Determination of the domain of the admissible matrix elements in the four-dimensional $\mathcal{PT}$–symmetric anharmonic model

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Abstract

Many manifestly non-Hermitian Hamiltonians (typically, $\mathcal{PT}$–symmetric complex anharmonic oscillators) possess a strictly real, “physical” bound-state spectrum. This means that they are (quasi-)Hermitian with respect to a suitable non-standard metric $\Theta \neq I$. The domain $\mathcal{D}$ of the existence of this metric is studied here for a nontrivial though still non-numerical four-parametric “benchmark” matrix model.
1 Non-Hermitian observables with real spectra

Quite a few realistic quantum models are characterized by a mere “fragile” stability of their bound states. For example, the reality of the energies of certain nuclear-physics models may be lost after an “inessential” change of its coupling strengths [1]. Such a phenomenon is rendered possible when the Hamiltonian merely remains Hermitian with respect to a nonstandard scalar product, i.e., with respect to a “nontrivial metric” \( \Theta \neq I \) in an underlying “physical” Hilbert space. This means that all the operators of observables \( H \) must obey an unusual rule

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

Such a property of (typically: Hamiltonian) \( H \) guarantees the reality of the spectrum and may be called quasi-Hermiticity.

Practical objections may occur against the use of a nontrivial metric \( \Theta \neq I \). One of their sources lies in the fact that many phenomenological models in Quantum Mechanics are based on a differential-operator realization of their Hamiltonians. Thus, whenever one works with a one-dimensional differential-operator Hamiltonian (in units \( \hbar = 2m = 1 \)),

\[
H = -\frac{d^2}{dx^2} + V(x) = H^\dagger, \quad x \in (-\infty, \infty) \tag{2}
\]

one usually prefers the most economical \( \Theta = I \) scenario since even its simplest alternatives require a number of additional mathematical considerations [2]. Moreover, up to the very recent past it has been intuitively expected that the transition to any non-Hermitian generalization of the class of differential-operator Hamiltonians (2) would be accompanied by a complexification of their spectrum and by a decaying-state re-interpretation of the corresponding wave functions. The latter misunderstanding even survived the publication of a few studies [3, 4] which paid attention to specific examples

\[
H = -\frac{d^2}{dx^2} + U(x) + i W(x) \neq H^\dagger, \quad x \in (-\infty, \infty). \tag{3}
\]

where the two independent real potentials \( U(x) = U(-x) \) and \( W(x) = -W(-x) \) happened to generate the real bound-state spectra [5] and where their spatial symmetry/antisymmetry has been re-interpreted as a combined parity-plus-time-reversal (called “\( PT \)”) symmetry of the Hamiltonian [6].

The scepticism (well sampled, e.g., on the Streater’s webpage [7]) did not fully die out even after publication of several analytic, semi-classical and numerical studies.
of some new $\mathcal{PT}$-symmetric models (3) in 1998 (cf., e.g., [8, 9, 10]). Their authors demonstrated that the entire spectrum seems to remain real in comparatively large domains $D$ of parameters. At present, fortunately, we witness a reconciliation and final acceptance of the idea that the complex differential Hamiltonians may possess the real bound-state spectra, indeed. The two sets of the fresh 2006 “state-of-the-art” reports may be found in the August dedicated issue of J. Phys. A: Math. Gen. (vol. 39, number 32, pp. 9963 – 10261) and in the September dedicated issue of Czech. J. Phys. (vol. 56, number 9, pp. 885 – 1064).

One of the paradoxes accompanying such a development of the subject is that in contrast to the popularity of the various anharmonic-type models (based, first of all, on their high relevance in field theory [11]), much less attention has been paid to the finite-dimensional matrix versions of the non-Hermitian quantum Hamiltonians [12]. One of the reasons is that in the matrix models (encountered, quite naturally, in variational calculations [1]) one usually deals with “too many” independent matrix elements. The selection and/or preference of some of them might look “too arbitrary” in the context of physics and/or “too ambiguous” in the language of mathematics.

