Complex symmetric Hamiltonians and exceptional points of order four and five

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

(Received 4 April 2018; published 13 September 2018)

A systematic elementary linear-algebraic construction of non-Hermitian Hamiltonians $H = H(\gamma)$ possessing exceptional points $\gamma = \gamma^{(\mathrm{EP})}$ of higher orders is proposed. The implementation of the method leading to EPs of orders $K = 4$ and $K = 5$ is described in detail. Two distinct areas of applicability of our user-friendly benchmark models are conjectured: (1) in *quantum* mechanics of non-Hermitian systems and (2) in their experimental simulations via *classical* systems (e.g., coupled waveguides).

DOI: 10.1103/PhysRevA.98.032109

I. INTRODUCTION

The recent increase in popularity of Schrödinger equations

$$i\,\partial_t|\psi\rangle = H\,|\psi\rangle \tag{1}$$

with non-Hermitian (and, say, parameter-dependent) Hamiltonians

$$H = H(\gamma) \neq H^{\dagger}(\gamma) \tag{2}$$

opened (or reopened) a number of mathematical questions [1]. It also evoked many challenges in theoretical quantum physics [2,3] as well as in experimental classical physics and optics [4].

Within the community of quantum physicists many new, promising phenomenological models have been conjectured and studied, ranging from their ordinary differential versions (to which attention was attracted, in 1998, by the pioneering letter by Bender and Boettcher [5]) up to their truly sophisticated quantum-field descendants (cf., e.g., an exhaustive review [6] of this most ambitious project).

The Bender and Boettcher toy-model Hamiltonians $H_{(\mathrm{BB})}(\gamma) = -d^2/dx^2 + V_{(\mathrm{BB})}(x,\gamma)$ were chosen non-self-adjoint but, for technical reasons, $\mathcal{PT}$-symmetric, $H_{(\mathrm{BB})}\mathcal{PT} = \mathcal{PT}H_{(\mathrm{BB})}$, with parity $\mathcal{P}$ and antilinear time reversal $\mathcal{T}$. Several unexpected features of these unconventional quantum Hamiltonians (e.g., the often occurring reality of spectra) inspired mathematicians and enhanced their interest in a systematic study of similar models (cf. *pars pro toto*, a truly nice monograph [7]).

The idea proved inspiring also beyond quantum physics. In classical optics, for example, the Bender and Boettcher $\mathcal{PT}$-symmetric Schrödinger equation was found to be equivalent to the classical Maxwell equation in a paraxial approximation [8]. The complex function $V(x)$ acquired a new physical meaning of the complex refraction index admitting both the gain and the loss of the beam intensity. A quick growth in popularity of the Maxwell-equation-related models followed. One of the reasons behind their successful tests in the laboratory may be seen in the current progress in nanotechnologies. This helped physicists to simulate various *ad hoc* features and forms of non-Hermiticity (e.g., $\mathcal{PT}$ symmetry) *experimentally*, say, in the context of the physics of photonic molecules [9] or for devices composed of coupled waveguides [10].

In our present paper we felt inspired by the mutual enrichment between quantum and nonquantum considerations, especially when related to the concept of the exceptional point (EP; cf. p. 64 in [11]). In Sec. II we recall the particular role played by the EPs in quantum physics. As an illustration we recall the $\mathcal{PT}$-symmetric version of the Bose-Hubbard many-body model in its non-Hermitian version, which was proposed and studied, in 2008, by Graefe *et al.* [12] (cf. Sec. II A). In the subsequent subsection, II B, an explanation is added of the less widely known possibility of full theoretical compatibility between the non-Hermiticity of a quantum Hamiltonian in an auxiliary, "false but friendly" [13] Hilbert space (endowed with an unphysical but more easily calculated inner product) and the unitarity of the evolution it generates in another, amended Hilbert space using a nontrivial Hilbert-space metric $\Theta \neq I$ in the definition of the necessary correct and physical inner product.

In alternative, nonquantum applications the theoretical as well as the phenomenological role of the EPs is different. In Sec. III we explain why the change of perspective enhances the appeal of non-Hermiticity in experimental physics as well as in the mathematics of elementary algebraic construction methods. In Sec. IV, in particular, our main message is then based on the turn of attention from the Bose-Hubbard model to a more general family. Complex and symmetric tridiagonal-matrix non-Hermitian Hamiltonians are considered. Using straightforward linear-algebraic methods, a systematic search for EP singularities is performed. Their exhaustive classification is shown fully nonnumerically at $N = 4$ and $N = 5$.

An extensive review and analysis of the various physical aspects of these mathematical results are finally given in Sec. V, with all of this material summarized in Sec. VI.

II. QUANTUM SYSTEMS WITH EXCEPTIONAL POINTS

Drawing attention to the occurrence and unfolding of exceptional points we intend to consider the class of finite-dimensional matrix Hamiltonians, (2), with dimension

*znojil@ujf.cas.cz

$N < \infty$ and with the special complex-symmetric structure,

$$H_{mn}(\gamma) = H_{nm}^{*}(\gamma). \tag{3}$$

In the context of pure mathematics this choice could have been suggested by a review paper [14] and talk [15]. From these sources one deduces, e.g., an intimate relationship between the complex symmetry of matrices and the $\mathcal{PT}$ symmetry of operators.

Equally strong encouragement of our study was provided by physicists, especially via papers [12–16], in which the class of complex symmetric Hamiltonians was further narrowed to their tridiagonal-matrix subfamily such that

$$H_{mn}(\gamma) = 0 \quad \text{whenever} \quad |m-n| \geqslant 2. \tag{4}$$

What attracted our attention to the finite-dimensional Hilbert spaces was also certain older quantum models and results on the physics of atomic nuclei (a recommended compact review may be found in Ref. [17]). Last but not least, we should mention that during our study we found a deeper physical inspiration in Refs. [18,19] and in several other recent studies of optical waveguides with gain and loss.

A. $\mathcal{PT}$-symmetric Bose-Hubbard model of Graefe *et al.* [12]

In the phenomenological context the proposal and study of the $\mathcal{PT}$-symmetric Bose-Hubbard model in Ref. [12] were motivated by the search for an elementary simulation of the process of the Bose-Einstein condensation. Up to the purely numerically tractable interaction term the non-Hermitian Hamiltonian of the model was chosen in the form

$$H_{(\mathrm{BH})}(\gamma) = 2\,(-i\gamma\, L_z + L_x) \tag{5}$$

of the complex linear combination of the two angular-momentum generators $L_{z,x}$ of the real Lie algebra $su(2)$. The underlying representation theory enables one to treat operator (5) as decomposed into an infinite family of finite-dimensional $N \times N$ matrices

$$H^{(2)}_{(\mathrm{BH})}(\gamma) = \begin{bmatrix} -i\gamma & 1 \\ 1 & i\gamma \end{bmatrix}, \tag{6}$$

$$H^{(3)}_{(\mathrm{BH})}(\gamma) = \begin{bmatrix} -2\,i\gamma & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 2\,i\gamma \end{bmatrix}, \tag{7}$$

etc. An inessential change of parameter $\gamma \to \sqrt{z}$ can be recommended in the subsequent items, i.e., in

$$H^{(4)}_{(\mathrm{BH})}(z) = \begin{bmatrix} -3\,i\sqrt{z} & \sqrt{B} & 0 & 0 \\ \sqrt{B} & -i\sqrt{z} & \sqrt{A} & 0 \\ 0 & \sqrt{A} & i\sqrt{z} & \sqrt{B} \\ 0 & 0 & \sqrt{B} & 3\,i\sqrt{z} \end{bmatrix} \tag{8}$$

with $B = 3$ and $A = 4$ as well as in

$$H^{(5)}_{(\mathrm{BH})}(z) = \begin{bmatrix} -4\,i\sqrt{z} & \sqrt{B} & 0 & 0 & 0 \\ \sqrt{B} & -2\,i\sqrt{z} & \sqrt{A} & 0 & 0 \\ 0 & \sqrt{A} & 0 & \sqrt{A} & 0 \\ 0 & 0 & \sqrt{A} & 2\,i\sqrt{z} & \sqrt{B} \\ 0 & 0 & 0 & \sqrt{B} & 4\,i\sqrt{z} \end{bmatrix} \tag{9}$$

with $B = 4$ and $A = 6$, etc. Such a change of notation is motivated by the simplification of the respective secular equations (see below). Still, the possibility of an alternative choice of sign of $\gamma \to -\sqrt{z}$ should be kept in mind as a helpful symmetry of the Bose-Hubbard model (see also the first picture in paper [12]). Due to this symmetry and due to the reality of the spectra, all of the matrices, (6)–(9), etc., may be declared eligible, together with their $\gamma \to -\gamma$ counterparts, as nonnumerical toy-model generators of quantum evolution.

