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### Tridiagonal $\mathcal{PT}$ -symmetric *N*-by-*N* Hamiltonians and a fine-tuning of their observability domains in the strongly non-Hermitian regime

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#### Abstract

A generic  $\mathcal{PT}$ -symmetric Hamiltonian is assumed tridiagonalized and truncated to  $N < \infty$  dimensions,  $H \to H^{(\text{chain model})}$ , and all its up-down symmetrized special cases with J = [N/2] real couplings are considered,  $H^{(\text{chain model})} \to H^{(N)}$ . Using symbolic manipulation and extrapolation techniques we find out that in the strongly non-Hermitian regime the secular equation gets partially factorized at all N. This enables us to reveal a finetuned alignment of the dominant couplings implying an asymptotically sharply spiked shape of the boundary of the J-dimensional quasi-Hermiticity domain  $\mathcal{D}^{(N)}$  in which all the spectrum of energies  $E_n^{(N)}$  remains real and observable.

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#### 1. Introduction

Unexpectedly often, many general theoretical considerations as well as practical phenomenological applications of quantum mechanics rely on the exceptionally friendly mathematics connected with the one-dimensional harmonic oscillator  $H^{(HO)}$ . In particular, the equidistance of its energies (say, E = 1, 3, 5, ... in suitable units) proves fairly favorable in perturbation theory where it simplifies the practical calculations of the spectra of the various anharmonic oscillators

$$H^{(\text{AHO})} = H^{(\text{HO})} + H^{(\text{perturbation})}.$$
 (1)

Even when one restricts attention to the mere *finite-dimensional* perturbations written in terms of the eigenvectors  $|m^{(HO)}\rangle$  of  $H^{(HO)}$  itself,

$$H^{(\text{perturbation})} = \sum_{m,n=1}^{N} |m^{(\text{HO})}\rangle \tilde{W}_{m,n}^{(N)} \langle n^{(\text{HO})}|, \qquad (2)$$

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the finite-dimensional matrix example (1) + (2) may produce a lot of theoretical inspiration as sampled, e.g., in chapter two of Kato's classical book on perturbation theory where many low-dimensional Hermitian as well as non-Hermitian sample matrices were considered [1].

The parallel, purely phenomenological inspiration by the truncated equation (2) need not be less exciting. For example, the authors of an explicit numerical exercise [2] felt inspired by the recent growth of popularity of the  $\mathcal{PT}$ -symmetric [3] and pseudo-Hermitian [4] models and analyzed their *strongly-perturbed* sample with

$$\tilde{W}_{m,n}^{(N)} = i \langle m^{(\text{HO})} | x^3 \exp[-\alpha H^{(\text{HO})}] | n^{(\text{HO})} \rangle, \qquad m, n = 1, 2, \dots, N.$$
(3)

They found out that as long as  $H^{(\text{HO})} = x^2 + p^2$  is positive, a very good approximation of the nonlinear-differential-equation  $N = \infty$  results is achieved via the series of truncated, purely algebraic and linear  $N < \infty$  equations (2).

In our recent papers [5] and [6], we took one step forward. Assuming that one could annihilate *any* far-off-diagonal element of *any* given matrix  $H^{(AHO)}$  via a finite sequence of elementary Jacobi rotations [7] we restricted our attention to the mere 'irreducible', *tridiagonal* anharmonic-oscillator-type models:

$$H^{(\text{chain})} = H^{(\text{HO})} + \sum_{\substack{m,n=1\\|m-n|=1}}^{N} |m^{(\text{HO})}\rangle W^{(N)}_{m,n} \langle n^{(\text{HO})}|.$$
(4)

In the  $\mathcal{PT}$ -symmetric scenario (guaranteed, in the normalization accepted in [5], by the mere antisymmetry  $W_{m,m+1}^{(N)} = -W_{m+1,m}^{(N)} \equiv g_m$  among the *real* matrix elements) we shifted the origin of the energy scale and arrived at the *N*-dimensional and tridiagonal 'chain-model' matrices  $\langle m^{(\text{HO})} | H^{(\text{chain})} | n^{(\text{HO})} \rangle \equiv H_{m,n}^{(\text{chain})}$ :

$$H^{(\text{chain})} = \begin{bmatrix} 1 - N & g_1 & 0 & 0 & \dots & 0 \\ -g_1 & 3 - N & g_2 & 0 & \dots & 0 \\ 0 & -g_2 & 5 - N & \ddots & \ddots & \vdots \\ 0 & 0 & -g_3 & \ddots & g_{N-2} & 0 \\ \vdots & \vdots & \ddots & \ddots & N - 3 & g_{N-1} \\ 0 & 0 & \dots & 0 & -g_{N-1} & N - 1 \end{bmatrix} \neq (H^{(\text{chain})})^{\dagger}.$$
(5)

For the sake of simplicity we decided to pay attention solely to the up–down-symmetric special cases  $H^{(N)}$  of  $H^{(\text{chain})}$  where we choose

$$g_{N-k} = g_k \ge 0, \qquad k = 1, 2, \dots, J$$
 (6)

at both the even N = 2J and the odd N = 2J + 1.

In subsection 2.1, we shall start our present continuation of the latter study of the toy model (5) + (6) by a brief review of the results of paper [5]. We point out there that the model  $H^{(N)}$  itself has been introduced as partially tractable by an algebraic, symbolic-manipulation-based non-numerical extrapolation method. We remind the readers that at any dimension N = 2J or N = 2J + 1, the spectrum  $\{E_n^{(N)}\}$  remains real and observable inside a *J*-dimensional domain  $\mathcal{D} = \mathcal{D}^{(N)}$  of the matrix elements which is compact and all contained inside a bigger domain  $\mathcal{S}^{(N)}$  defined by the following elementary inequality [5]:

$$\frac{N^3 - N}{2} \ge 2\sum_{n=1}^{J-1} g_n^2 + \begin{cases} g_J^2, & N = 2J, \\ 2g_J^2, & N = 2J+1. \end{cases}$$
(7)

There exists just a finite set of the 'maximal-coupling' intersections of the two surfaces, i.e., of the (J - 1)-dimensional boundaries  $\partial D^{(N)}$  and  $\partial S^{(N)}$ . We succeeded in determining the coordinates of these points (called, in [5], extremely exceptional points, EEP) in a closed form:

$$g_n^{(\text{EEP})} = \sqrt{n(N-n)}, \qquad n = 1, 2, \dots, J.$$
 (8)

In subsection 2.2, we shall extend the review by adding some empirical observations published in our most recent numerical study [6] and concerning the behavior of the energies  $E_n^{(N)}$ , predominantly, *far off* the EEP extremes. In particular, we shall recollect there the lucky guess of the ansatz

$$g_n = g_n^{(\text{EEP})} \sqrt{(1 - \xi_n(t))}, \qquad \xi_n(t) = t + t^2 + \dots + t^{J-1} + G_n t^J \tag{9}$$

which extrapolates, to all J, the rigorous fine-tuning rule derived, in [5], at J = 2. In the numerical context of [6] it merely served as a bookkeeping tool in our experiments with the various choices of the rescaled couplings  $G_n$ . In what follows we intend to describe several much deeper and more far-reaching consequences of this type of an ansatz.