In what follows we intend to fill the gap and to study a model which tries to circumvent both these “traps” by containing just a few “relevant” free parameters and by being still surprisingly rich in its mathematical structure and consequences. Moreover, its “derivation” from the differential operator (3) (cf. section 2) gives it a certain generic character while leaving it still purely non-numerical and exactly solvable. Last but not least, the not quite expected closed-form feasibility of its mathematical analysis (cf. sections 3 and 4) is quite well matched by some of its appealing phenomenological features, a few remarks on which are added here in our final section 5.

2 Matrix toy models

2.1 Variational origin

In order to interconnect the differential and finite-dimensional $N$-state Hamiltonians let us start from their most elementary differential harmonic-oscillator example $H_0$ with the eigenstates $|n\rangle, n = 0, 1, 2, \ldots$ or, in the coordinate representation,

$$
\langle x | 2m \rangle = N_{(m, +)} e^{x^2/2} H_{2m}(x^2), \quad \langle x | 2m + 1 \rangle = x N_{(m, -)} e^{x^2/2} H_{2m+1}(x^2)
$$

(4)
where the symbols $\mathcal{H}_n$ denote the well known Hermite polynomials [13]. The subscripts $\pm$ in the normalization factors $\mathcal{N}_{(m,\pm)}$ are added to emphasize that our basis states (4) are, simultaneously, eigenstates of the operator of parity $\mathcal{P}$ with eigenvalues $(-1)^n$. The action of the complex conjugation $\mathcal{T}$ (mimicking the time reversal [8]) preserves these basis states once the normalization factors $\mathcal{N}_{(m,\pm)}$ are chosen real.

The $\mathcal{PT}$--symmetry $\mathcal{H}\mathcal{PT} = \mathcal{PT}\mathcal{H}$ of a given Hamiltonian (say, (3)) with real spectrum enables us to normalize all the eigenstates $|\psi_n\rangle$ of $\mathcal{H}$ in such a way that

$$\mathcal{PT} \langle x | \psi_n \rangle = + \langle x | \psi_n \rangle .$$

(5)

In effect, the fixed parity of our harmonic-oscillator basis (4) is generalized to the $\mathcal{PT}$--symmetry of eigenstates. Once we accept such a convention (speaking about “unbroken $\mathcal{PT}$--symmetry of wave functions”) we may decompose

$$|\psi\rangle = |\psi_+\rangle - i |\psi_-\rangle$$

(6)

with real expansion coefficients $\phi_m$ and $\chi_m$ in the variational ansatz of the form

$$|\psi_+\rangle = \sum_{m=0}^{N_+} |2m\rangle \phi_m, \quad |\psi_-\rangle = \sum_{m=0}^{N_-} |2m+1\rangle \chi_m, \quad N_+ + N_- = N \to \infty .$$

The partitioning of our basis with $|2n\rangle \equiv |n_+\rangle$ and $|2m + 1\rangle \equiv |m_-\rangle$ and its variational truncation with $N \gg 1$ transform Hamiltonian (3) into a finite-dimensional partitioned complex matrix

$$\tilde{H} = \begin{pmatrix} S & i B \\ i C & L \end{pmatrix}$$

where the untilded letters denote the submatrices with real matrix elements,

$$S_{mn} = \langle 2m | -\frac{d^2}{dx^2} + U(x) | 2n \rangle = (S^T)_{mn} ,$$

(7)

$$L_{mn} = \langle 2m + 1 | -\frac{d^2}{dx^2} + U(x) | 2n + 1 \rangle = (L^T)_{mn} ,$$

(8)

$$B_{mn} = \langle 2m | \mathcal{W}(x) | 2n + 1 \rangle \neq (B^T)_{mn} \equiv C_{mn} = \langle 2m + 1 | \mathcal{W}(x) | 2n \rangle .$$

(9)

The superscript $^T$ denotes transposition.
2.2 Real matrix Schrödinger equations

After we insert (6) in Schrödinger equation $\hat{H}|\psi\rangle = E|\psi\rangle$ we reveal that the resulting partitioned matrix form of Schrödinger equation for bound states is real and non-Hermitian,

$$
\begin{pmatrix}
\vec{\phi} \\
\vec{\chi}
\end{pmatrix} = E
\begin{pmatrix}
\vec{\phi} \\
\vec{\chi}
\end{pmatrix}, \quad H = \begin{pmatrix}
S & B \\
-B^T & L
\end{pmatrix}.
$$

(10)

No mathematical contradiction appears in the latter picture since the metric $\Theta$ naturally becomes singular on the boundary $\partial D$ of the domain $D$.