B. The procedure of Hermitization

In conventional studies of quantum evolution one usually requires it to be unitary. For our sample generators $H^{(N)}_{(\mathrm{BH})}(\gamma)$ (i.e., for the diagonalizable, hiddenly Hermitian Bose-Hubbard Hamiltonians), this means that the spectrum must be real. The authors of Ref. [12] emphasized that the latter condition is satisfied if and only if $-1 < \gamma < 1$. For the conventional nonnegative $\gamma \geqslant 0$ and real $z \geqslant 0$ they concluded that every element $H^{(N)}_{(\mathrm{BH})}(z)$ in the sequence is exactly solvable and, moreover, that each toy-model Hamiltonian $H^{(N)}_{(\mathrm{BH})}(z)$ in the family possesses a unique and real exceptional point $z^{(\mathrm{EP})} = 1$ of order N.

For the admissible parameters $\gamma \in (-1, 1)$ one can find a (nonunique) Hermitian and positive matrix of the Hilbert-space metric Θ such that

$$H^{\dagger}\,\Theta = \Theta\, H, \tag{10}$$

i.e., such that $H = H^{(N)}_{(\mathrm{BH})}(\gamma)$ may be declared Hermitian with respect to an amended inner product $\langle\cdot|\Theta\,\cdot\rangle$. The details of the theory using nontrivial metrics $\Theta \neq I$ may be found, say, in reviews [2] and [17]. For our present purposes it is only necessary to emphasize that the first principles of the theory remain unchanged. Thus, any observable phenomenon must still be represented by a hiddenly Hermitian operator Λ such that $\Lambda^{\dagger}\,\Theta = \Theta\,\Lambda$. In other words, only the initial knowledge of the Hamiltonian-dependent metric $\Theta = \Theta(H)$ makes the model theoretically complete.

Needless to add, the necessary guarantee of validity of Eq. (10) is far from trivial in practice. The difficulty of the construction of $\Theta = \Theta(H)$ is, incidentally, one of the reasons why the matrix phenomenological models with small dimensions $N \ll \infty$ are so important, both in the theory and in its applications.

1. Construction of a metric at $N = 2$

At $N = 2$ we may insert the quantum Hamiltonian $H^{(2)}_{(\mathrm{BH})}(\gamma)$ of Eq. (6) into Eq. (10). The routine solution of this linear algebraic problem yields *all* of the eligible (i.e., positive definite) metrics. Up to an overall inessential multiplicative factor they are all defined by the following one-parametric formula:

$$\Theta^{(2)}(\beta) = I^{(2)} + \begin{bmatrix} 0 & \beta + i\gamma \\ \beta - i\gamma & 0 \end{bmatrix}, \quad -\sqrt{1-\gamma^2} < \beta < \sqrt{1-\gamma^2}. \tag{11}$$

Obviously, in the arbitrarily small vicinities of $\gamma = \gamma^{(EP)}$ such a metric only exists, in the spirit of Ref. [20], after the minimally anisotropic metric constant choice of $\beta = 0$.

2. Construction of a metric at $N = 3$

A fully analogous treatment of the next quantum system with Hamiltonian (7) (in which we abbreviate $g = \sqrt{2}\gamma$) will lead to the two-parametric family of metrics

$$\Theta^{(3)}(\beta, \delta) = I^{(3)} + \begin{bmatrix} 0 & \beta + i\,g & \delta + i\,g\,\beta \\ \beta - i\,g & \delta + g^2 & \beta + i\,g \\ \delta - i\,g\,\beta & \beta - i\,g & 0 \end{bmatrix}. \tag{12}$$

In the spirit of Ref. [20] one may again prefer a "minimally anisotropic" choice of $\beta = 0$ and $\delta = 0$, which yields the metric with eigenvalues

$$\theta_0 = 1, \quad \theta_\pm = 1 + \frac{1}{2}g^2 \pm \frac{1}{2}\sqrt{8\,g^2 + g^4}. \tag{13}$$

Obviously, the resulting special metric $\Theta^{(3)}(0, 0)$ still exists up to the maximal admissible (i.e., real-energy-admitting) non-Hermiticity limit of $g \to g^{(EP)} = 1$.

An entirely analogous procedure will also work at any higher matrix dimension N.

III. EXCEPTIONAL POINTS IN NONQUANTUM OPTICS

Schrödinger-like equations and their solutions appear in many nonquantum branches of physics. Thus, in the physical context of classical optics the quantum effects may be simulated via microwave devices [21] or coupled waveguides [22]. Once these devices prove to be characterized by a symmetry between the gain and the loss in the medium, the mathematics of solutions becomes shared with quantum theories exhibiting the combined parity times the time reversal symmetry *alias* $\mathcal{PT}$ symmetry [6]. Thus, after one leaves the unitary quantum mechanics and turns one's attention to classical optics, the related Schrödinger-to-Maxwell change in the meaning of the Schrödinger-like evolution equation, (1), is accompanied by slightly easier, formally less restrictive mathematics. For example, "wave-function" solutions $|\psi\rangle$ no longer need to be normalizable.

In the new context it is crucial that the evolution generated by the Hamiltonian-resembling operators $H = H^{(N)}(\gamma)$ need not be required unitary. The spectra of "energies" may be complex, while the components of the "wave functions" themselves may become directly measurable [4]. Last but not least, simplification of the mathematics may be accompanied by the feasibility of experimental setups in which the generators are allowed to be time dependent, $H = H(t)$ [23].

A. Two coupled waveguides

Theoretical studies of nonstationary systems as well as realizations of experiments remain highly nontrivial. Fortunately, this direction of research also leads to multiple surprising results reconnecting quantum and classical physics. For illustration one may recall the really surprising recent discovery of the failure of applicability of the intuitive adiabatic hypothesis in a non-Hermitian setting [18], which was first reported during the 15th International Workshop on Pseudo-Hermitian Hamiltonians in Quantum Physics, in Palermo [24] in 2015.

For explanation, just a version of the 2×2 toy model of Eq. (6) proved sufficient. In a recent compact review [19] the authors described an interesting application of the new phenomenon to the description of scattering of classical (say, electromagnetic) waves through a two-mode waveguide device. A comparatively satisfactory theoretical explanation of the phenomenon of breakdown of the adiabatic approximation has been achieved via numerical solution of the manifestly time-dependent $N = 2$ evolution rule, (1).

On this background a number of "elusive effects" has been predicted, resulting from the fact that the Hamiltonian matrix itself is symmetric but not real. Indeed, the requirement of its reality would make it Hermitian so that all of the elusive effects would disappear. Theoretically the device was described by a slightly modified version,

$$H(\delta, g, \gamma_1, \gamma_2) = \begin{bmatrix} \delta - i\gamma_1/2 & g \\ g & -i\gamma_2/2 \end{bmatrix}, \tag{14}$$

of the most elementary model, (6). All four parameters (*viz.*, δ, responsible for the so-called detuning; g, denoting mutual symmetric coupling of the modes; and γ_1 and γ_2, gauging the losses in the medium of the two respective waveguides) were chosen real.