In the preliminary steps taken in section 3 we shall start the analysis of our bound-state problem by the direct, brute-force algebraic solution of its secular equations

$$\det(H^{(N)} - EI^{(N)}) = 0 \tag{10}$$

at N = 4 (subsection 3.1), at N = 5 (subsection 3.2) and at N = 6 (subsection 3.3). In section 4, we shall change the variables in the manner prescribed by equation (9). This will lead to the much more compact strong-coupling leading-order formulae at the two sample dimensions N = 4 (subsection 4.1) and N = 5 (subsection 4.2). Certain indications of the possibility of a successful extrapolation of these formulae with respect to the dimension N will follow in section 5 sampling N = 6 (subsection 5.1) and N = 7 (subsection 5.2).

The climax of our present paper comes in sections 6 (where we extend the above results to all the even dimensions N = 2J) and 7 (where the parallel extrapolations are outlined in the case of any odd N = 2J + 1). The remaining text is just discussions (section 8) and summary (section 9) which emphasize that our present, perturbation-theory-simulating attention paid to the interval of *small t* fills in fact the gap between the algebraic t = 0 approach of paper [5] and its numerical large-t pendant of letter [6].

#### 2. A brief review of the state of art

Our continuing interest in the family (5) has several reasons. Firstly, in possible applications, special cases of  $H^{(N)}$  could play the role of a non-standard spin model (cf their N = 2 samples in [8, 9]) or of a Hamiltonian of a system where a 'de-frozen', new degree of freedom can emerge (with N = 3 see [10]). At any higher dimension N, every  $H^{(N)}$  is, using the language of the review paper [11], quasi-Hermitian and, therefore, eligible, say, as a Hamiltonian of a quantum chain. Inside  $\mathcal{D}^{(N)}$  and in a suitably specified physical Hilbert space  $\mathcal{H}^{(N)}$ , all our models  $H^{(N)}$  obey all the postulates of Quantum Mechanics in a way illustrated, at N = 2, in [9]. Due to their finite matrix form, all of them appear particularly suitable for an illustration of some subtleties of perturbation theory, especially in the weak-coupling dynamical regime where all their off-diagonal elements  $g_n$  remain small [1]. In the sense explained in [5], all of our toy Hamiltonians  $H^{(N)}$  are also interesting as  $\mathcal{PT}$ -symmetric [3, 12] and/or parity-pseudo-Hermitian [4] candidates for operators of observables which are capable of exhibiting multiple confluences of their (in Kato's language) 'real exceptional points' [6, 13, 14]. Last but not least, our non-Hermitian matrices  $H^{(N)}$  are, through the above-mentioned variational

and perturbative considerations [15], directly and closely related to the popular *differential*  $\mathcal{PT}$ -symmetric quantum Hamiltonians of Bender *et al* [12] and others [16]–[21].

#### 2.1. Observations made in paper [5]

In 'paper I' [5] we felt inspired by the exceptional transparency of the geometry of the 'physical' domains of quasi-Hermiticity  $\mathcal{D}^{(N)}$  in the strong-coupling regime and at the smallest dimensions N. In such a setting, the first non-numerical result of [5] was that *all* the eigenenergies become complex whenever the anharmonicity becomes sufficiently strong. Such a type of observation was interpreted as very important because the crucial point of making *any*  $\mathcal{PT}$ -symmetric Hamiltonian H 'physical' (i.e., responsible for observable and stable bound states) lies in the specification of the 'allowed' range  $\mathcal{D} = \mathcal{D}(H)$  of its free parameters.

In paper I we showed that the *non-numerical* construction of  $\mathcal{D}(H)$  proves feasible in an EEP, 'maximal-coupling' limit  $H = H_{(\text{EEP})}^{(N)}$  of our tridiagonal matrices  $H^{(N)}$  at *all* their dimensions N. The proof was based on an elementary observation that for every individual model  $H^{(N)}$  with a fixed dimension N, the spectrum is determined by the polynomial secular equation for the squared energy  $s = E^2$ ,

$$det[H^{(N)} - EI^{(N)}] = s^{J} - P_{1}^{(N)}(g_{1}, \dots, g_{J})s^{J-1} + P_{2}^{(N)}(g_{1}, \dots, g_{J})s^{J-2} - \dots + (-1)^{J}P_{J}^{(N)}(g_{1}, \dots, g_{J}) = 0.$$
(11)

We recollected that due to the polynomiality of the latter equation, the sum of the *physical* (i.e., nonnegative) roots  $s_i$  must be equal to the first coefficient,

$$P_1^{(N)}(g_1, \dots, g_J) = s_1 + s_2 + \dots + s_J \ge 0.$$
(12)

As a consequence, the closure of the domain  $\mathcal{D}^{(N)}$  must lie *inside* the closure of another, bigger domain  $\mathcal{S}^{(N)}$  which is defined, much more simply, by the upper estimate (12). The shape of the surface of  $\mathcal{S}^{(N)}$  is a hyperellipsoid or a hypersphere (cf [5] or equation (7)). This enabled us to define the EEP vortices as the points where the couplings are maximal, i.e., where the boundary  $\partial \mathcal{D}^{(N)}$  of the quasi-Hermiticity domain *intersects* the circumscribed 'upper-estimate' hypersurface  $\partial \mathcal{S}^{(N)}$ . In this context, a key technical result of paper I consisted in the derivation of *the closed formula* for all of the EEP coordinates (namely, of equation (8)).

In the present continuation of paper I, we intend to pay attention to the shape of the hypersurfaces  $\partial D^{(N)}$  in the vicinity of their EEP extremes. This is a well-motivated project since, in spite of the reality (i.e., 'mathematical' observability) of the energies of the system in its solvable EEP limit, the 'physical' version of the same (i.e., strong-coupling) observability concept requires more than that. Obviously, during any measurement we should stay *in the interior* of the domain  $D^{(N)}$ , requiring that a small random perturbation of the couplings *cannot* induce a spontaneous complexification of some energies and a subsequent sudden collapse of the system.

#### 2.2. Observations made in paper [6]

Later on, we complemented the algebraic constructions of [5] by the purely numerical study [6] of the possible complexification patterns of the spectra of our chain models  $H^{(\text{chain})}$ . We can summarize that

• the perturbed harmonic-oscillator spectrum  $\{E_n\}$  remains all real in the weakly anharmonic regime characterized by a 'sufficient' smallness of all the elements or couplings  $H_{m,m+1}^{(N)}$  at all *m*;

• the pairs  $(E_n, E_{n+1})$  of energies coincide and complexify whenever their mutual coupling  $H_{n,n+1}^{(N)}$  exceeds certain *n*-dependent 'exceptional-point' value [1].

A particularly amusing empirical (though easily explained) observation made in [6] was that one can preserve the reality of the spectrum even when crossing the no-interaction boundary via a breakdown of the rule given by equation (9):

 $g_k \sim \sqrt{\lambda}, \qquad (\lambda > 0) \longrightarrow (\lambda < 0).$  (13)

Although such a switch between the *real* and *purely imaginary* couplings will not be considered in what follows, we shall still use the parametrization (13) in its strong-coupling real form (9) where  $\lambda = 1 - t$  is assumed large while the new, formal auxiliary parameter  $t \in (0, 1)$ remains, preferably, sufficiently small, characterizing our  $\mathcal{PT}$ -symmetric and up/down symmetric chain models  $H^{(N)}$  in their most interesting, strongly non-Hermitian dynamical regime.

In [6], the use of the parameters  $\lambda$  or t has been shown to facilitate the study of the spectra, real or complex, at any N. In addition, the use of the 'renormalized' coupling strengths  $G_n$  opened the way toward a systematic (namely, combinatorial) classification of the nonequivalent energy-complexification patterns or, if you wish, of the non-equivalent scenarios of a 'quantum catastrophe'. Moreover, we found that once we fix a real J-plet of optional parameters  $G_n$  in ansatz (9), the range of the remaining free parameter  $t \in (-\infty, \infty)$  splits into four specific subintervals.