In general, the solutions of eq. (10) must be constructed numerically. The well known exception is represented by the two-state models [14]. The two-dimensional version of our present simplified eq. (10) has also thoroughly been discussed in our recent letter [15]. In the corresponding two by two matrix Schrödinger equation

$$
\begin{pmatrix}
S & B \\
-B & L
\end{pmatrix}
\begin{pmatrix}
\phi \\
\chi
\end{pmatrix} = E
\begin{pmatrix}
\phi \\
\chi
\end{pmatrix}
$$

(11)

parameters $s, b$ and $l$ are real and, by assumption, the even and odd unperturbed energies are nondegenerate, $s \neq l$. Via a suitable scaling we may achieve that $l - s = 2$. A shift of the energy scale $E \rightarrow E + const$ leads to the completely symmetric arrangement of our entirely general $H$ with $s = -1$ and $l = 1$. We recall the secular equation $\det(H - E) = 0$ and deduce the energy levels,

$$
E = E_{\pm} = \pm \sqrt{1 - b^2}.
$$

(12)

Thus, for our single-parametric family $H = H(b)$ of the $N = 2$ Hamiltonians the domain $D = D(N)$ of the (single) free parameter $b$ where the energies are real coincides with the (closed) interval of $b \in D(2) \equiv [-1, 1]$. At both the ends of this interval our Hamiltonian ceases to be diagonalizable. For this reason the domain of the quasi-Hermiticity of $H$ is often being re-defined as a mere open set or interior $D^{(0)}(2) = (-1, 1)$. Under both these conventions, one finds complex energies in the vicinity of every element of the boundary $\partial D \equiv \partial D^{(0)}$ [16].

2.3 Anharmonic-oscillator-like four-by-four matrix model

In the harmonic-oscillator model itself the evaluation of the matrix elements remains trivial and one arrives at the simplest illustrative example $H_0$ containing just a
decoupled pair of diagonal submatrices,

\[ S_{mn}^{(0)} = \langle 2m \mid H_0 \mid 2n \rangle = \delta_{mn} \cdot (4n + 1), \quad (13) \]

\[ L_{mn}^{(0)} = \langle 2m + 1 \mid H_0 \mid 2n + 1 \rangle = \delta_{mn} \cdot (4n + 3). \quad (14) \]

For all the Hermitian generalizations of \( H_0 \) with unbroken parity (\( \mathcal{P} H = H \mathcal{P} \)) equation (10) would stay decoupled (\( B = B^T = 0 \)). This means that the parity-preserving and Hermitian anharmonicities may be considered “trivial” in leaving the matrices \( S \) and \( L \) decoupled and diagonalizable by the separate unitary transformations in the respective even-parity and odd-parity subspaces.

We intend to employ just the diagonalized and purely harmonic submatrices (13) and (14), studying merely the role of the off-diagonal anharmonic-oscillator-like coupling matrices \( B \) in what follows. Thus, we shall start from the general \( \mathcal{PT} \)-symmetric model (10) with

\[
H = \begin{pmatrix}
1 & 0 & \cdots & B_{11} & B_{12} & \cdots \\
0 & 5 & \cdots & B_{21} & \cdots \\
\vdots & \vdots & \ddots & \vdots & \ddots \\
-B_{11} & -B_{21} & \cdots & 3 & 0 & \cdots \\
-B_{12} & \cdots & 0 & 7 & \ddots \\
\vdots & \vdots & \ddots & \vdots & \ddots & \ddots
\end{pmatrix} . \quad (15)
\]