The model yields a pair of instantaneous eigenenergies $E_\pm(z) = E_\pm[\delta(z), g(z), \gamma_1(z), \gamma_2(z)]$ which are distinct and complex in general. The secular equation is trivial, yielding the two values $E_\pm(z)$ in closed form. These values may be perceived as evaluations of a two-sheeted analytic function $\mathbb{F}(z)$. According to Kato [11] such an explicit representation of the spectrum also enables us to localize the so-called "exceptional points" $z^{(EP)}$ at which the two levels of the energy happen to merge, $E_+(z^{(EP)}) = E_-(z^{(EP)})$.

In [19], the authors performed the search. In their 2×2 matrix model, (14), the analytic-function representation of the energies appeared to have the square-root form near $z^{(EP)}$, with $\mathbb{F}(z) \sim \sqrt{z - z^{(EP)}}$. In an experimental setup the "no-detuning" choice of $\delta = 0$ and the z-independent choice of the losses $\gamma_{1,2}$ enabled the authors to determine the degeneracy-responsible EP couplings in closed form:

$$g = g[z^{(EP)}] = \tfrac{1}{4}(\gamma_1 - \gamma_2). \tag{15}$$

The existence of the nondiagonalizable EP limit of the Hamiltonian

$$\lim_{z \to z^{(EP)}} H[\delta(z), g(z), \gamma_1(z), \gamma_2(z)] = \frac{1}{4}\begin{bmatrix} -2\,i\gamma_1 & \gamma_1 - \gamma_2 \\ \gamma_1 - \gamma_2 & -2\,i\gamma_2 \end{bmatrix} \tag{16}$$

has also been found to be detectable, experimentally, due to the mathematical property of the eigenvalues which form, in the EP vicinity, the so-called cycle of period 2 (cf. p. 65 in [11]). In the context of physics the latter mathematical peculiarity of the model enabled the authors to reveal the limits of the applicability of the conventional adiabatic hypothesis in the non-Hermitian and non-stationary dynamical setting [19].

Multiple analogous searches for the signatures of the two-sheeted nature of the energy Riemann surfaces have been performed, recently, by many independent experimental groups [25]. In the language of mathematics the existence of the EP2 singularity means that one might perform such a variation of the parameters that the system would be forced to circumscribe its EP2 branch point and to move to the second sheet of the Riemann surface. In order to force the wave function to return to its initial value, one has to circumscribe the EP2 singularity twice.

In an alternative experimental setup one could try to force the system to pass strictly through the EP2 singularity. This would lead to the coalescence $|\psi_0(z^{(\mathrm{EP})})\rangle = |\psi_1(z^{(\mathrm{EP})})\rangle$ of wave functions, tractable as a simulation of a quantum phase transition [26]. Beyond the quantum world, the effect is equally interesting. In the context of waveguides, for example, one could even force the classical photons to stop at EP2 [27].

An analogous theoretical as well as experimental analysis would become much less easily accessible in the general dynamical scenarios characterized by Kato's EPs of order $K > 2$. Any experimental study of dynamical $K > 2$ mode switching would require rather sophisticated equipment, say, complicated but still tractable waveguide systems as sampled, say, in Fig. 6 in Ref. [28].

B. Three coupled waveguides

In Ref. [29] the authors contemplated an experimentally feasible arrangement of a coupled *triplet* of semiconductor waveguides. Their system (exhibiting, in addition, the so-called $\mathcal{PT}$-symmetric distribution of the gain and loss in the medium of the waveguides) found a formal theoretical description in another elementary schematic Hamiltonian, *viz.*, matrix (7). This is a complex and symmetric matrix, not too dissimilar to its two-dimensional predecessor, (6). In Ref. [29] we may read that "in principle the approach of extending the system with additional waveguides ...can be continued [but] ...all further extensions should first be studied in [simplified] approaches."

These sentences may be reread as the most concise formulation of the aims of the present paper. One still has to expect that any extension of the EP2-related results to the case of the K-sheeted Riemann-surface scenarios with $K > 2$ will be complicated. Even in the case of $K = 3$ proper design of the experimental setup required a careful fine-tuning of the parameters [16,30]. On the positive side, strong encouragement comes from the observation that decisive theoretical progress was achieved after the scope of the experiment-oriented searches was restricted to tridiagonal complex symmetric models as sampled by Eq. (7) above. In this sense, a decisive theoretical step forward was made by the authors of Ref. [16]. Subsequently, the practical experimental appeal of the tridiagonal matrix model has been emphasized in [10] and [29].

All of the latter $K = 3$ projects were aimed at a slow motion along a path over a three-sheeted Riemann surface while circumscribing, three times, the carefully localized exceptional point of order 3 (EP3). The details may be found in Fig. 3 in Ref. [29]. What the latter study revealed was, first, the phenomenon of the characteristic permutation of the components of $|\psi\rangle$. This offered a signature of the coalescence of all three eigenfunctions at $z = z^{(\mathrm{EP3})}$. It also appeared to make sense to change the parameters in

$$H = H^{(3)}(z) = \begin{bmatrix} -i\sqrt{z} & \sqrt{A(z)} & 0 \\ \sqrt{A(z)} & 0 & \sqrt{A(z)} \\ 0 & \sqrt{A(z)} & i\sqrt{z} \end{bmatrix}.$$

This simplified the secular polynomial as well as its three energy roots, $E_\pm(z) = \pm\sqrt{2\,A(z) - z}$ and $E_0 = 0 \neq E_0(z)$. One could spot the EP3 singularity at $z = z^{(\mathrm{EP3})} = 1$ and $A(1) = 1/2$,

$$\lim_{z\to z^{(\mathrm{EP3})}} H^{(3)}(z) = H^{(3)}_{(\mathrm{EP3})} = \begin{bmatrix} -i & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & i \end{bmatrix}. \tag{17}$$

An extensive analysis of consequences may be found in Ref. [16]. It led us to conclude that the models using $K > 3$ deserve to be studied along similar lines.

IV. TRIDIAGONAL COMPLEX SYMMETRIC HAMILTONIANS REVISITED

Theoretical papers [12,31] paid attention to systems which are assigned a multisheeted Riemann surface $\mathbb{F}$ admitting the existence and, perhaps, experimental detection of EPs of the Kth order. At any integer K one can work, locally, with the K-sheeted analytic function $\mathbb{F}(z) \sim (z - z^{(\mathrm{EP})})^{1/K}$ representing the energy eigenvalues. In what follows we try to support this point of view constructively.

A. 4 × 4 Hamiltonian matrices

Let us pick up $K = 4$ and contemplate the eligible Hamiltonian matrices in the tridiagonal and complex symmetric form of Eq. (8). The key merit of this choice is that it yields energies $E = \pm\sqrt{x}$ determined in terms of roots of the exactly solvable secular equation

$$x^2 + 10\,xz - 2\,Bx - Ax + 9\,z^2 + 6\,Bz - 9\,zA + B^2 = 0. \tag{18}$$

The availability of the closed formula

$$x_\pm = B - 5\,z + \frac{1}{2}A \pm \frac{1}{2}\sqrt{-64\,Bz + 4\,BA + 64\,z^2 + 16\,zA + A^2} \tag{19}$$

reduces the search for the EP4 confluence of the roots $x_\pm(z^{(\mathrm{EP4})}) = 0$ to the analysis of Eq. (19), yielding the following two algebraic equations for three unknowns:

$$B - 5\,z + 1/2\,A = 0,$$
$$-64\,Bz + 4\,BA + 64\,z^2 + 16\,zA + A^2 = 0. \quad (20)$$

They have the two independent EP4 solutions, *viz*., the well-known Bose-Hubbard solution of Ref. [12],

$$B^{(\mathrm{EP4})} = 3z, \quad A^{(\mathrm{EP4})} = 4z, \quad (21)$$

and the new solution

$$B^{(\mathrm{EP4})} = -27z, \quad A^{(\mathrm{EP4})} = 64z. \quad (22)$$

As long as both of these solutions are nonnumerical, they may easily be analyzed in detail.