- (1) In an 'unobservable' regime, some of the energies are not real (so that  $H^{(N)}$  itself is not quasi-Hermitian, QH) at  $t \in (-\infty, t_{(OH)}(G_1, G_2, \dots, G_J))$ .
- (2) The genuine quasi-Hermitian and  $\mathcal{PT}$ -symmetric regime is encountered in the range of  $t \in (t_{(QH)}(G_1, G_2, \ldots, G_J), t_{(PH)}(G_1, G_2, \ldots, G_J))$  where one stays safely inside  $\mathcal{D}^{(N)}$ . The value of the parity-pseudo-Hermiticity boundary  $t_{(PH)}$  is given by the decision [5] that the matrix  $H^{(N)}$  remains real,  $\max_n \xi_n(t) \leq 1$ .
- (3) In the next interval of  $t \in (t_{(PH)}(G_1, G_2, \dots, G_J), t_{(H)}(G_1, G_2, \dots, G_J))$ , the matrix  $H^{(N)}$  ceases to be real *and* its  $\mathcal{P}$  (i.e., parity-) pseudo-Hermiticity 'strengthens' to an  $\eta$ -pseudo-Hermiticity. An N = 4 illustrative example of the 'modified parity'  $\eta$  (which may further vary with *t*) was given in [6].
- (4) Hermitian regime enters the scene at  $t \in (t_{(H)}(G_1, G_2, \dots, G_J), \infty)$ . One has  $\xi_n(t) > 1$  at all *n* so that all the couplings  $g_n$  become purely imaginary.

In this setting, one notes a certain complementarity between the results of [5, 6]. In the former (and older) text we intended to stay safely inside *the closure* of the domain  $\mathcal{D}^{(N)}$ . In this framework, we showed that the choice of the optimal proportionality coefficients (8) in equation (13) implies that we can minimize  $t_{(QH)} = 0$ . In this sense we found the *maximal* interaction strengths which are still compatible with the reality of the spectrum. In contrast, the scope of paper [6] was broader and covered (i.e., sampled, numerically) *all* the four eligible intervals of the auxiliary parameter *t*.

In what follows we shall show how the successful localization of the exceptional boundary point with  $t_{(QH)} = 0$  in [5] can be extended to a certain approximative closed-formula description of all the (J - 1)-dimensional boundary set  $\partial \mathcal{D}^{(N)}$  in a vicinity of this point. This will definitely clarify, *inter alii*, how the necessary physical stability of our model can be guaranteed via a constructive, leading-order specification of an *interior, strong-coupling* part of the domain  $\mathcal{D}^{(N)}$ .

#### 3. The method of explicit constructions

#### 3.1. Guiding example: N = 4

In the first nontrivial N = 4 example we set  $g_1 = \sqrt{3(1-\beta)}$ ,  $g_2 = \sqrt{4(1-\alpha)}$  and consider

$$H^{(4)} = \begin{pmatrix} -3 & \sqrt{3-3\beta} & 0 & 0\\ -\sqrt{3-3\beta} & -1 & 2\sqrt{1-\alpha} & 0\\ 0 & -2\sqrt{1-\alpha} & 1 & \sqrt{3-3\beta}\\ 0 & 0 & -\sqrt{3-3\beta} & 3 \end{pmatrix}$$

with  $\alpha, \beta \in (0, 1)$ . This leads to the secular equation

$$s^{2} - (6\beta + 4\alpha)s - 36\beta + 36\alpha + 9\beta^{2} = 0$$
(14)

with the doublet of available elementary roots,

$$s_{\pm} = 3\beta + 2\alpha \pm 2\sqrt{3\beta\alpha + \alpha^2 + 9\beta - 9\alpha}.$$
(15)

As long as the energies are square roots of these roots we must guarantee that  $s_{\pm} \ge 0$ . *Vice versa*, the latter two inequalities may be understood as an implicit definition of the domain  $\mathcal{D}^{(4)} = \mathcal{D}^{(4)}(\alpha, \beta)$ . More details may be found elsewhere [15].

In an attempt to clarify the origin of ansatz (9) let us now introduce an auxiliary, redundant parameter t and set  $\alpha = ta$  and  $\beta = tb$ , treating t as a radius of the EEP vicinity and preserving just the leading-order terms in t. Then, conditions  $s_{\pm} \ge 0$  degenerate to the two elementary rules

$$b \ge a + \mathcal{O}(t), \qquad a \ge b + \mathcal{O}(t)$$

which may be interpreted as a requirement of a fine-tuned balance between *a* and *b* (or  $\alpha$  and  $\beta$ ) near the EEP extreme. We may conclude that our ansatz (9) is optimal and that *inside*  $\mathcal{D}^{(4)}$ , the value of  $\alpha$  can only differ from  $\beta$  in the *next* order in the small *t*,

$$\beta = t + Bt^2, \qquad \alpha = t + At^2. \tag{16}$$

Tractable as an exact change of variables  $(\alpha, \beta) \longrightarrow (A, B)$ , such a rule *strictly* replaces the inequalities  $s_{\pm} \ge 0$  by the *t*-parametrized pair of the necessary and sufficient conditions of the physical acceptability of  $H^{(4)}$ ,

$$t^{2}A^{2} + 5tA + 3t^{2}AB + 4 + 3tB + 9B - 9A \ge 0,$$
(17)

$$t^{2} + 2t^{3}B + t^{4}B^{2} - 4t^{2}B + 4t^{2}A \ge 0.$$
(18)

In the vicinity of the EEP extreme, we can omit the higher-order terms from equations (17) and (18). This reduces this pair of inequalities to the compact leading-order estimate

$$\frac{4}{9} \ge A - B \ge -\frac{1}{4}.\tag{19}$$

This leading-order rule defines  $\mathcal{D}^{(4)}$  reliably near the EEP vertex. Indeed, in a graph-drawing scenario we may suppress the redundancy and fix  $t \equiv \beta$  (i.e., set B = 0). This converts (19) into the explicit leading-order formulae which define the two branches of the boundary  $\partial \mathcal{D}^{(4)}$ ,

$$\alpha^{(\text{upper})}(\beta) = \beta + \frac{4}{9}\beta^2 + \mathcal{O}(\beta^3), \qquad \alpha^{(\text{lower})}(\beta) = \beta - \frac{1}{4}\beta^2 + \mathcal{O}(\beta^3).$$
(20)

These two curves osculate at EEP so that the domain  $\mathcal{D}^{(4)}$  appears sharply spiked near this extreme.

It makes sense to believe that such a geometric property of the domain D is generic. At the higher matrix dimensions N, precisely this hypothesis has been formalized by the



Figure 1. The *t*-dependence of energies, with two choices of A at N = 4.

tentative ansatz (9). For a graphical illustration of its consequences we decided to sample the N = 4 spectrum in figure 1. At B = 0 it compares the quadruplet of the energies which are real at all  $t \ge 0$  (and which correspond to the 'admissible' choice of the rescaled coupling A = 4/9 - 20/100 which lies safely inside  $\mathcal{D}^{(4)}$ ) with another quadruplet obtained at a 'forbidden' A = 4/9 + 2/100 (i.e., slightly outside  $\mathcal{D}^{(4)}$ , violating the upper bound in equation (19)) which remains all complex at all the positive small  $t < t_{(OH)}(A)$ .