We shall restrict our attention to the “first nontrivial” four-level system with the truncated dimensions \( N_+ = N_- = 2 \). For the sake of convenience we shall also symmetrize the unperturbed spectrum via a shift of the origin on the energy scale, \( (1, 3, 5, 7) \to (-3, -1, 1, 3) \) and arrive at the Schrödinger-equation

\[
\begin{pmatrix}
-3 & 0 & c & b \\
0 & 1 & a & d \\
-c & -a & -1 & 0 \\
-b & -d & 0 & 3
\end{pmatrix}
\begin{pmatrix}
\phi_0 \\
\phi_1 \\
\chi_0 \\
\chi_1
\end{pmatrix}
= E
\begin{pmatrix}
\phi_0 \\
\phi_1 \\
\chi_0 \\
\chi_1
\end{pmatrix} . \quad (16)
\]

In comparison with the current two-state analyses, a combined effect mediated by the simultaneous growth of all the four real parameters \( a, b, c \) and \( d \) will be more complicated of course. At the same time, the levels coupled by an off-diagonal matrix element will still follow the pattern revealed at \( N = 2 \). This means that, say, the growth of \( c \) will cause a mutual attraction of the energy levels \(-3\) and \(-1\), etc.
Obviously, the separate effects of attraction will compete. One even might encounter the usual crossing of levels, not accompanied by any instability and/or subsequent complexification of the pairs of the levels involved. This is the reason why the “first nontrivial” $N = 4$ model deserves a deeper analysis.

3 Constructive analysis of the four-by-four model

A priori we may say that the influence of the variation of all the quadruplet of coupling constants in (16) is tractable non-numerically since the spectrum of energies coincides with the set of roots of the secular determinant

$$\det \begin{pmatrix} -3 - E & 0 & c & b \\ 0 & 1 - E & a & d \\ -c & -a & -1 - E & 0 \\ -b & -d & 0 & 3 - E \end{pmatrix} = 0 .$$  \hspace{1cm} (17)

The exact energies remain obtainable using closed formulae since the corresponding secular polynomial is of the mere fourth order,

$$E^4 - \left(10 - a^2 - b^2 - c^2 - d^2\right) E^2 - 4 \left(c^2 - d^2\right) E + C(a, b, c, s) = 0$$  \hspace{1cm} (18)

where we abbreviated

$$C(a, b, c, d) = 9 - 9 a^2 - b^2 + 3 c^2 + 3 d^2 + a^2 b^2 + c^2 d^2 - 2 a b c d .$$

Still, the use of the closed formulae does not facilitate our insight in the structure of the spectrum too much as it proves prohibitively uncomfortable. Our experience is that virtually any alternative analytic approach to eq. (18) proves preferable.

3.1 Quadruple mergers of the energy levels

We intend to describe the mechanism of a complexification of the energies in the manner which would separate the essential and inessential influence of the variations of the parameters. Thus, in a formal language we shall search for the values of the matrix elements $a$ bis $d$ at which an abrupt, qualitative change of the spectrum could occur.

In this sense, the most interesting situation occurs at the “points of maximal nonhermiticity”’(PMN) at which all the four energy levels coincide, $E_0 = E_1 = E_2 =$
\[ E_3 = z = z^{(PMN)}. \] In the light of an “up-down” symmetry of our unperturbed spectrum \((-3, -1, 1, 3)\) we may fix \(z^{(PMN)} = 0\). A change of this value could only be caused by a (presumably, perturbative) modification of our model.

Under the assumption \(z = 0\) our secular equation should read \((E - z)^4 = E^4 = 0\) so that the quadratic term in eq. (18) must vanish,

\[ a^2 + c^2 + b^2 + d^2 = 10. \] (19)

This means that all the four PMN parameters must lie on a four-dimensional sphere with radius \(\sqrt{10}\). Similarly, from the condition of the vanishing of the linear term we deduce that \(c^2 = d^2\). Finally, the condition \(C(a, b, c, d) = 0\) reads

\[ 9 - b^2 - 9a^2 + 3d^2 + 3c^2 + c^2d^2 - 2cba + a^2b^2 = 0 \]

and degenerates to the factorized relation

\[ C(a, b, c, d) = \left(d^2 - ab + 3\right)^2 - \left(b - 3a\right)^2 = \left(d^2 - \alpha\right)\left(d^2 - \beta\right) = 0 \] (20)

where \(\alpha = (b + 3)(a - 1)\) and \(\beta = (b - 3)(a + 1)\). This means that at any fixed value of \(d^2 > 0\) we get all its solutions \((a, b)\) as points in the \(a - b\) plane which lie on the four branches of the two hyperbolas \(d^2 = \alpha(a, b)\) and \(d^2 = \beta(a, b)\) as displayed for illustration in Figure 1, with their two centers marked by the bigger circles and with the two intersections marked by the small circles (units and axes are dropped here as irrelevant).