1. Bose-Hubbard model revisited

Once we pick up the first solution and set, tentatively, $B = 3$ and $A = 4$, we arrive at the one-parametric family of Hamiltonians

$$H = H^{(4)}(z) = \begin{bmatrix} -3\,i\sqrt{z} & \sqrt{3} & 0 & 0 \\ \sqrt{3} & -i\sqrt{z} & 2 & 0 \\ 0 & 2 & i\sqrt{z} & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 3\,i\sqrt{z} \end{bmatrix} \quad (23)$$

with energies

$$E_{\pm,\pm}(z) = \pm(2 \pm 1)\sqrt{1-z}.$$

All four of them remain real for $z \in (0, 1)$, and all of them vanish at $z = z^{(\mathrm{EP4})} = 1$. Beyond this point, all of the levels become purely imaginary so that the model is to be assigned the physical interpretation of an open quantum system or of a device in classical optics.

Within the interval of $z \in (0, 1)$, on the contrary, the guaranteed reality of the spectrum leads to the possibility of the construction of a metric which would render possible a consistent unitary-evolution interpretation of the system in the quantum setting. The authors of Ref. [12], unfortunately, left this construction of $\Theta(H)$ as well as the discussion of its properties to the readers as an elementary exercise. Here, we return to this point in Sec. V C 2 below.

2. Jordan blocks

By definition, the Bose-Hubbard Hamiltonian, (23), ceases to be diagonalizable at the EP4 singularity. It can only be assigned there the canonical four-dimensional nondiagonal Jordan-block representation. In general, at any EP energy degeneracy of order K we may postulate

$$H^{(K)}(z^{(\mathrm{EPK})})Q^{(K)} = Q^{(K)}J^{(K)}(E). \quad (24)$$

The symbol $J^{(K)}(E)$ stands here for the $K \times K$ Jordan block,

$$J^{(K)}(E) = \begin{bmatrix} E & 1 & 0 & \dots & 0 \\ 0 & E & 1 & \ddots & \vdots \\ 0 & 0 & E & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \dots & 0 & 0 & E \end{bmatrix}. \quad (25)$$

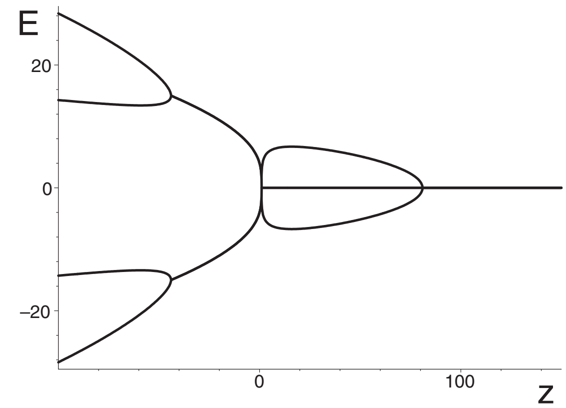

FIG. 1. Real parts of eigenvalues $E_n(z)$ of the non-Hermitian $N = 4$ matrix $H^{(N)}(z)$ of Eq. (26).

The other symbol, $Q = Q^{(K)}$, is Hamiltonian dependent. It denotes the object called the transition matrix. For example, in our present Bose-Hubbard illustrative example with $E = E^{(\mathrm{EP4})} = 0$ and $z^{(\mathrm{EP4})} = 1$ it is entirely routine to evaluate

$$Q^{(4)} = \begin{bmatrix} 6\,i\,z^{3/2} & -6\,z & -3\,i\sqrt{z} & 1 \\ -6\,z^{3/2}\sqrt{3} & -4\,i\,z\sqrt{3} & \sqrt{3}\sqrt{z} & 0 \\ -3\,i\,z^{3/2}\sqrt{3}\sqrt{4} & \sqrt{3}z\sqrt{4} & 0 & 0 \\ 3\,z^{3/2}\sqrt{4} & 0 & 0 & 0 \end{bmatrix}.$$

This transition matrix plays a key role in the perturbation-expansion analysis of Schrödinger equations (1) in the vicinity of EPs of any order $K \geqslant 2$. The physical consequences as well as the mathematical details are explained in Ref. [12] and, beyond the Bose-Hubbard illustrative example, in Ref. [31].

3. Generalized Bose-Hubbard model

Our first new, non-Bose-Hubbard result is that we may insert $B = -27$ and $A = 64$ into Eq. (8). This yields the EP4-supporting complex symmetric toy model

$$H^{(4)}(z) = \begin{bmatrix} -3\,i\sqrt{z} & 3\,i\sqrt{3} & 0 & 0 \\ 3\,i\sqrt{3} & -i\sqrt{z} & 8 & 0 \\ 0 & 8 & i\sqrt{z} & 3\,i\sqrt{3} \\ 0 & 0 & 3\,i\sqrt{3} & 3\,i\sqrt{z} \end{bmatrix} \quad (26)$$

with energies

$$E_{\pm,\pm}(z) = \pm\sqrt{5 - 5\,z \pm 4\sqrt{-44 + 43\,z + z^2}}. \quad (27)$$

The analysis is again straightforward. Graphically, the z dependence of the real and imaginary parts of the eigenvalues of matrix (26) is displayed in Figs. 1 and 2, respectively. The plots show that all four energies vanish at $z = 1$ (EP4). The inner square-root expression remains purely imaginary at smaller positive $z \in (0, 1)$ so that all four related energies are complex. Otherwise, the inner square-root expression is real so that one only has to distinguish between the interval $z \in (1, 81)$ (in which we have two real and two purely imaginary energies) and the interval $z \in (81, \infty)$.

In the latter interval all four energy roots are purely imaginary so that an *ad hoc* premultiplication of matrix (26) by

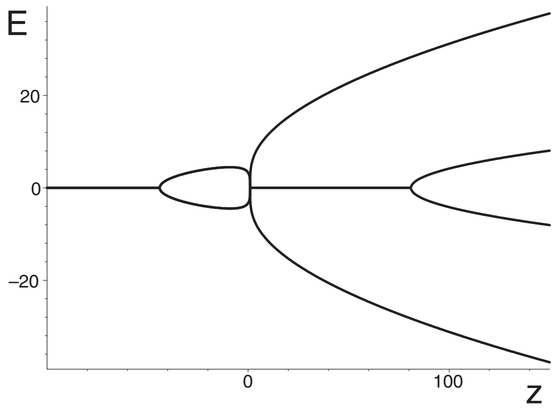

FIG. 2. Imaginary parts of eigenvalues $E_n(z)$ of the non-Hermitian $N = 4$ matrix $H^{(N)}(z)$ of Eq. (26).

an imaginary unit would make the spectrum real, rendering the resulting complex symmetric matrix $\tilde{H}^{(4)}(z) = i\,H^{(4)}(z)$ eligible as a correct and physical hidden Hermitian generator of unitary evolution in a new, slightly exotic quantum model with just two imaginary matrix elements.

One can summarize that at positive $z \geqslant 0$ the model exhibits the EP4 degeneracy at $z = 1$ and the EP2 degeneracy at $z = 81$. It is worth adding that at $z = 1$ the model satisfies Eq. (24) with the following transition matrix:

$$Q^{(4)} = \begin{bmatrix} 216\,i z^{3/2} & -36\,z & -3\,i\sqrt{z} & 1 \\ 72\,z\sqrt{-3\,z} & -12\,i\sqrt{z}\sqrt{-3\,z} & 3\sqrt{-3\,z} & 0 \\ -9\,iz\sqrt{-3\,z}\sqrt{64} & 3\sqrt{-3\,z}\sqrt{64}\sqrt{z} & 0 & 0 \\ -27\,z^{3/2}\sqrt{64} & 0 & 0 & 0 \end{bmatrix}.$$

In the case of the hiddenly Hermitian Hamiltonian $\tilde{H}^{(4)}(z)$ only two of the energies vanish in the limit $z \to z^{(\mathrm{EP2})} = 81$ so that a perturbation study of its vicinity would only be based on the use of a transition matrix of rank 2.