#### 3.2. Inessential changes at N = 5

At the first nontrivial odd dimension N = 5 with  $g_1 = b = 2\sqrt{1-\beta}, \beta \in (0, 1)$  and  $g_2 = a = \sqrt{6(1-\alpha)}, \alpha \in (0, 1)$ , our model

$$H^{(5)} = \begin{pmatrix} -4 & 2\sqrt{1-\beta} & 0 & 0 & 0\\ -2\sqrt{1-\beta} & -2 & \sqrt{6-6\alpha} & 0 & 0\\ 0 & -\sqrt{6-6\alpha} & 0 & \sqrt{6-6\alpha} & 0\\ 0 & 0 & -\sqrt{6-6\alpha} & 2 & 2\sqrt{1-\beta}\\ 0 & 0 & 0 & -2\sqrt{1-\beta} & 4 \end{pmatrix}$$

leads to the secular polynomial of the fifth degree in E which is divisible by E. Thus, one of the roots, namely, the energy  $E_2 = 0$  may be treated as trivial. The remaining four energies E may be computed from the two roots  $s = E^2$  of the quadratic equation

$$s^{2} - P_{1}^{(5)}(g_{1}, g_{2})s + P_{2}^{(5)}(g_{1}, g_{2}) = 0$$
(21)

where one easily evaluates

$$P_1^{(5)}(g_1, g_2) = 8\beta + 12\alpha, \qquad P_2^{(5)}(g_1, g_2) = 48\alpha\beta - 144\beta + 144\alpha + 16\beta^2.$$

We may skip the details—near EEP the construction of  $\mathcal{D}^{(5)}$  is strikingly analogous to its N = 4 predecessor.

#### 3.3. Inessential changes at N = 6

At N = 6, three parameters  $\alpha$ ,  $\beta$ ,  $\gamma \in (0, 1)$  enter the three coupling constants  $g_1 = c = \sqrt{5(1 - \gamma)}, \qquad g_2 = b = 2\sqrt{2(1 - \beta)}, \qquad g_3 = a = 3\sqrt{1 - \alpha}$  which specify the dynamics via the Hamiltonian

$$H^{(6)} = \begin{bmatrix} -5 & g_1 & 0 & 0 & 0 & 0 \\ -g_1 & -3 & g_2 & 0 & 0 & 0 \\ 0 & -g_2 & -1 & g_3 & 0 & 0 \\ 0 & 0 & -g_3 & 1 & g_2 & 0 \\ 0 & 0 & 0 & -g_2 & 3 & g_1 \\ 0 & 0 & 0 & 0 & -g_1 & 5 \end{bmatrix}.$$
 (22)

The shape of the associated domain of quasi-Hermiticity  $\mathcal{D} = \mathcal{D}(a, b, c)$  can be deduced from the secular equation

$$\det(H^{(6)} - EI^{(6)}) = s^3 - 3P_1^{(6)}s^2 + 3P_2^{(6)}s - P_3^{(6)} = 0, \qquad s = E^2$$
(23)

(note the slightly modified notation) re-written as the relation

 $[s - s_1(a, b, c)][s - s_2(a, b, c)][s - s_3(a, b, c)] = 0$ 

between its roots  $s_k(a, b, c)$ . As long as they define the energies  $E_{\pm k} = \pm \sqrt{s_k(a, b, c)}$ , all of them must be nonnegative in  $\mathcal{D}^{(6)}$ . For this reason, we have to satisfy three requirements  $P_k^{(6)} \ge 0, k = 1, 2, 3$  plus a certain slightly more complicated fourth condition (with the derivation left to the reader as an exercise).

From a geometric point of view, the construction of the boundary  $\partial D^{(6)}$  of the physical domain remains similar to its N = 4 predecessor. Thus, equation

$$P_1^{(6)} = -(a^2 + 2b^2 + 2c^2 - 35)/3 = 0$$

determines the ellipsoid which circumscribes the domain  $\mathcal{D}^{(6)}$ . In contrast, the geometric interpretation of the further circumscribed surfaces (given by equations  $P_2^{(6)} = 0$  etc) is much less straightforward. For this reason, we intend to employ ansatz (9) and to replace the variables  $\alpha$ ,  $\beta$ ,  $\gamma$  by the new triplet *A*, *B*, *C* defined by the J = 3 version of the recipe,

$$\alpha = t + t^2 + At^3, \qquad \beta = t + t^2 + Bt^3, \qquad \gamma = t + t^2 + Ct^3.$$
 (24)

The auxiliary variable t is redundant but useful because we intend to keep it small.

#### 4. The method of rescaled couplings

Our above exact result (16) can be reinterpreted as a tentative ansatz with the obvious generalization (9). The use of the latter rule requires an assumption of the smallness of  $|t| \ll 1$ . This could simplify our secular equation (10), near the EEP extremes at least.

#### 4.1. Guiding example: N = 4

In the new notation our secular equation (i.e., our implicit definition of the N = 4 energies) degenerates to the leading-order relation

$$s^{2} - 10ts + (36A - 36B + 9)t^{2} + \mathcal{O}(t^{3}) = 0.$$

After we introduce a new coupling parameter  $\omega = \omega^{(J)} = 36(A - B)$ , this equation for the unknown quantity L = s/t acquires a transparent *t*-independent leading-order form which may be partially factorized:

$$L^{2} - 10L + 9 + \omega = (L - 1)(L - 9) + \omega = 0.$$
(25)

It is important that the roots of equation (25) are known exactly,

$$L_{\pm} = 5 \pm \sqrt{16} - \omega$$

4.1.1. The leading-order localization of the boundary  $\partial D^{(4)}$ . Obviously, the growth of  $\omega > 0$  beyond its 'upper limit'  $\omega_{UL} = 16$  makes all the four roots *L* (i.e., all the related leading-order energies) complex. In the alternative scenario, the decrease of  $\omega < 0$  below its 'lower limit'  $\omega_{UL} = -9$  makes just one of the roots (namely,  $L_{-}$ ) negative.

Both these estimates coincide with the above-derived formula (19). We may conclude that the use of our perturbation-type ansatz (16) reproduces, completely, the leading-order information about the spiked shape of the boundary  $\partial D^{(4)}$  near the EEP extreme.

We could also speak about the quadruplet of the *t*-dependent energies  $E_0(t), \ldots, E_3(t)$  studied in the strong-coupling regime. This dynamical regime is characterized by the small auxiliary quantities *t* which, in effect, measure the 'distance' of our model  $H^{(4)}$  from its EEP t = 0 extreme. In such an alternative language, the pair of  $E_1(t)$  and  $E_2(t)$  will complexify somewhere near  $\omega \sim \omega_{LL}$ , etc (cf [6] for a more complete discussion and for a combinatorial classification of all the possible scenarios of complexification at any *N*).

4.1.2. A linearized localization of  $\partial D^{(4)}$  at small  $\omega$ . In the symmetric-coupling regime with A = B one stays safely inside the 'physical' interior of  $D^{(4)}$ . Once we assume that the difference  $\omega \sim A - B$  is small, the extraction of all the energy roots becomes facilitated. In the leading-order approximation their  $\omega$ -dependence remains linear,

$$L_{-} = 1 + \frac{\omega}{8} + \mathcal{O}(\omega^2), \qquad L_{+} = 9 - \frac{\omega}{8} + \mathcal{O}(\omega^2).$$
 (26)

These formulae still offer a *qualitatively correct* perturbative explanation of the *complexification pattern* of the energies. Indeed, even from the oversimplified approximation  $s = E^2 = Lt + O(t^2)$  using closed formulae (26) one can deduce the rough estimates of the critical  $\omega_{UL}^{(1)} = 32$  (or about 23.4 in the second-order approximation in  $\omega$ ) and  $\omega_{LL}^{(1)} = -8$  (or -9.37 in the second-order approximation), yielding even a reasonably good quantitative prediction.