Once we return to the former constraint (19) we may conclude that the points on the hyperbolas are spurious unless they lie also on the centered circle with the radius \(\sqrt{10 - 2d^2}\). Hence, under our spectrum-symmetry assumption \(z = 0\) there exist four PMN matrix-element solutions which induce a “maximal”, quadruple merger of the real energy levels, in a finite interval of values of the free parameter \(d^2\) of course. In our illustrative Figure 1 (where we choose \(d^2 = 8/5\)) we see that and how the resulting points of the boundary \(\partial D\) in the \(a - b\) plane (denoted by symbols \(C2a, C2b, C5a\) and \(C5b\)) emerge as intersections of the central circle with the respective hyperbolic segments \(C2 - C3\) and \(C5 - C6\).

### 3.2 Simplified four-by-four model with \(c^2 = d^2\)

In terms of the abbreviations

\[ A = 5 - d^2 - \frac{1}{2}\left(a^2 + b^2\right), \quad B = \left(d^2 - ab + 3\right)^2 - \left(b - 3a\right)^2 \]
the symmetry assumption \( c^2 = d^2 \) makes our original secular eq. (18) simpler,

\[
E^4 - 2AE^2 + B = 0,
\]

and much more easily solvable by the compact formula,

\[
E_{\pm,\pm} = \pm \sqrt{A \pm \sqrt{A^2 - B}}.
\]  

(21)

This means that the necessary and sufficient condition of the reality of the energies is given by the pair of requirements

\[
A \geq 0
\]  

(22)

and

\[
A^2 \geq B \geq 0.
\]  

(23)

Conditions (22) and (23) represent an exceptionally transparent implicit definition of the quasi-Hermiticity domain \( D \) and/or of its boundary set \( \partial D \) of all the complexification points.

Complementing the discussion presented in paragraph 3.1 above we might notice that \( B \equiv C(a, b, d, d) \) in our older notation. This means that the two hyperbolas of Figure 1 represent precisely the boundary curves of the domain \( D \) of validity of condition \( B \geq 0 \) of eq. (23). One can easily verify that its subdomain where \( d^2 \leq \alpha(a, b) \) and \( d^2 \leq \beta(a, b) \) consists of two disjoint subsubdomains \( D(+, A/B) \) with the respective boundary curves \( A1 - A2 - A3 \) and \( B1 - B2 - B3 \). Similarly, the second, single and simply connected subdomain \( D(-, C) \) of \( D \) where \( d^2 \geq \alpha(a, b) \) and \( d^2 \geq \beta(a, b) \) is specified by its two pieces of boundary \( C1 - C2 - C3 \) and \( C4 - C5 - C6 \) in Figure 1. Obviously, just the latter subdomain has a non-vanishing overlap with the interior of the circumscribed circle (19).

We can summarize that the bound-state energies of the model can only remain real inside the latter overlap. In order to arrive at a corresponding sufficient condition, one has to recall the last constraint \( A^2 \geq B \) of eq. (23). In its entirely explicit form it reads

\[
\left(8 + a^2 - b^2\right)^2 \geq 4d^2 \left[16 - (a + b)^2\right].
\]

Its exhaustive discussion and geometric interpretation gets facilitated and becomes more or less elementary in its alternative representation

\[
(2 + \sigma \delta)^2 \geq d^2 \left(4 - \sigma^2\right).
\]

in the new, rotated coordinates \( \sigma = a + b \) and \( \delta = a - b \).
4 Special case: $\mathcal{PT}$–symmetric band matrices

4.1 Perturbative considerations

A re-numbering of the basis (i.e., an interchange of its second and third element) makes the matrix in eq. (17) equivalent (i.e., isospectral) to another Hamiltonian,

$$
H(a, b, c, d) = \begin{pmatrix}
-3 & c & 0 & b \\
-c & -1 & -a & 0 \\
0 & a & 1 & d \\
-b & 0 & -d & 3 \\
\end{pmatrix}.
$$