B. 5 × 5 Hamiltonian matrices

With $N = 5$ and with the Bose-Hubbard choice of $B = 4$, $A = 6$, and $z \geqslant 0$ in (9) we have to deal with the tridiagonal complex symmetric Hamiltonian possessing, up to a constant level $E_0 = 0$, the following four z-dependent energy eigenvalues:

$$E_{\pm,\pm}(z) = \pm(3 \pm 1)\sqrt{(1 - z)}.$$

They stay real for $z \in (0, 1)$, and all of them vanish at $z = 1$. The EP5 presence is readily verified. The z-dependent quadruplet becomes purely imaginary at any $z > 1$ [12]. At $z = z^{(\mathrm{EP5})} = 1$ the Hamiltonian ceases to be diagonalizable. With transition matrix

$$Q^{(5)} = \begin{bmatrix} 24 & 24\,i & -12 & -4\,i & 1 \\ 48\,i & -36 & -12\,i & 2 & 0 \\ -24\sqrt{6} & -12\,i\sqrt{6} & 2\sqrt{6} & 0 & 0 \\ -48\,i & 12 & 0 & 0 & 0 \\ 24 & 0 & 0 & 0 & 0 \end{bmatrix}$$

it may still be shown to satisfy Eq. (24).

1. Bose-Hubbard model revisited

Even if we do not specify parameters A and B, the 5×5 complex symmetric tridiagonal matrix Hamiltonian, (9), preserves the symmetry of the energies $E = \pm\sqrt{x}$. Keeping in mind the z-independent root $x_0 = 0$, i.e., $E_0 = 0$ we still have an utterly elementary secular equation:

$$x^2 + 20\,xz - 2\,xB - 2\,Ax + 2\,AB - 32\,zA + 64\,z^2 + 16\,zB + B^2 = 0. \quad (28)$$

It is straightforward to deduce that

$$x_\pm = B - 10\,z + A \pm \sqrt{-36\,zB + 36\,z^2 + 12\,zA + A^2}.$$

The search for the EP5 confluence proceeds again via the pair of relations

$$-36zB + 36\,z^2 + 12zA + A^2 = 0, \quad B - 10z + A = 0, \quad (29)$$

with solutions

$$B^{(\mathrm{EP5})} = 4z, \quad A^{(\mathrm{EP5})} = 6z \quad (30)$$

and

$$A^{(\mathrm{EP5})} = -54z, \quad B^{(\mathrm{EP5})} = 64z. \quad (31)$$

This means that the conclusions may be expected to remain qualitatively the same as those at $N = 4$ above.

2. Generalized Bose-Hubbard model

The non-Bose-Hubbard choice of $B = 64$ and $A = -54$ yields the "anomalous" Hamiltonian

$$H^{(5)}(z) = \begin{bmatrix} -4\,i\sqrt{z} & 8 & 0 & 0 & 0 \\ 8 & -2\,i\sqrt{z} & 3\,i\sqrt{6} & 0 & 0 \\ 0 & 3\,i\sqrt{6} & 0 & 3\,i\sqrt{6} & 0 \\ 0 & 0 & 3\,i\sqrt{6} & 2\,i\sqrt{z} & 8 \\ 0 & 0 & 0 & 8 & 4\,i\sqrt{z} \end{bmatrix}.$$

Up to the constant "observer energy" $E = 0$, the quadruplet of its nontrivial energies reads

$$E_{\pm,\pm}(z) = \pm\sqrt{-10\,z + 10 \pm 6\sqrt{z^2 - 82\,z + 81}}.$$

They vanish at $z = 1$ (EP5). One can detect the occurrence of two coupled EP2 singularities at $z = 81$, with the two nonvanishing, purely imaginary energies $E_\pm^{(\mathrm{EP2})} = \pm\sqrt{-800}$ in Eq. (24).

The classification of the reality or imaginarity of the energies proceeds as before. One finds four complex energy roots in the interval of $z \in (1, 81)$, the quadruplet of the purely imaginary roots at the larger $z \in (81, \infty)$, and, finally, two real and two imaginary energies at the smallest eligible $z \in (0, 1)$. Evaluation of the EP5 transition matrix

$$Q^{(5)} = \begin{bmatrix} -3456 & -576\,i & 48 & -4\,i & 1 \\ -1728\,i & -144 & -48\,i & 8 & 0 \\ -1728\,i\sqrt{6} & 144\sqrt{6} & 24\,i\sqrt{6} & 0 & 0 \\ 1728\,i & -432 & 0 & 0 & 0 \\ -3456 & 0 & 0 & 0 & 0 \end{bmatrix}$$

completes the whole construction.

V. DISCUSSION

Once a Hamiltonian admits complex eigenvalues, we lose the possibility of its Hermitization, i.e., of the unitarity of quantum evolution based on the introduction of a suitable *ad hoc* metric $\Theta = \Theta(H)$ amending the Hilbert space. Two consistent physical interpretations of the model remain available. In one we can treat the model as an incomplete, effective description of the so-called open quantum system (cf. [3,32]. In an alternative interpretation one returns to classical physics and one accepts the loss of unitarity as a characteristic feature of the evolution process in question.

In the present paper we have considered both the real- and the complex-spectrum scenarios. We have pointed out the similarities as well as the differences. A number of technical challenges has been considered, indicating that the most difficult part of the buildup of an acceptable *quantum* non-Hermitian unitary model may be seen in its necessary Hermitization, i.e., in the construction of the Hamiltonian-dependent metric $\Theta(H)$. In comparison, the most difficult part of the proposals of the analogous *classical-physics* models relates to their realization in the laboratory.

Let us now add a few remarks. We stress a few of the most important differences, mathematical as well as phenomenological. We also intend to emphasize the existence of shared features including (1) the phenomenological relevance of the EP singularities and (2) the practical feasibility of predictions.

A. Physics represented by classical non-Hermitian Hamiltonians

Within the nonquantum setup the most difficult obstacles are currently well known to emerge in the design of experimental realizations. The absence of the necessity of the construction of the physical inner products simplifies the mathematics. The majority of the existing experiments seems to be connected with the most elementary picture of non-Hermitian eigenvalue degeneracies *alias* phase transitions (we restricted our consideration to the finite-dimensional models mainly for this reason).

The mathematical core of our message may be seen in the construction of the models in which just a few eigenvalues merge at an elementary exceptional point of order K (EPK) with a not too large K. We just returned to our constructive studies of quantum models possessing higher-order exceptional points [33], and we just omitted the requirement of reality of the spectrum. This change of perspective was inspired by the recent growth of interest in sophisticated experiments localizing the exceptional points of higher order in classical systems. We felt mostly inspired by the recent conference report [29] in which exceptional points of third order (EP3) were studied in a system of coupled waveguides. We also noted that in Ref. [34], optical microcavities were identified as prime candidates for the sensing applications of EPs. The third-order exceptional points were identified, in Ref. [35], for a system of three coupled microrings made from a semiconductor material. Using the same, rather restricted and more or less purely numerical mathematics, researchers also considered waves coupled in acoustic cavities with asymmetric losses in which realization of the fourth-order EP4 proved feasible [36].

We decided to concentrate on the not yet fully clarified theoretical aspects of similar experiments. In contrast to the difficulties of the practical fine-tuning of parameters in experiments, the construction of nonquantum theoretical models supporting Kth-order exceptional points may already be declared well advanced at present. These developments proceeded along several independent lines. Physicists tested and, subsequently, widely accepted that, first, one can hardly move beyond the $N = 3$ matrix models without the heuristically helpful requirement of $\mathcal{PT}$ symmetry [37].

The acceptance of $\mathcal{PT}$ symmetry opened the way towards the not entirely expected nonnumerical (albeit computer-assisted and symbolic-manipulation-based [38]) constructions of suitable Hs and, in particular, to the localization of their EPs via closed formulas [33,39,40]. Another efficient EP-construction tool has been found in the standard self-adjoint toy models known and used in condensed-matter physics. Via straightforward replacement of some of their real parameters with purely imaginary or complex quantities it was possible to preserve the underlying algebraic solvability features. Interesting generalizations were obtained for the $\mathcal{PT}$-symmetrized Su-Schrieffer-Heeger model [41], the Aubry-André and Harper models [42], etc.