4.1.3. A systematic build-up of higher-order corrections. Whenever we keep the t-dependent version of our N = 4 secular equation (14) in full precision, we can construct the perturbation series for the energies at the small t in the standard manner, with

$$E_3 = -E_0 = \sum_{k=0}^{\infty} t^{k+1/2} E_3^{(k)}, \qquad E_2 = -E_1 = \sum_{p=0}^{\infty} t^{p+1/2} E_2^{(p)}$$

and with

$$E_3^{(0)} = \sqrt{2\sqrt{9B - 9A + 4} + 5},$$
  
$$E_3^{(1)} = \frac{1}{2\sqrt{2\sqrt{9B - 9A + 4} + 5}} \left(\frac{3B + 5A}{\sqrt{9B - 9A + 4}} + 3B + 2A\right)$$

etc, or with

$$E_2^{(0)} = \sqrt{5 - 2\sqrt{9B - 9A + 4}},$$
  
$$E_2^{(1)} = \frac{1}{2\sqrt{5 - 2\sqrt{9B - 9A + 4}}} \left(2A + 3B - \frac{3B + 5A}{\sqrt{9B - 9A + 4}}\right),$$

etc. These formulae offer another source of insight in the mechanisms of complexification of the spectrum at the boundary  $\partial D^{(4)}$ .

4.2. A change of the pattern at N = 5

The insertion of ansatz (16) in secular equation (21) gives

$$P_1^{(5)}(b,a) = 20t + 8t^2B + 12t^2A.$$

This confirms our expectations that the necessary non-negativity of this expression is guaranteed at all the not too large |A|,  $|B| \ll 1/t$ . Similarly we are able to evaluate and demand that, in full precision,

$$P_2^{(5)}(b,a) = 144t^2A - 144t^2B + 64t^2 + 16t^4B^2 + 48t^3A + 48t^4AB + 80t^3B \ge 0.$$

Obviously, the higher-order corrections may only be needed quite far from the EEP extreme. In the dominant order in t we may conclude that

$$s^{2} - 20ts + (144A - 144B + 64)t^{2} + \mathcal{O}(t^{3}) = 0.$$

Once we put  $s = Lt + O(t^2)$  again, we get

 $L^{2} - 20L + 64 + \varepsilon = (L - 4)(L - 16) + \varepsilon = 0, \qquad \varepsilon = 144(A - B).$ (27)

In the regime with a small  $\varepsilon$  (of any sign), we easily get the leading-order  $\varepsilon$ -dependence of both the roots,

$$L_{-} = 4 + \frac{\varepsilon}{12} + \mathcal{O}(\varepsilon^2), \qquad L_{+} = 16 - \frac{\varepsilon}{12} + \mathcal{O}(\varepsilon^2).$$

Marginally, it is amusing to note that in the trivial case with  $A - B = \varepsilon = 0$  the positive doublet of energies (as well as its negative counterpart) has a tendency of moving directly to the corresponding weak-coupling harmonic-oscillator limit. Our leading-order approximation  $E_{\pm} = +\sqrt{(10 \pm 6)t + O(t^2)}$  behaves as if being, paradoxically, exact at t = 1.

4.2.1. Toward the boundary  $\partial D^{(5)}$ . In a way paralleling our above N = 4 considerations let us switch to a larger, positive  $\varepsilon \sim A - B > 0$ . The two dominant energies  $E_3 \ge E_2 > 0$  will then decrease and increase with the growth of  $\varepsilon$ , respectively. One can predict an ultimate coincidence and a subsequent complexification of this doublet at a non-vanishing Kato's exceptional point localized at some 'boundary coordinate'  $t = t_{(QH)} > 0$  of quasi-Hermiticity.

For the opposite, negative and decreasing  $\varepsilon < 0$  the approximative results are similar and do not lead to any contradictions. We may summarize that near the shared EEP maximum of  $g_1$  and  $g_2$ , the growth of the difference between A and B would lead us out of the physical domain  $\mathcal{D}^{(5)}$ . In the other words, the boundary  $\partial \mathcal{D}^{(5)}$  near EEP is of a sharply spiked form as well.

#### 5. Extrapolation hypothesis

Let us now turn attention to the models with J = 3. We intend to offer some quantitative arguments in favor of the intuitive idea that the exceptional-point boundaries  $\partial D^{(6)}$  and  $\partial D^{(7)}$  have a form of a surface of a deformed cube with protruded, razor-sharp edges (=double exceptional points) and with the spiked, strong-coupling vertices (i.e., triple exceptional points).

We expect that such an intuitively transparent geometric interpretation of the shape of  $\mathcal{D}^{(6)}$  and  $\mathcal{D}^{(7)}$  will provide a firm ground for extrapolations toward higher dimensions in subsequent sections of this paper.

#### 5.1. Expectable observations at N = 6

After transition from N = 4 to N = 6, symbolic manipulations on a computer become rather lengthy. Still, they enable us to evaluate, in closed form, the approximate secular-equation coefficients

$$\begin{aligned} P_1^{(6)} &= P_1^{(6)}(c, b, a) = 35t + 35t^2 + \mathcal{O}(t^3), \\ P_2^{(6)} &= P_2^{(6)}(c, b, a) = 259t^2 + (216A + 518 + 144B - 360C)t^3 + \mathcal{O}(t^4) \end{aligned}$$

and

$$P_3^{(6)} = P_3^{(6)}(c, b, a) = (3600A + 1200C - 4800B + 225)t^3 + (3600B - 1800C + 675 - 1800A)t^4 + O(t^5).$$

The resulting shortened leading-order secular equation is finally obtained and reads

 $s^{3} - 35ts^{2} + 259t^{2}s - (225 - \omega^{(3)})t^{3} = 0, \qquad \omega^{(3)} = 1200(-3A + 4B - C).$ 

After we put  $s = E^2 = Lt + O(t^2)$ , its partial factorization remains feasible,

$$(L-1)(L-9)(L-25) + \omega = 0.$$
<sup>(28)</sup>

In a way paralleling the previous N = 4 example, a transparency of this equation facilitates the analysis of the relationship between the variations of the coupling-dependent quantity  $\omega \sim 4B - C - 3A$  and of the physical spectrum of energies  $E_0 = -E_5 \leq E_1 = -E_4 \leq E_2 = -E_3$ , inside the domain of its reality at least.

