will be forced to perform the phase transition of the first kind [34]. *Any* perturbation making the exponent arbitrarily small but negative should be considered, in this setting, irrespective of its norm, infinitely large and entirely out of the scope of any consistent unitary quantum theory.

The purely numerical nature of model (43) appeared to be one of its increasingly serious shortcomings. Even the warmly welcomed reality of the spectrum at $\delta \geqslant 0$ was merely one of the necessary conditions of the compatibility of Eq. (43) with its unitary-evolution interpretation. In a rigorous sense, the status of quantum model (43) is not yet fully clarified. One of the main reasons for doubts was formulated by Siegl and Krejčiřík [43]. After a detailed mathematical analysis, the ordinary-differential model (43) was found not to fit fully in the framework of the quasi-Hermitian quantum mechanics (cf. also several compact reviews of the current state of the art in [5]). The source of potential instability has been found, at any generic $\delta > 0$, in an anomalously large and next-to-unpredictable influence of perturbations.

The difficulties of such type were already predicted by mathematicians [18]. In our present paper, the resolution of the problem was based on Ref. [2], i.e., on the exclusive use of bounded Hamiltonians. Without such a constraint, one would have to clarify, systematically, all of the relevant mathematical subtleties. A concise review of the results of such an approach was written, recently, by Antoine and Trapani [20].

B. Towards the models with complex energies

The description of the latter irregularities has been based on the study of pseudospectra. Their use may be expected to tame the anomalies in the majority of the nonquantum applications of the theory. Among them, let us mention here the discovery of the failure of the adiabaticity hypothesis for non-Hermitian Hamiltonians [36]. Recently, this discovery was complemented by a deeper insight in [37]. The slightly modified team of authors paid attention to the mode switching in waveguides. In a toy-model-based analysis of the system, they simulated the evolution by a Schrödinger-type equation (3) with a suitable complex-symmetric (CS) Hamiltonian $H^{(CS)}$ with complex spectrum. Surprisingly enough, the authors worked with a three-parametric family of these Hamiltonians, but they merely supported their observations by the brute-force numerical calculations. This appeared to be one of the sources of inspiration of our present perturbation-theory considerations. We were persuaded that in similar analyses of the emergence of various non-Hermiticity-related instabilities, quantum or nonquantum, the direct use of a suitably adapted Rayleigh-Schrödinger perturbation-expansion technique might prove insightful and also technically not too difficult.

We believe that in spite of our present restriction of attention to the mere models with real spectra, one of the eligible branches of the future study of Hamiltonians $H^{(CS)}$ could be based on their EP-related split $H^{(CS)} = H_0^{(CS)} + V^{(CS)}$, where

$$H_0^{(CS)} = \frac{1}{4}\begin{bmatrix} -2\,i\gamma_1 & \gamma_1-\gamma_2 \\ \gamma_1-\gamma_2 & -2\,i\gamma_2 \end{bmatrix} \tag{44}$$

would have the complex spectrum. Thus, it would still fit in our present nondiagonalizable scenario based on the use of the transition matrix

$$Q^{(CS)} = \frac{1}{4}\begin{bmatrix} -i\gamma_1+i\gamma_2 & 4 \\ \gamma_1-\gamma_2 & 0 \end{bmatrix}$$

leading to the complex Jordan-block simplification of Hamiltonian (44),

$$\begin{aligned} S^{(CS)} &= Q^{-1}H_0^{(CS)}Q \\ &= \begin{bmatrix} -1/4\,i\gamma_1 - 1/4\,i\gamma_2 & 1 \\ 0 & -1/4\,i\gamma_1 - 1/4\,i\gamma_2 \end{bmatrix}. \end{aligned} \tag{45}$$

Even though the spectrum is now complex, the method of perturbing such an EP Hamiltonian remains the same.

Classical physics perspective

In classical physics and optics, the perception of the unitarity is specific, and not of central importance. Recently, the growth of interest in the Hamiltonians with complex energies has been motivated by the growing appeal of the direct experimental relevance of the concept of the spontaneously broken $\mathcal{PT}$ symmetry in a nonquantum setting. The easiness of the realization of $\mathcal{PT}$ symmetry in the form of an interplay between gain and loss in the optical and/or other media led to a boom of the study of its multiple counterintuitive phenomenological features and consequences [15].

In Eq. (43), for example, infinitely many energies cease to be real when the exponent becomes small but negative. Still, one observes that the low-lying part of the spectrum remains real and that there exists an infinite series of the critical negative exponents,

$$\begin{aligned} &\delta^{(\text{critical})}(1) < \delta^{(\text{critical})}(2) < \cdots < \delta^{(\text{critical})}(M) \\ &\quad < \cdots < \delta^{(\text{critical})}(\infty) = 0, \end{aligned}$$

which are, precisely, the above-mentioned EP singularities. At these points, the Hamiltonian ceases to be diagonalizable. At every subscript M, the emergence of the related Jordan block of dimension $K = 2$ reflects the degeneracy of the pair of energies E_{2M-1} and E_{2M}, which are real at $\delta > \delta^{(\text{critical})}(M)$ and which form a complex-conjugate pair at $\delta < \delta^{(\text{critical})}(M)$ (cf. [11] for more details).