In the $\mathcal{PT}$-symmetrized Bose-Hubbard model of Graefe *et al.* [12] the authors were particularly successful when they recalled the representation theory of angular momentum algebra. This facilitated their study of the unfolding of EP degeneracy under perturbations. In the present paper, another feature of the model (*viz*., the matrix tridiagonality and complex symmetry of the Hamiltonian) was found to be almost equally useful for generalizations, especially at lower-dimension N's. Along these lines we discovered the existence of a family of new, in general nonunitary and non-Bose-Hubbard, models possessing higher-order exceptional points.

B. Mathematics behind exceptional-point unfolding

The turn of our attention to classical optics enabled us to avoid various mathematical challenges connected with the proper probabilistic interpretation of evolving state vectors $|\psi\rangle$ in the consequent quantum setting. We did not need to consider the Hermitian-conjugate form of Eq. (1) which must be solved in the full-fledged non-Hermitian quantum mechanics [43]. We also did not need to insist on the reality of the eigenvalues of H itself, which may be necessary for the very observability of quantum systems. At the same time, our interest in the systems near EPs may be perceived as shared by both classical and quantum physicists, in both cases being separated into their experimental and theoretical subcategories.

One of the most interesting questions emerging in the vicinity of EPs concerns the role of perturbations in the removal of an EP-related spectral degeneracy. A key mathematical subtlety of such an "EP unfolding" reflects the fact that one has to distinguish between the unfolding of a single EP of order K and the unfolding of a family of lower-order EPs of the respective orders K_1, ..., K_n such that $K_1 + \ldots + K_n = K$. In mathematical language, one has to speak here about the so-called "cycles" [11]. For our present purposes, the optimal clarification of physics behind such a scenario may be mediated by examples.

1. The cycles and their degeneracy at $N = 3$

In the constructive analysis of the non-Hermitian 3×3 matrix toy-model Hamiltonian of Ref. [16] the authors emphasized that the existence of the standard, EP3-related Jordan-block canonical form

$$J^{(3)}(E) = \begin{bmatrix} E & 1 & 0 \\ 0 & E & 1 \\ 0 & 0 & E \end{bmatrix} \quad (32)$$

of their three-dimensional tridiagonal toy-model Hamiltonian implies that in the vicinity of the EP3 singularity the eigenenergies may be perceived as represented by the analytic function which lives on a three-sheeted Riemann surface (see, e.g., pp. 63–65 in [11]) for details). This is a purely theoretical feature of the model which is in a one-to-one correspondence with the possibility of the experimental confirmation that whenever one succeeds in circumscribing the singularity, three circles are needed for the system to return to its initial state, i.e., in the language of quantum mechanics, to the initial wave function. In parallel, the authors of Ref. [16] also added the remark that after some other choice of the parameters in their Hamiltonian, one can encounter an alternative scenario in which the system returns to its initial state after a mere *two* circles.

Explanation of the apparent paradox is easy: the $K = 2$ nature of the new situation will merely reflect the partial survival of the diagonalizability of the Hamiltonian. The canonical form of H will be mediated by Eq. (24), in which one obtains the $K = 2$ Jordan-block result of the following form:

$$J^{(1+2)}(E', E) = \begin{bmatrix} E' & 0 & 0 \\ 0 & E & 1 \\ 0 & 0 & E \end{bmatrix}. \quad (33)$$

Thus, a cycle of lower order appears here due to the accidental degeneracy $E' \to E$ between a non-EP and an EP energy level.

2. Degenerate cycles at $N = 4$

Similar effects may be encountered also at higher matrix dimensions N of course. The explanation is given by the relationship between the number of circles and the respective dimensions K_j of the canonical Jordan blocks given by the so-called periods of the cycles of the eigenvalues in the vicinity of degenerate EPs (cf., e.g., p. 65 and eq. (1.6) in [11]).

The canonical form of our present $N = 4$ complex symmetric Hamiltonian, (8), can mimic the reduction phenomenon at the EP2 parameters $B = -27$, $A = 64$, and $z = 81$, yielding, via Eq. (24), the mere $K = 2$ Jordan-block canonical representation

$$J^{(1+1+2)}(E', E'', E) = \begin{bmatrix} E' & 0 & 0 & 0 \\ 0 & E'' & 0 & 0 \\ 0 & 0 & E & 1 \\ 0 & 0 & 0 & E \end{bmatrix}, \quad E = 0. \quad (34)$$

This means that, hypothetically, the system returns to its original state after the mere two circles circumscribing the EP singularity.

Along the same lines one could even get an exhaustive classification of the alternative scenarios. For four-dimensional Hamiltonians, for example, one could complement the abovementioned EP4 and single-EP2 scenarios by the single-EP3 possibility

$$J^{(1+3)}(E', E) = \begin{bmatrix} E' & 0 & 0 & 0 \\ 0 & E & 1 & 0 \\ 0 & 0 & E & 1 \\ 0 & 0 & 0 & E \end{bmatrix} \quad (35)$$

or, finally, by its double-EP2 alternative

$$J^{(2+2)}(E', E) = \begin{bmatrix} E' & 1 & 0 & 0 \\ 0 & E' & 0 & 0 \\ 0 & 0 & E & 1 \\ 0 & 0 & 0 & E \end{bmatrix}. \quad (36)$$

An exhaustive classification of the five-dimensional (or higher) nonequivalent scenarios would be slightly more complicated but equally straightforward.

C. Physics behind the quantum non-Hermitian models

In quantum systems one has to deal with several paradoxical new aspects of the old question of the stability or instability of systems exposed to small perturbations. In the quantum unitary-evolution setting the emergence of instabilities *alias* quantum catastrophes, is not always sufficiently well understood or explained in the literature, despite being one of the most characteristic consequences of the occurrence of EPs. Along these lines, a complementary inspiration of our research was provided also by the conventional Hermitian treatment of quantum information. The $\mathcal{PT}$-symmetrization recipe opened the way, e.g., towards the perfect-transfer-of-states protocol, which has been based on the choice and treatment of the Hamiltonian as an angular momentum in an external magnetic field [44].

There exist two remarkable by-products of the latter choices of H. One of them lies in the exact, nonnumerical description of the critical behavior at the EP2 singularities even after a fairly nontrivial hypercube-graph generalization of the model. This might prove inspiring in the future. Another source of inspiration may be found in Ref. [28], where the authors developed a recursive bosonic quantization technique which is able to generate the generalized classes of the $\mathcal{PT}$-symmetric networks and other classical photonic structures exhibiting numerous interesting topological and symmetry features (cf., e.g., Fig. 2 in [28]).

Once one's attention turns to non-Hermitian quantum systems, one reveals the existence of a number of paradoxes, often created by the lack of the necessary mathematical insight. The physics of quantum systems represented by non-Hermitian phenomenological observables $H^{(N)}$, $\Lambda^{(N)}$, ... (with real spectra and with any matrix dimension N, finite or infinite) becomes particularly interesting in the vicinity of their EP-singularity boundaries. For illustration, a few quantitative studies of the emergence of related quantum phase transitions may be found in [33]. The authors of some other studies did not always keep in mind the fundamental requirements for the consistent probabilistic interpretation of their quantum models. This may lead to misunderstandings, indeed.

1. The strength-of-perturbation paradox

The physics represented by non-Hermitian operators is still under intensive development. In most cases, one just has to avoid certain more or less elementary misunderstandings. Many of them have been clarified in a review [2]. One encounters subtler forms also in the more recent literature. For example, in Ref. [45] the authors claim to have detected "unexpected wild properties of operators familiar from *PT*-symmetric quantum mechanics," and as a consequence, they "propose giving the mathematical concept of the pseudospectrum a central role in quantum mechanics with non-Hermitian operators." The phenomenologically disturbing "immanent instability" claims are also illustrated, by the authors of Ref. [45], via a number of $N = \infty$ ordinary differential models.