(24)

Once the coupling of the most distant levels vanishes, $b = 0$, and once we re-install the symmetry $c = d$, we arrive at a perceivably simpler two-parametric Hamiltonian

$$
H(a, c) = \begin{pmatrix}
-3 & c & 0 & 0 \\
-c & -1 & -a & 0 \\
0 & a & 1 & c \\
0 & 0 & -c & 3 \\
\end{pmatrix}.
$$

(25)

It is particularly suitable for perturbative analysis. For example, its one-parametric special case

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

possesses the easily evaluated energies

$$
E_{\pm 1} = \pm \left[ -6 \alpha^2 + 5 - 2 \left(5 \alpha^4 - 12 \alpha^2 + 4\right)^{1/2} \right]^{1/2},
$$

$$
E_{\pm 3} = \pm \left[ -6 \alpha^2 + 5 + 2 \left(5 \alpha^4 - 12 \alpha^2 + 4\right)^{1/2} \right]^{1/2}.
$$

In the regime of a small $\alpha^2$ the quickly decreasing curve

$$
|E_{\pm 3}| = 3 - 2 \alpha^2 - \alpha^4 - \frac{7}{6} \alpha^6 + O(\alpha^8)
$$

gets closer and closer to the slowly increasing curve

$$
|E_{\pm 1}| = 1 + \alpha^4 + \frac{3}{2} \alpha^6 + O(\alpha^8).
$$

The energy curves finally intersect, pairwise, at a certain critical strength,

$$
\alpha^{(CS)} = \sqrt{\frac{2}{5}}, \quad E_{\pm 1}^{(CS)} = E_{\pm 3}^{(CS)} = \pm \sqrt{\frac{13}{5}} \sim \pm 1.612451550.
$$

Beyond this boundary, i.e., at $\alpha^2 > 2/5$, all the four energies become complex.
4.2 Facilitation of the construction of the metric $\Theta$

There exists a clear contrast between the robust reality of the energies resulting from a Hermitian Hamiltonian $H = H^\dagger$ and the globally fragile character of the reality of the spectrum in the models which are non-Hermitian and, in particular, $\mathcal{PT}$-symmetric. We emphasized in section 1 that this contrast finds a formal representation in the transition to a nontrivial physical metric $\Theta \neq I$.

On the formal level the operator $\Theta$ may be different for different Hamiltonians so that both the Hamiltonian $H$ and the metric $\Theta$ may depend on certain variable parameters. One expects, in particular, that the spectrum of $H$ ceases to be real out of the domain $\mathcal{D}$ of these parameters. Of course, a necessary deeper study of all these possibilities is much easier at finite dimensions $N$ when the linear equation (1) determines all the eligible metrics $\Theta$.

The straightforward linear-algebraic construction of $\Theta$ remains ambiguous. For our present, drastically simplified $N = 4$ input Hamiltonians $H$ the complete solution and discussion of the problem remains feasible. For illustration let us consider the one-parametric model (26) and solve the related problem

$$H^\dagger(\alpha) \Theta = \Theta H(\alpha)$$

(27)

by brute force. This gives the following nontrivial four-parametric real symmetric matrix solution

$$\Theta(p, q, r, s) = \begin{pmatrix}
\Theta_{11} & \Theta_{12} & r & \Theta_{14} \\
\Theta_{12} & p & \Theta_{23} & s \\
r & \Theta_{32} & \Theta_{33} & \Theta_{34} \\
\Theta_{14} & s & \Theta_{34} & q
\end{pmatrix}$$