5.1.1. Toward the boundary  $\partial \mathcal{D}^{(6)}$ . The discussion is easier at the small  $\omega^{(3)}$  where all the three roots of equation (28) are almost linear in  $\omega$ ,

$$L_1 = 1 - \frac{\omega}{8 \cdot 24} + \mathcal{O}(\omega^2), \qquad L_2 = 9 + \frac{\omega}{8 \cdot 16} + \mathcal{O}(\omega^2), \qquad L_3 = 25 - \frac{\omega}{16 \cdot 24} + \mathcal{O}(\omega^2).$$

At  $\omega \approx 0$  and at the smallest  $t \neq 0$  we have  $E_0 \sim -5\sqrt{t}$ ,  $E_1 \sim -3\sqrt{t}$ ,  $E_2 \sim -\sqrt{t}$ ,  $E_3 \sim \sqrt{t}$ ,  $E_4 \sim 3\sqrt{t}$  and  $E_5 \sim 5\sqrt{t}$ . With the decrease of  $\omega < 0$  the levels  $E_1$  and  $E_2$  (and also  $E_3$  and  $E_4$ ) get closer to each other and, in a way which parallels the similar observation made at N = 4, they finally complexify at the critical  $\omega_{(LL)} \approx -323.1387184$  near  $E_3 \approx E_4 \approx 2.147400716\sqrt{t}$ . In the light of the obvious fact that the growth of every coupling  $g_k$  causes an attraction of the corresponding levels [9], the interpretation of the above rule is easy and consistent because the decrease of  $\omega$  means not only a smaller B < (3A+C)/4 but also, at any given t,  $g_1$  and  $g_3$ , an enhancement of the coupling  $g_2$  between the levels which complexified.

In the opposite direction, the increase of  $\omega > 0$  causes the decrease of the smallest root  $L_s(\omega) \left(=E_{2,3}^2/t\right)$  of equation (28) while the other two roots  $L_m(\omega) \left(=E_{1,4}^2/t\right)$  and  $L_d(\omega) \left(=E_{0,5}^2/t\right)$  start approaching each other. In this way, the first and dominating complexification involves the pair  $E_{2,3}$  (with  $E_{2,3} \approx 0$ ) because it takes place exactly at  $\omega_{(\rm UL)} = 225$ , i.e., much earlier than the subsequent ultimate completion of all the complexification process with  $E_5 \approx E_4 \approx 4.326\,893\,054\sqrt{t}$  near  $\omega_{(\rm UL[4.5])} \approx 1081.657\,240$ .

#### 5.2. Expectable changes at N = 7

With N = 7 and with the J = 3 rule (24), we employ the symbolic manipulations on a computer and get 5 terms in

$$P_1^{(7)}(a, b, c) = 56t + 56t^2 + \mathcal{O}(t^3)$$

16 terms in

$$P_2^{(7)}(a, b, c) = 784t^2 + \mathcal{O}(t^3)$$

and 33 terms in

$$\mathcal{Q}_{2}^{(7)}(a, b, c) = (7200C - 21600B + 14400A + 2304)t^{3} + \mathcal{O}(t^{4})$$

The resulting shortened leading-order secular equation reads

$$s^{3} - 56ts^{2} + 784t^{2}s - (2304 - \varepsilon)t^{3} = 0, \qquad \varepsilon = 7200(-C + 3B - 2A).$$

With s = Lt it factorizes as follows:

$$(L-4)(L-16)(L-36) + \varepsilon = 0.$$
(29)

5.2.1. Toward the boundary  $\partial D^{(7)}$ . The three closed solutions of equation (29) may be expanded in the powers of  $\varepsilon$ ,

$$L_1 = 4 - \frac{\varepsilon}{384} + \mathcal{O}(\varepsilon^2), \qquad L_2 = 16 + \frac{\varepsilon}{240} + \mathcal{O}(\varepsilon^2), \qquad L_3 = 36 - \frac{\varepsilon}{640} + \mathcal{O}(\varepsilon^2).$$

A balanced return to the unperturbed values occurs now along a 'middle line' with  $\varepsilon = 0$ , i.e., for B = (2A + C)/3.

For the diminished Bs (i.e., for a stronger coupling  $b = g_2$  between  $E_1$  and  $E_2$ ), we are getting closer to the boundary surface along which the levels  $E_1$  and  $E_2$  merge and subsequently complexify. This behavior is confirmed by our formula because the shift  $\varepsilon$  becomes negative in such a scenario.

The growth of  $\varepsilon > 0$ , in contrast, may be assigned to the diminished A or C. In the former case, the growth of  $a = g_1$  implies that  $E_1 \rightarrow 0$  while the alternative growth of  $c = g_3$  results, naturally and expectedly, in the merger of  $E_2$  with  $E_3$ .

## 6. Arbitrary even dimension and the localization of boundaries $\partial \mathcal{D}^{(2J)}$ in the EEP vicinity

We saw that in many a respect one should pay separate attention to the models with even and odd N. Thus, we shall search for a successful extrapolation of our low-N 'experiments' in two separate sections, starting with the family where N = 2J.

Our first assumption concerns the values of the rescaled couplings  $G_n$  (abbreviated, occasionally, as A, B etc) which will be assumed bounded while the scaling parameter t itself will be assumed small.

Our second, main assumption is that our older equations (25) and (28) are exactly the respective N = 4 and N = 6 special cases of the general leading-order secular equation:

$$(L-1^2)(L-3^2)(L-5^2)\cdots(L-[2J-1]^2)+\omega^{(J)}=0.$$
(30)

We tested this hypothesis together with the ansatz (9) by extensive symbolic manipulations which confirmed its validity at *all* the integers N = 2J in a way documented in table 1. This table also summarizes the corresponding resulting explicit formulae for the *J*-dependent quantities  $\omega^{(J)}$ . Using the same extrapolation philosophy as above, we may extract the universal algebraic definition of the coupling-characterizing expression  $\omega^{(J)}$  as given by the following extrapolated conjecture *at all the positive integers J*:

$$\omega^{(J)} = 2(2J-1)(2J-1)! \sum_{n=1}^{J} (-1)^{J-n+1} {2J-2 \choose J-2+n} \theta(n) G_n.$$
(31)

| Table 1. Auxiliary functions of couplings $\omega^{(0)}$ (even $N = 2J$ ). |           |                                    |  |  |  |  |  |
|--|-----------|------------------------------------|--|--|--|--|--|
| J  | Dimension | $\omega^{(J)}/[2(2J-1)(2J-1)!]$    |  |  |  |  |  |
| 2  | 4         | A - B                              |  |  |  |  |  |
| 3  | 6         | -3A + 4B - C                       |  |  |  |  |  |
| 4  | 8         | 10A - 15B + 6C - D                 |  |  |  |  |  |
| 5  | 10        | -35A + 56B - 28C + 8D - E          |  |  |  |  |  |
| 6  | 12        | 126A - 210B + 120C - 45D + 10E - F |  |  |  |  |  |
| :  | :         |                                    |  |  |  |  |  |
| :  | •         |                                    |  |  |  |  |  |

**Table 1.** Auxiliary functions of couplings  $\omega^{(J)}$  (even N = 2J).

**Table 2.** Auxiliary functions of couplings  $\varepsilon^{(J)}$  (odd N = 2J + 1).

| J | Dimension | $\varepsilon^{(J)}/[2(2J-1)(2J)!]$ |
|---|-----------|------------------------------------|
| 2 | 5         | A - B                              |
| 3 | 7         | -2A + 3B - C                       |
| 4 | 9         | 5A - 9B + 5C - D                   |
| 5 | 11        | -14A + 28B - 20C + 7D - E          |
| 6 | 13        | 42A - 90B + 75C - 35D + 9E - F     |
| ÷ | :         |                                    |
|   |           |                                    |

This is our first main result deduced via an interpolation of the computed coefficients at the first few dimensions *N*, complemented by a subsequent (and, of course, much easier) verification of the hypothesis at a number of the higher *N*. Formula (31) contains just the usual combinatorial numbers (given by the standard Pascal-triangle recurrences) and the anomalous scaling factor  $\theta(n)$  which is equal to one at n > 1 and to one half at n = 1.