Despite the use of a high-quality functional analysis the authors' correct mathematical results are accompanied by their misleading physical interpretation. We cannot endorse their claims. The point lies very close to our above discussion: One must distinguish between the classical, Maxwell-equation systems and the unitary quantum models. Exclusively in the classical case the picture of the "wild" physics is realistic (cf. also a number of further examples of the non-Hermiticity-caused instabilities in [7]). In the quantum-physics approach, in contrast, it would be necessary to amend the inner-product metric $I \to \Theta$, making the quantum version of the theory consistent by means of the necessary transition from the auxiliary, "user-friendly" but "false" Hilbert space $\mathcal{H}^{(F)}$ to its correct, physical, "standard" alternative $\mathcal{H}^{(S)}$.

The latter transition is not considered in [45]. This leads to the misleading conclusions. Their essence lies in the use of the "false" pseudospectrum:

$$\Lambda_\epsilon^{(F)}(A) = \{\lambda \in \mathbb{C} \mid \exists \psi \in \mathcal{H}^{(F)} \setminus \{0\}, \exists V : (A+V) \psi = \lambda\psi, ||V||_{\mathcal{H}^{(F)}} \leqslant \epsilon\}.$$

This definition is inappropriate, based on the use of the norm of the perturbation V in the *manifestly unphysical* Hilbert space $\mathcal{H}^{(F)}$. The analysis of the latter, ill-defined (or, better, unphysical) pseudospectrum is, in the unitary quantum-theory setting, irrelevant. The calculation does not take into account the realistic metric, i.e., the different geometry of the unique physical Hilbert space $\mathcal{H}^{(S)}$.

In the quantum world the influence of perturbations must necessarily be characterized by another, correctly defined, *metric-dependent* pseudospectrum:

$$\Lambda_\epsilon^{(S)}(A) = \{\lambda \in \mathbb{C} \mid \exists \psi \in \mathcal{H}^{(S)} \setminus \{0\}, \exists V : (A+V) \psi = \lambda\psi, ||V||_{\mathcal{H}^{(S)}} \leqslant \epsilon\}.$$

In spite of the technically much more complicated nature of the latter, amended pseudospectrum, one cannot expect its evaluation to lead to the "unexpected wild properties" of any admissible $\mathcal{PT}$-symmetric operators [31]. Indeed, whenever one satisfies the (necessary) hidden-Hermiticity constraint, (10), and whenever the perturbations remain small in the correct physical geometry of Hilbert space $\mathcal{H}^{(S)}$, one *does not* encounter any instabilities.

2. The Bose-Hubbard unfolding paradox

In the non-Hermitian but $\mathcal{PT}$-symmetric Bose-Hubbard quantum model the authors of Ref. [12] studied the phenomenon of the unfolding (i.e., of the removal of degeneracy) of the higher-order exceptional-point energy under a well-defined perturbation V. Unfortunately, they also did not formulate the task in a consistent manner, i.e., in the correct physical Hilbert space $\mathcal{H}^{(S)}$ with metric $\Theta^{(\text{correct})}(H_0 + V)$. For this reason, the description of the unfolding of the multiply degenerate (i.e., higher-order EP) Bose-Hubbard bound-state energies $E_n(\gamma^{(\text{EP})})$ after perturbation {cf. sections 4 (numerical results) and 5 (perturbation results) in Ref. [12]} must be characterized as incomplete. The main reason is that the self-consistent nature of perturbation theory in the non-Hermitian quantum picture makes the calculations, in effect, nonlinear. We have to keep in mind that

$$\Theta_0 = \Theta(H_0) \neq \Theta^{(\text{correct})}(H_0 + V) = \Theta_0 + K(\Theta_0, H_0, V).$$

For each separate perturbation V we have to repeat the solution of Eq. (10). For "sufficiently small" perturbations (whatever that means) we can simplify the process and neglect the higher-order terms. Equation (10) gets replaced by

$$H_0^\dagger K - K H_0 = \Theta_0 V - V^\dagger \Theta_0, \tag{37}$$

i.e., by the implicit definition of the leading-order form of K. Whenever one skips this apparently merely technical step, the results cannot be declared physical.

In the $\mathcal{PT}$-symmetric Bose-Hubbard case the criticism from Sec. V C 1 reapplies. The proper probabilistic interpretation cannot be provided without the knowledge of $\Theta^{(\text{correct})}(H_0 + V)$. Without this knowledge, the perturbed system is merely tractable as classical. Moreover, in [12], the perturbed eigenvalues cease to be real and form rings on the complex plane. The perturbed Bose-Hubbard quantum system ceases to be observable so that it must be declared nonunitary and unstable.

Beyond the concrete Bose-Hubbard model the generic change of non-Hermitian perturbations will always imply a nontrivial change of the metric Θ. The mutual relationship between these changes can be best studied in quantum systems with small $N \ll \infty$. The correlations become particularly relevant near the dynamical EP singularity. In the EP limit the eligible Hamiltonian-Hermitization metrics $\Theta(H)$ will cease to exist because all of the candidates for the metric [i.e., *all* of the solutions of Eq. (10)] will cease to be invertible. The geometry of the physical Hilbert space will become, in the EP vicinity, strongly anisotropic [20].

VI. SUMMARY

Although the notion of the exceptional point (EP) emerged, in the context of perturbation theory, in mathematics [11], it very quickly acquired applications in several branches of physics [46]. The conference "The Physics of Exceptional Points" in 2010 [47] covered, for example, domains of physics as different as the study of Bose-Einstein condensates and of light-matter interactions, the behavior of molecules during photodissociation, the phase transitions related to the spontaneous breakdown of $\mathcal{PT}$ symmetry, and questions of stability in many-body quantum systems as well as in classical magnetohydrodynamics. Still, the most immediate motivation of the meeting seems to have been provided by the series of speculations and experiments [25] which demonstrated the presence of an EP singularity in the eigenvalue and eigenvector spectra of various classical devices. In [48], for example, two modes of a certain classical electromagnetic microwave billiard [i.e., eigenvectors $\psi_1(z)$ and $\psi_2(z)$ of its "Hamiltonian" $H(z)$] were shown to coalesce, at the EP singularity (i.e., at a parameter $z = z^{(\mathrm{EP})}$), with a phase difference of $\pi/2$.

The EP singularity in question was shown to be of the square-root type (abbreviated EP2). From the point of view of elementary linear algebra this means that the 2×2 matrix $H(z^{(\mathrm{EP})})$ ceased to be diagonalizable and that it acquired the canonical form of a 2×2 Jordan block. In the language of functional analysis the related two eigenvalues, $E_1(z)$ and $E_2(z)$, of $H(z)$ with $z \neq z^{(\mathrm{EP2})}$ could be called "cyclic," of period 2 (cf. p. 64 in [11]). The importance of this feature in physics can be deduced from the very logo of the conference [47]. In an illustration of the consequences of cyclicity this logo samples the intensity of the electromagnetic field in the microwave during a step-by-step variation of parameter $z = z(t)$. The parameter is made to circumscribe its critical value $z^{(\mathrm{EP2})}$ so that one can see that the billiard can only return to its initial state after two circles.

In the present paper we have emphasized that under the assumption of complex symmetry and tridiagonality of Hamiltonians, the transition to the more general $N \times N$ matrices $H^{(N)}(z^{(\mathrm{EP})})$ can be found, both theoretically and experimentally, feasible. Decisive encouragement can be sought in the purely empirical fact that in the dedicated literature, virtually all of the successful benchmark Hamiltonians $H^{(N)}(z)$ are being chosen, even at the lowest dimensions, $N = 2$ and $N = 3$, in the very specific complex symmetric and tridiagonal matrix forms exhibiting a number of features shared with the angular-momentum representation methods, say, of Refs. [12] and [39] or [28]. In this spirit we have performed here an extended search using a straightforward linear algebraic method. Considering just a few-parametric class of the eligible candidates $H^{(N)}(z)$ we filled the gap, on the side of theory, up to $N = 4$ and $N = 5$. The resulting models appeared, unexpectedly, to be exactly solvable. We believe that experimental simulations based on these matrices will prove equally user-friendly in the future, especially in the vicinity of the various EP-limiting cases.