(28)

of the sixteen quasi-Hermiticity conditions (27). In the solution which is routine we may employ the notation

$$\Theta_{11} = \frac{1}{6}(-9p + 3q + 10r + s) + \frac{1}{\alpha^2}(2r - s),$$

$$\Theta_{14} = -\frac{(r + s)\alpha}{3},$$

$$\Theta_{33} = \frac{1}{6}(-3p - 3q + 4r + s) + \frac{s}{\alpha^2},$$

$$\Theta_{12} = \frac{\alpha}{6}(3p - 3q - 4r - s) + \frac{1}{\alpha}(-2r + s),$$

$$\Theta_{23} = \frac{\alpha}{6}(-3p + 3q + 2r - s) - \frac{s}{\alpha},$$

$$\Theta_{34} = \frac{\alpha}{6}(3p - 3q - 4r - s) - \frac{s}{\alpha},$$

which specifies the unindexed matrix elements as independent parameters.
4.3 Construction of the surface \( \partial \mathcal{D} \) near the nonperturbative PMN regime

In the light of our previous results, Hamiltonian \( H(a, c) \) of eq. (25) possesses the quadruply degenerate energy \( E = E^{(PMN)} = 0 \) at the four PMN points with coordinates \( a = a^{(PMN)} = \pm 2 \) and \( c = c^{(PMN)} = \pm \sqrt{3} \). In the vicinity of one of them (let us pick up, say, the lower left one) we may set \( a = a^{(PMN)} (-1 + a') \) and \( c = c^{(PMN)} (-1 + c') \) with some small measures of deviation \( a' \) and \( c' \).

In the zeroth order of perturbative analysis this ansatz just reproduces the PMN solution \( a' = c' = 0 \). On the first-order level of precision the result \( a' = c' \) remains indeterminate. We have to switch to an improved ansatz containing a new, auxiliary small parameter \( t \),

\[
\begin{align*}
a &= a^{(PMN)} \left[ -1 + t + \alpha t^2 + O \left( t^3 \right) \right], \\
c &= c^{(PMN)} \left[ -1 + t + \gamma t^2 + O \left( t^3 \right) \right].
\end{align*}
\]

Its insertion in the polynomial secular equation \( \det \left[ H(a, c) - E \right] = 0 \) (which is of the second order in \( s = E^2 \)) leads just to a re-arranged version of the solutions derived in paragraph 3.2. In particular, on the second order level of precision we obtain the following simplified version of eq. (22),

\[
10 t + (-5 + 4 \alpha + 6 \gamma) t^2 + O \left( t^3 \right) \geq 0
\]

which only requires that our small parameter must be non-negative, \( t \geq 0 \). The second half (23) of the implicit definition of the quasi-Hermiticity subdomain \( \mathcal{D} \) in the \( a-c \) plane is more informative and gives the final, comprehensive estimate

\[
\gamma + \frac{8}{9} + O(t) \geq \alpha \geq \gamma - \frac{1}{2} + O(t).
\]

This formula characterizes the “allowed” parameters \( a \) and \( c \) which remain compatible with the reality of the energies. Its form is suitable for the parametric graphical plotting of the boundary \( \partial \mathcal{D} \). The result is sampled in Figure 2 showing that in the vicinity of the PMN matrix elements the domain \( \mathcal{D} \) has the shape of an extremely narrow spike. Its vertex \( \left( a^{(PMN)}, c^{(PMN)} \right) \) represents the simultaneous maximum of the size of these elements, saturating the circumscribed-sphere inequality (22) at the same time.
Towards more-dimensional models

A broad class of modifications of the standard harmonic oscillators may be characterized by a certain user-friendliness of their perturbative study. *A priori*, this experience may be extended to the quasi-Hermitian models where their \(N\)-state matrix Hamiltonian is just a small perturbation of the ordinary harmonic oscillator. Beyond this perturbative regime, unfortunately, the effects of the non-Hermitian components become less predictable. Firstly, in contrast to the usual textbook quantum theory where \(\Theta = I\), our present use of \(\Theta \neq I\) (i.e., of a manifest non-Hermiticity of \(H\)) may mean that the domain \(\mathcal{D}\) (where \(H\) represents an observable) is finite and that many of the textbook perturbation-theory theorems and algorithms may cease to be applicable [16].

In particular, our present study of a specific four-state toy model revealed that certain deeply non-perturbative mathematical as well as physical phenomena may occur along the boundary \(\partial \mathcal{D}\). Thus, we may expect that perturbation theory can offer a reliable qualitative description of the most relevant consequences of the variation of the matrix elements only in the regime far from the boundary \(\partial \mathcal{D}\). In its vicinity, on the contrary, perturbative considerations must be used with much more care and in an accordingly modified form.