The geometric interpretation of formula (31) could be discussed in an immediate parallel with the texts on the special cases with N = 4 and N = 6 in sections 4.1 and 5.1, respectively. At the general *J*, a careful inspection of the first few secular equations (30) seems to indicate that at the smallest *ts*, the complexification of the spectrum *always* proceeds

- through the single merger, at the zero energy, of the 'middle' levels  $E_{J-1}$  and  $E_J$  (at some  $\omega_{(\text{UL})}^{(J)} > 0$  for  $J = 1, 3, 5, \ldots$  and at some  $\omega_{(\text{LL})}^{(J)} < 0$  for  $J = 2, 4, 6, \ldots$ );
- through the two simultaneous, symmetric mergers of the negative  $E_{J-3}$  with  $E_{J-2}$  and of the positive  $E_{J+1}$  with  $E_{J+2}$  (at  $\omega_{(LL)}^{(J)} < 0$  for  $J = 1, 3, 5, \ldots$  and at  $\omega_{(UL)}^{(J)} > 0$  for  $J = 2, 4, 6, \ldots$ ).

#### 7. All odd dimensions and the boundaries $\partial \mathcal{D}^{(2J+1)}$ in the EEP vicinity

When the dimension is odd, N = 2J + 1, the application of the ansatz (9) simplifies the problem significantly as well. This ansatz can be perceived again as an equivalence transformation based on a mere change of the variables,  $g_n \to G_n$ . It maps the domain  $\mathcal{D}^{(N)}(g_1, \ldots, g_J)$  of quasi-Hermiticity of  $H = H^{(2J+1)}(g_1, \ldots, g_J)$  into another, equivalent manifold  $\mathcal{D}^{(2J+1)}(G_1, \ldots, G_J)$  of the acceptable parameters in  $H = H^{(2J+1)}(G_1, \ldots, G_J)$ .

For all the odd dimensions N we may ignore the persistent 'middle' bound-state energy  $E_J^{(2J+1)} = 0$ . *Mutatis mutandis*, this enables us to use the same J and to apply the same (or at least very similar) geometric, algebraic and analytic considerations as above.

**Table 3.** Coefficients  $C_{(J)}^{(J)}$  of equations (33) and (34).

| $\mathcal{C}_{(n)}$ or equations (be) and (b). |     |    |    |     |     |      |     |     |     |   |   |  |
|--|-----|----|----|-----|-----|------|-----|-----|-----|---|---|--|
|  | n = |    | -3 | -2  | -1  | 0    | 1   | 2   | 3   | 4 | 5 |  |
| J  |     |    |    |     |     |      |     |     |     |   |   |  |
| (1)  |     |    |    | (0) | (0) | (-1) | (1) | (0) | (0) |   |   |  |
| 2  |     |    |    |     | -1  | -1   | 1   | 1   |     |   |   |  |
| 3  |     |    |    | -1  | -3  | -2   | 2   | 3   | 1   |   |   |  |
| 4  |     |    | -1 | -5  | -9  | -5   | 5   | 9   | 5   | 1 |   |  |
| 5  |     | -1 | -7 | -20 | -28 | -14  | 14  | 28  | 20  | 7 | 1 |  |
|  |     |    |    |     |     |      |     |     |     |   |   |  |
| :  |     |    |    |     |     |      |     |     |     |   |   |  |
|  |     |    |    |     |     |      |     |     |     |   |   |  |

One of the most visible differences between the models  $H^{(2J)}$  and  $H^{(2J+1)}$  may be traced to the fact that in place of the (hyper)ellipsoids pertaining to the even dimensions we have to deal with the *simpler* (hyper)spheres  $S^{(N)}$  at all N = 2J + 1. In the same comparison, in contrast, the leading-order secular equation

$$(L-2^2)(L-4^2)(L-6^2)\dots(L-[2J]^2) + \varepsilon^{(J)} = 0$$
(32)

pertaining to the odd N = 2J + 1 is slightly more complicated. This is demonstrated by table 2 showing that the general formula for the factors  $\varepsilon^{(J)}$ 

$$\varepsilon^{(J)} = 2(2J-1)(2J)! \sum_{n=1}^{J} (-1)^{J-n} C^{(J)}_{(n)} G_n$$
(33)

is perceivably less explicit. The reason is that the elementary combinatorial coefficients in equation (31) are replaced now by no-name integer coefficients  $C_{(n)}^{(J)}$ .

Fortunately, the latter coefficients can be understood as an immediate generalization of the current combinatorial numbers since, firstly, they exhibit a left-right antisymmetry  $C_{(1-n)}^{(J)} = -C_{(n)}^{(J)}$  at n = 1, 2, ... and, secondly, these coefficients may be generated by the recurrences

$$C_{(n)}^{(J)} = C_{(n-1)}^{(J-1)} + 2C_{(n)}^{(J-1)} + C_{(n+1)}^{(J-1)}$$
(34)

from the initial row  $C_{(n)}^{(J)}$  at J = 1 which contains a unit at n = 1 and zero for n > 1 (cf table 3). Thirdly, a decomposition of the sum (34) in the two steps specifies the coefficients  $C_{(n)}^{(J)}$  as a subset of the triangle generated by the usual combinatorial three-term recurrences. The latter generation pattern is sampled in table 4. One notes that both the three-term recurrences and their illustrative table 4 differ from their standard Pascal-triangle predecessors merely in an anomalous, left–right antisymmetric initialization.

Once we return to our leading-order energies  $E_n^{(2J+1)}$  we may say, on the basis of equation (32), that their *leading-order* complexification *always* seems to proceed in one of the following two ways:

- through the two simultaneous, symmetric mergers of the negative  $E_{J-2}$  with  $E_{J-1}$  and of the positive  $E_{J+1}$  with  $E_{J+2}$  (at  $\varepsilon_{(LL)}^{(J)} < 0$  for  $J = 1, 3, 5, \ldots$  and at  $\varepsilon_{(UL)}^{(J)} > 0$  for  $J = 2, 4, 6, \ldots$ );
- through the two simultaneous, symmetric mergers of the negative  $E_{J-3}$  with  $E_{J-2}$  and of the positive  $E_{J+2}$  with  $E_{J+3}$  (at  $\varepsilon_{(\text{UL})}^{(J)} > 0$  for  $J = 1, 3, 5, \ldots$  and at  $\varepsilon_{(\text{LL})}^{(J)} < 0$  for  $J = 2, 4, 6, \ldots$ ).

In the other words, the implicit definition (32) of the spectrum has a similar geometric interpretation and implications for the shape of the boundary  $\partial D^{(2J+1)}$  as its even-dimensional predecessor (30) did.

| J   |    |    |    |    |    |    | п  | = | 1        |   | 2        |   | 3        |   |   |
|-----|----|----|----|----|----|----|----|---|----------|---|----------|---|----------|---|---|
| (1) |    |    |    |    |    |    | -1 |   | 1        |   |          |   |          |   |   |
| _   |    |    |    |    |    | -1 |    | 0 |          | 1 |          |   |          |   |   |
| 2   |    |    |    |    | -1 |    | -1 |   | 1        |   | 1        |   |          |   |   |
| _   |    |    |    | -1 |    | -2 |    | 0 |          | 2 |          | 1 |          |   |   |
| 3   |    |    | -1 |    | -3 |    | -2 |   | <u>2</u> |   | <u>3</u> |   | <u>1</u> |   |   |
| _   |    | -1 |    | -4 |    | -5 |    | 0 |          | 5 |          | 4 |          | 1 |   |
| 4   | -1 |    | -5 |    | -9 |    | -5 |   | <u>5</u> |   | <u>9</u> |   | <u>5</u> |   | 1 |
|     |    |    |    |    |    |    |    |   |          |   |          |   |          |   |   |
| :   |    |    |    |    |    |    |    |   |          |   |          |   |          |   |   |

**Table 4.** Pascal-like triangle, with coefficients  $C_{(m)}^{(J)}$  underline

#### 8. Discussion

#### 8.1. Kato's exceptional points

In Kato's book [1], certain  $\kappa$ -dependent one-parametric families of *N*-by-*N* matrices were discussed, with elements defined as holomorphic functions of  $\kappa$  in a complex domain  $D_0$ . It has been noted there that up to not too many 'exceptional points'  $\kappa^{(EP)} \in D_0$ , the number of eigenvalues of any such matrix  $H(\kappa)$  is equal to a constant.