ACKNOWLEDGMENT

This work was supported by GAČR Grant No. 16-22945S.

[1] *Non-Selfadjoint Operators in Quantum Physics: Mathematical Aspects*, edited by F. Bagarello, J.-P. Gazeau, F. H. Szafraniec, and M. Znojil (Wiley, Hoboken, NJ, 2015).

[2] A. Mostafazadeh, Int. J. Geom. Meth. Mod. Phys. **7**, 1191 (2010).

[3] N. Moiseyev, *Non-Hermitian Quantum Mechanics* (Cambridge University Press, Cambridge, UK, 2011).

[4] R. El-Ganainy, K. G. Makris, M. Khajavikhan *et al.*, Nat. Phys. **14**, 11 (2018).

[5] C. M. Bender and S. Boettcher, Phys. Rev. Lett. **80**, 5243 (1998).

[6] C. M. Bender, Rep. Prog. Phys. **70**, 947 (2007).

[7] L. N. Trefethen and M. Embree, *Spectra and Pseudospectra* (Princeton University Press, Princeton, NJ, 2005).

[8] K. G. Makris, R. El-Ganainy, D. N. Christodoulides, and Z. H. Musslimani, Phys. Rev. Lett. **100**, 103904 (2008).

[9] R. El-Ganainy, M. Khajavikhan, and Li Ge, Phys. Rev. A **90**, 013802 (2014).

[10] J. Schnabel, H. Cartarius, J. Main, G. Wunner, and W. D. Heiss, Phys. Rev. A **95**, 053868 (2017).

[11] T. Kato, *Perturbation Theory for Linear Operators* (Springer-Verlag, Berlin, 1966).

[12] E. M. Graefe, U. Günther, H. J. Korsch, and A. E. Niederle, J. Phys. A: Math. Theor. **41**, 255206 (2008).

[13] M. Znojil, Symm. Integr. Geom. Methods Appl. (SIGMA) **5**, 001 (2009).

[14] S. R. Garcia and M. Putinar, Trans. Am. Math. Soc. **358**, 1285 (2005).

[15] S. R. Garcia, conference talk, cf. http://mxn.ujf.cas.cz/∼esfxnsa.

[16] G. Demange and E.-M. Graefe, J. Phys. A: Math. Theor. **45**, 025303 (2012).

[17] F. G. Scholtz, H. B. Geyer, and F. J. W. Hahne, Ann. Phys. (NY) **213**, 74 (1992).

[18] T. J. Milburn, J. Doppler, C. A. Holmes, S. Portolan, S. Rotter, and P. Rabl, Phys. Rev. A **92**, 052124 (2015).

[19] J. Doppler, A. A. Mailybaev, J. Böhm *et al.*, Nature **537**, 76 (2016).

[20] D. Krejčiřík, V. Lotoreichik, and M. Znojil, Proc. R. Soc. A **474**, 20180264 (2018).

[21] M. Philipp, P. von Brentano, G. Pascovici, and A. Richter, Phys. Rev. E **62**, 1922 (2000); C. Dembowski, H.-D. Gräf, H. L. Harney, A. Heine, W. D. Heiss, H. Rehfeld, and A. Richter, Phys. Rev. Lett. **86**, 787 (2001).

[22] R. El-Ganainy, K. G. Makris, D. N. Christodoulides, and Z. H. Musslimani, Opt. Lett. **32**, 2632 (2007); Ch. E. Rüter, K. G. Makris, R. El-Ganainy *et al.*, Nat. Phys. **6**, 192 (2010).

[23] M. Znojil, Phys. Rev. D **78**, 085003 (2008).

[24] http://www.math.unipa.it/˜phhqp15/.

[25] M. Lawrence, N. Xu, X. Zhang, L. Cong, J. Han, W. Zhang, and S. Zhang, Phys. Rev. Lett. **113**, 093901 (2014); T. Gao, E. Estrecho, K. Y. Bliokh *et al.*, Nature **526**, 554 (2015); H. Xu, D. Mason, L. Jiang, and J. G. E. Harris, *ibid.* **537**, 80 (2016).

[26] E. Caliceti and S. Graffi, in [1], pp. 189–240; M. Znojil, Ann. Phys. (NY) **336**, 98 (2013); D. I. Borisov, Acta Polytech. **54**, 93 (2014); D. I. Borisov, F. Růžička, and M. Znojil, Int. J. Theor. Phys. **54**, 4293 (2015); D. I. Borisov and M. Znojil, in *Non-Hermitian Hamiltonians in Quantum Physics*, edited by F. Bagarello, R. Passante, and C. Trapani, Springer Proceedings

in Physics, Vol. 184 (Springer, Berlin, 2016), pp. 201–217, arXiv:1303.4876v3.
[27] T. Goldzak, A. A. Mailybaev, and N. Moiseyev, Phys. Rev. Lett. **120**, 013901 (2018).
[28] M. H. Teimourpour, R. El-Ganainy, A. Eisfeld, A. Szameit, and D. N. Christodoulides, Phys. Rev. A **90**, 053817 (2014).
[29] J. Schnabel, H. Cartarius, J. Main *et al.*, Acta Polytech. **57**, 454 (2017).
[30] W. D. Heiss, J. Phys. A: Math. Theor. **41**, 244010 (2008); W. D. Heiss and G. Wunner, *ibid.* **49**, 495303 (2016).
[31] M. Znojil, Phys. Rev. A **97**, 032114 (2018).
[32] I. Rotter, J. Phys. A: Math. Theor. **42**, 153001 (2009).
[33] M. Znojil, J. Phys. A: Math. Theor. **45**, 444036 (2012); G. Lévai, F. Růžička, and M. Znojil, Int. J. Theor. Phys. **53**, 2875 (2014); M. Znojil, Symmetry **8**, 52 (2016).
[34] W.-J. Chen, S. K. Özdemir, G.-M. Zhao, J. Wiersig, and L. Yang, Nature **548**, 192 (2017).
[35] H. Hodaei, A. U. Hassan, S. Wittek, H. Garcia-Gracia, R. El-Ganainy, D. N. Christodoulides, and M. Khajavikhan, Nature **548**, 187 (2017).
[36] K. Ding, G. Ma, M. Xiao, Z.-Q. Zhang, and C.-T. Chan, Phys. Rev. X **6**, 021007 (2016).
[37] M. Znojil, Phys. Lett. B **647**, 225 (2007); Phys. Lett. A **367**, 300 (2007).
[38] M. Znojil, Phys. Rev. A **82**, 052113 (2010).
[39] M. Znojil, J. Phys. A: Math. Theor. **40**, 4863 (2007).
[40] M. Znojil, J. Phys. A: Math. Theor. **40**, 13131 (2007); Phys. Lett. B **650**, 440 (2007).
[41] F. Růžička, Int. J. Theor. Phys. **54**, 4154 (2015).
[42] A. K. Harter, T. E. Lee, and Y. N. Joglekar, Phys. Rev. A **93**, 062101 (2016).
[43] M. Znojil, Ann. Phys. (NY) **385**, 162 (2017).
[44] X. Z. Zhang, L. Jin, and Z. Song, Phys. Rev. A **85**, 012106 (2012).
[45] D. Krejčiřík, P. Siegl, M. Tater, and J. Viola, J. Math. Phys. **56**, 103513 (2015).
[46] M. V. Berry, Czech. J. Phys. **54**, 1039 (2004); W. D. Heiss, *ibid.* **54**, 1091 (2004); J. Phys. A: Math. Theor. **45**, 444016 (2012); V. M. Martinez Alvarez, J. E. Barrios Vargas, and L. E. F. Foa Torres, Phys. Rev. B **97**, 121401(R) (2018).
[47] http://www.nithep.ac.za/2g6.htm. Accessed 28 January 2018.
[48] C. Dembowski, B. Dietz, H.-D. Gräf, H. L. Harney, A. Heine, W. D. Heiss, and A. Richter, Phys. Rev. Lett. **90**, 034101 (2003).