Several purely theoretical questions emerge near \(\partial \mathcal{D}\) also in the areas of non-quantum physics exemplified, say, by magnetohydrodynamics [17], cosmology [18], crystal optics [19] or statistical physics [20]. In parallel, the points of \(\partial \mathcal{D}\) play an important role in the purely mathematical framework of perturbation theory [21] or supersymmetric considerations [22]. For all these reasons our present constructive study of the boundaries \(\partial \mathcal{D}\) may prove relevant in many different applications, after an appropriate generalization of our schematic model if necessary.

In this context, our study of the first nontrivial \(N = 4\) model offered several useful hints. We saw that our understanding and reconstruction of the shape of the boundary \(\partial \mathcal{D}\) will play a key role in the appropriate necessary modifications and applications of perturbation techniques. In such a context, it is of course unpleasant that the number of the relevant matrix elements (i.e., of the freely variable parameters at hand) grows very quickly with the dimension \(N\) since \(\dim \mathcal{D} = \text{entier}[N^2/4]\) in general. This makes the present \(N = 4\) model quite exceptional because in the very next \(N = 6\) model one already has \(\dim \mathcal{D} = 9\), etc.

In the purely formal setting, a sufficiently well-motivated reduction of the number
of the “relevant” matrix elements should be proposed in the future, therefore. The very first steps in this direction have only been made very recently – in ref. [23] certain additional symmetries have been introduced via certain non-Hermitian parity-type operators $\mathcal{P} \neq \mathcal{P}^\dagger$, etc.

In the more realistic considerations the relevance of the present model relates to the situations where some of the energy levels of a quantum system get close to each other. A number of experimental as well as theoretical challenges is encountered. On one side, during a variation of parameters the so called avoided level crossings may be observed in some nonrelativistic systems like atomic nuclei [24]. On the other side, a confluence of the two energy levels (at a point of $\partial \mathcal{D}$) may be followed by their subsequent complexification.

In the vicinity of a point of $\partial \mathcal{D}$ a nontrivial innovation of the physics of the model is often needed in its phenomenological applications. For illustration we may recollect an electron in a critically strong field where the single-particle Dirac equation must necessarily be replaced by its field-theoretical extension including many new degrees of freedom [25]. In a related brief comment [26] we emphasized that even on the level of the practical analyses of quantum systems using some oversimplified phenomenological models it is not always easy to draw the clear separation line between the avoided and unavoidable level crossings. A reliable separation of the two seem strongly model-dependent at present. All the future extension of the scope of the quantitative analysis of the models will be welcome, therefore.

A deeper study of the phenomenon of the complexification of the energies to larger dimensions will be well motivated not only by its purely mathematical appeal but also by the very pragmatic needs of a clarification of the possible and eligible patterns of the spectra in phenomenological models. In this sense, our present selection of the specific illustrative $\mathcal{PT}$–symmetric Hamiltonians $\mathcal{H}$ in a certain “first nontrivial” matrix form may be perceived as a natural starting point of such an effort.

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Figure captions

Figure 1. The centered circle (19) and the two hyperbolas
$C(a, b, d, d) = 0$ with the respective centers at $(a, b) = (-1, 3)$
and $(a, b) = (1, -3)$ (marked by medium circles) in $a - b$ plane
at $c^2 = d^2 = 1.6$

Figure 2. Spiked shape of the physical domain $D(a, c)$ near its
lower left corner
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Figure 1

\[ B_1 = C_5 \]

\[ B_2 = C_4 \]

\[ A_2 = C_2 \]

\[ (a,b) = (1,-3) \]

\[ (a,b) = (-1,3) \]

\[ C_2a \]

\[ C_5a \]

\[ C_5b \]

\[ (a,b) = (1,-3) \]

\[ A_2 = C_2 \]

\[ A_3 \]

\[ C_6 \]

\[ D(+,A) \]

\[ D(-,C) \]

\[ D(+,B) \]

\[ B_3 \]

\[ B_1 \]

\[ C_3 \]

\[ C_4 \]

\[ D(-,C) \]