One of Kato's illustrative two-by-two examples possessing just a real pair of Kato's exceptional points was discussed in our recent paper [9]. In his/our example (=  $H^{(2)}$  in our present notation) we worked just with the real  $\kappa \equiv g_1$  and identified Kato's exceptional points as points of the boundary of the corresponding quasi-Hermiticity domain,  $\kappa^{(EP)} \in \partial D^{(2)}$ .

This was one of the important motivations of our continuing interest in the structure of the sets  $\partial D^{(N)}$  of the real exceptional points attached, in particular, to the real chain models  $H^{(N)}$  at the higher matrix dimensions *N*. In these particular models, the sets of the real Kato's exceptional points (i.e., the boundary sets  $\partial D$  of the models in question) exhibit a nice and transparent hierarchical pattern of confluence.

Among all the multiple exceptional points, an extreme is represented by the *J*-tuple confluence of these points at the strong-coupling extremal EEP vortices [5]. Of course, all the similar multiple confluence(s) of the exceptional-point hypersurfaces of various dimensions are in a close correspondence with some physical critical phenomena. We might emphasize that in our family  $H^{(N)}$ , a fine-tuning mechanism emerges which aligns the values of the physical couplings in a manifestly non-perturbative though still analytically tractable and presumably also generic and, in its qualitative aspects, not too model-dependent manner.

#### 8.2. Separable anharmonicities

On the more practical side of our present considerations and constructions it is worth emphasizing that Kato's abstract models of a generic dependence of the eigenvalues on a *single* variable parameter in  $H = H(\kappa) \neq H^{\dagger}$  need not always offer a better qualitative understanding of the situation.

For an explicit illustrative example, we may return to the differential-equation example of paper [2]. An inspection of table 1 of this paper reveals that once we vary just an arbitrarily chosen free parameter  $\alpha$  (as defined in equation (3)), no obvious pattern is detected in the complexifications *and* decomplexifications of the energy levels which occur in table in an apparently unpredictable and more or less chaotic manner.

What we would recommend in similar situations would be, in the light of our present experience, a deeper inspection of the separate matrix elements themselves, followed by a subsequent tentative re-definition of the spectrum as depending on some *more* (say, *J*) *independently* variable parameters in  $H = H(\kappa_1, \kappa_2, ..., \kappa_J) \neq H^{\dagger}$ . Only then one would have a right to expect that one finds an 'optimal' linear combination of  $\kappa_j$ s which would not cross the global boundary  $\partial D$  at random or, at least, which would stay *locally* more or less perpendicular to  $\partial D$ .

One could expect the existence of an 'optimal' size J of the set of the auxiliary parameters in many other manifestly non-Hermitian models based on the use of a complex potential V(x). Unfortunately, it is difficult to predict how such a type of analysis would prove efficient in practice. In this sense a return could be recommended to many older papers on the subject [16].

The problem looks interesting even as a purely mathematical puzzle of survival of the reality of the energies (i.e., in principle, of the observability of the system) *after* real potentials are replaced by their complex  $\mathcal{PT}$ -symmetric versions. An interest in such an apparent paradox has been evoked almost 10 years ago [12, 17] but it took several years before the necessary *rigorous* proofs of the reality of the spectrum became available [18].

Bad news is that too often, the reality proofs are fairly complicated [19]. In parallel, good news is that once all the energies stay real, one returns easily to the standard principles and formalism of Quantum Mechanics by using an ad hoc scalar product in the physical Hilbert space  $\mathcal{H}$ . This means that one merely replaces the usual overlaps  $\langle \phi | \psi \rangle$  by their generalizations  $\langle \phi | \Theta | \psi \rangle$  (this idea belongs to Scholtz *et al* [11]).

Although, as a rule, the physical Hilbert-space metric  $\Theta = \Theta^{\dagger} > 0$  proves complicated and non-local, people often succeed in its (e.g., perturbative [20]) construction. Of course, the explicit specification of the *whole* 'physical' domain  $\mathcal{D}$  seems to be an even more difficult task. That is why we recommended here the use of the finite-dimensional prototype matrices  $H^{(N)}$ .

It is obvious that our knowledge of the boundaries  $\partial \mathcal{D} = \partial \mathcal{D}(H)$  of the physical consistence of a generic  $\mathcal{PT}$ -symmetric Hamiltonian is necessary for any reliable physical prediction or for a consistent probabilistic interpretation of the results of quantum measurements. This boundary may have a fairly complicated shape even in the simplest, exactly solvable models [21]. At the same time, we believe that the present constructive clarification of the geometric structure of the corresponding 'prototype physical horizons'  $\partial \mathcal{D}^{(N)}(H^{(N)})$  (where even the diagonalizability of the matrices  $H^{(N)}$  themselves gets lost!) could accelerate the progress in the analysis of the more common Hs defined via potentials.

#### 9. Summary

Without any limitations imposed upon N, the series of *all* the models  $H^{(N)}$  has been shown to admit an innovative strong-coupling approximative treatment. In particular, the underlying polynomial secular equations were shown to degenerate to the closed leading-order form in the strong-coupling dynamical regime.

An appropriate technical tool for our simplification of the chain-model bound-state problem in question has been found in ad hoc perturbation ansatz (9) which reparametrizes all the coupling constants in a way inspired by their available closed-form  $t \rightarrow 0$  limit known from our previous paper [5].

Also our present methods were inspired by the same reference—we further developed the application of the brute-force symbolic-manipulation techniques as well as of the systematic formulations and verifications of extrapolation hypotheses. Marginally, we may add that one

of our results, namely, the implicit leading-order formula for the energies in odd dimensions N = 2J + 1 required a slightly unusual though straightforward and immediate generalization of the standard binomial coefficients. Our new combinatorial coefficients were shown closely related to a pair of alternative generalizations of the popular Pascal triangle.

Via a deeper analysis of the leading-order secular polynomials we were, subsequently, able to demonstrate, in the whole strong-coupling dynamical regime of  $H^{(N)}$ , how the determination of the asymptotic strong-coupling parts of the domains of quasi-Hermiticity  $\mathcal{D}^{(N)}$  degenerates to elementary approximative formulae at all the dimensions N.

Our main conclusion is that our class of models  $H^{(N)}$  could be understood, in many a respect, as representing or mimicking many generic features of the general  $\mathcal{PT}$ -symmetric and pseudo-Hermitian Hamiltonians. In this sense, in particular, our present quantitative description of the mechanism of complexification of the energies could find an important application as a guide to our understanding of the change of the dynamical regime called the spontaneous breakdown of  $\mathcal{PT}$ -symmetry [21].

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