An analogous situation is encountered with the nondiagonal Jordan block $H_0^{(CS)}$ of Eq. (44). After its small perturbation, one would have a tendency of forgetting about the EP-related nondiagonalizability and of a replacement of the nondiagonal Jordan block $H_0^{(CS)}$ by the apparently user-friendlier conventional diagonal matrix of eigenvalues. In this setting, the recommendation provided by our present paper is opposite—the unpleasant methodical discontinuity between the EP and non-EP scenarios is to be solved in favor of the former one.

In this sense, we believe that our present paper might inspire new perturbative studies. The constructive use of the smallness of the perturbations has intuitive appeal even near EPs. It might help in the technically less straightforward non-Hermitian scenarios, especially for the study of dynamics in the closest vicinity of the open-system toy-model EP Hamiltonians as sampled by Eq. (44).

VII. SUMMARY

In Kato's mathematical perturbation theory [19], the EP singularities play mainly just the formal role of marks of the end of the applicability of conventional weak-coupling expansions. The approximations of the weak-coupling type will necessarily fail near the EP radius of convergence. Although we often encounter some of the most interesting physical phenomena in such a dynamical regime, the authors of the related papers usually call the strong-coupling dynamics "nonperturbative." Such a terminology is misleading. There is no doubt that the weak-coupling approximations can only be fully successful *sufficiently far* from the natural EP boundaries. Still, there exist many examples of successful perturbation recipes of a strong-coupling type. One of them has been described and tested in our present paper.

Our interest in this problem was recently revitalized by the adiabaticity-failure numerical studies [36,37] as well as by the papers in which the existence of the non-Hermiticity-related instabilities was deduced using the *ad hoc* concept of the pseudospectrum [28,43,44]. In this context, we imagined that all of the similar identifications of the instabilities contain an internal contradiction because these identifications are made, exclusively, in the auxiliary Hilbert spaces in which neither the parametric domain $\mathcal{D}$ nor the physical metric operator $\Theta \neq I$ are properly taken into consideration. Thus, in spite of the well-known fact that the simplification $\Theta \to I$ is often admissible in nonquantum calculations, the difficulty of the quantum-theoretical necessity of the construction of $\Theta \neq I$ is often being circumvented rather than identified as the main task.

In the literature, the omission of the correct account of the anisotropic Θ's is often accompanied by the absence of the attention paid to the "methodical discontinuity" between the *nondiagonalizable nature* of the strong-coupling EP limit H_0 and the *diagonalizability* of any Hamiltonian defined inside the domain $\mathcal{D}$, i.e., after the strong-coupling perturbation is being turned on. In our present paper, we tried to remove a mental barrier by having kept the unperturbed Hamiltonian nondiagonal. Even after the inclusion of the perturbation, we kept the transition matrices Q unchanged.

The trick of having *the same* unperturbed basis before and after the perturbation has been shown to work well. We showed that it converted our perturbed-EP versions of the Schrödinger equation, via an appropriate perturbation-expansion ansatz, into an order-by-order solvable problem. The resulting non-Hermitian strong-coupling formalism acquired a self-consistent but still explicit-construction nature.

The main mathematical feature of the whole proposal may be seen in the fact that the "measure of the smallness" ϵ of the separate perturbations has the form which can vary, first of all, with the size and sign of the individual matrix elements of the perturbation in question. In addition, the form of the perturbation approximations has been revealed to also vary with the dimension K of the particular unperturbed Jordan block H_0. This formed a self-consistency pattern: The value of the expansion parameter ϵ has been found to coincide with a root of a perturbation-dependent secularlike polynomial of the Kth order. In parallel, parameter ϵ has been shown to order the wave-function components, making them arranged in a "step-by-step-unfolding" hierarchy [cf. Eq. (30)].

In the language of physics, our perturbation-approximation recipe puts several known facts into an entirely different perspective. This was illustrated via our family of $\mathcal{PT}$-symmetric $N \times N$ matrix Hamiltonians of Eqs. (9) and (10). The list of their remarkable features as available in Refs. [22,23] (and including their capability of a t-parametrized interpolation between the weak- and strong-coupling dynamical extremes) was complemented here by several items. The most remarkable one of them is seen in an easy constructive tractability of perturbations in the strong-coupling dynamical regime. Our models also exhibited a user friendliness in the secular polynomial context. The "generic" Kth-root value (29) of the perturbation-weighting parameter $\epsilon_{(K)}$ degenerated, for our admissible anharmonic oscillator and due to the specific tridiagonal-matrix structure of perturbations V, to the mere square-root expression given by Eq. (39) at $K = 3$ and by Eq. (41) at $K = 4$.

We may summarize that our illustrative non-Hermitian toy models (9) and (10) are sampling, in an almost optimal manner, the ways of suppression of the various forms of a phase-transition-onset instability. Counterintuitive as such resistance against perturbations may seem, its mechanism has been clarified as caused by the consequent use of the specific EP unfolding. Among all of the eligible generic energy-correction roots $\epsilon_{(K)} \sim \sqrt[K]{\lambda}$ of the degeneracy-removing secular Eq. (29), just one or two had to be selected. In other words, one has to keep in mind the fact that from the point of view of physics, the perturbation can only be realized in the *existing* physical Hilbert space which is characterized by a *nonsingular* inner-product metric Θ. From this perspective, the apparently high sensitivity of the perturbed spectrum to certain subtle details of the form of the perturbation should be understood as a mere mathematical artifact which we have, in our strong-coupling perturbation approach, fully under control.

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