Bound states emerging from below the continuum in a solvable $\mathcal{PT}$–symmetric discrete Schrödinger equation

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Abstract

The phenomenon of the birth of an isolated quantum bound state at the lower edge of the continuum is studied for a particle moving along a discrete real line of coordinates $x \in \mathbb{Z}$. The motion is controlled by a weakly nonlocal $2J$–parametric external potential $V$ which is non-Hermitian but $\mathcal{PT}$–symmetric. The model is found exactly solvable. The bound states are interpreted as Sturmians. Their closed-form definitions are presented and discussed up to $J = 7$.

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1 Introduction

The current growth of interest in the mathematical aspects of non-self-adjoint operators \cite{1, 2} has one of its roots in the increasing popularity of quantum physics of systems which exhibit a combined parity plus time-reversal invariance alias $\mathcal{PT}$–symmetry \cite{3, 4}. In this innovative branch of physics one can encounter discontinuities in the time-evolution processes \cite{3} and the critical situations in which a small change of a parameter $\lambda$ in a non-Hermitian but $\mathcal{PT}$–symmetric Hamiltonian $H(\lambda) \neq H^\dagger(\lambda)$ causes an abrupt change of the observable properties of the system in question \cite{6}. A broad class of the latter phenomena could be called “quantum catastrophes”. Their mathematical background may be found explained in the Kato’s monograph on linear operators \cite{7}. The points of the sudden change were given there the name of “exceptional points” (EP).

The localization of the singular EP values of $\lambda = \lambda_{(EP)}$ originally helped to determine the radii of the convergence of perturbation series. As long as the Hamiltonians in question were usually assumed self-adjoint, their EP parameters were complex, i.e., not carrying any immediate physical meaning (cf. Refs. \cite{8} for typical illustrative examples). The paradigm has been recently changed due to a dramatic increase of interest in non-Hermitian models. The EP singularities $\lambda_{(EP)}$ can be real in these models \cite{9}. Traditionally, people were connecting their occurrence with the physics of the so called “open systems”. Such a scenario may be found described in a number of reviews (cf., e.g., \cite{10, 11}), emphasizing that the open systems are, as a rule, unstable, resonant and quickly decaying or growing.

The comparatively recent interest in the $\mathcal{PT}$–symmetric theory of reviews \cite{4, 12, 13} has a perceivably different motivation and, in particular, an entirely different perception of the physical role of the real EP singularities. The difference is reflected by the terminology (used, say, in nuclear physics \cite{14}) by which the non-Hermitian Hamiltonians of the stable and unitary quantum systems are called quasi-Hermitian. This means that they share many of their observable features with the self-adjoint models of conventional textbooks.

One of the most characteristic distinctive features of quasi-Hermitian Hamiltonians $H(\lambda)$ is that they resemble their standard self-adjoint analogues merely inside certain domains (i.e., open sets) $\mathcal{D}$ of the admissible (and, say, real) values of the parameter or parameters $\lambda$. Naturally, the localization of the boundaries $\mathcal{D}$ of these domains (i.e., of the EP manifolds $\partial \mathcal{D}$) belongs to one of the main mathematical tasks for theoreticians.

In the literature the subjects is being developed with due care. There exist multiple model-based studies of $\mathcal{PT}$–symmetric Hamiltonians $H(\lambda)$ in which the $\mathcal{PT}$–symmetry gets spontaneously broken (\textit{pars pro toto}, see \cite{3, 15, 16}). This implies that at least some of the bound-state energies become complex after the passage of $\lambda$ through an EP element $\lambda_{(EP)}$ of the boundary $\partial \mathcal{D}$. In parallel, there also appeared a few studies \cite{17, 18, 19} in which the authors described another real-EP-related dynamical-evolution scenario. In it, the spontaneous breakdown of $\mathcal{PT}$–symmetry appeared inhibited and replaced by an
instantaneous recovery of the symmetry (cf., e.g., the toy models of Refs. [18, 20, 21] exhibiting the EP-related unavoided energy-level crossings).

We shall be interested in another, qualitatively different quantum-catastrophic scenario. It is encountered in the $\mathcal{PT}$–symmetric quantum systems in which an isolated and real energy level $E_n(\lambda)$ of a stable bound state grows with $\lambda$ and touches the lower boundary of the essential spectrum. Such a bound state may be perceived as disappearing (or, in an opposite direction, emerging) at the continuous-spectrum edge.

The mathematically rather sophisticated scenario of such a type is not too frequently studied in the literature (cf. its samples in [22, 23]). The gap will be partially filled in what follows. We shall consider a multiparametric family of $\mathcal{PT}$–symmetric Hamiltonians $H$ and we shall search for a constructive guarantee of the coexistence of bound states with the scattering solutions.

In section 2 we will introduce an ordinary difference Schrödinger equation which will prove useful for the purpose. In subsequent sections 3 and 4 we shall illustrate the basic technical merits of our replacement of the real coordinates in one dimension ($x \in \mathbb{R}$) by the discrete set of the grid points ($x_{new} \in \mathbb{Z}$). We shall show that in a way deviating from the conventional wisdom our preference of the difference Schrödinger equation is truly well motivated by certain simplifications of the relevant parts of the underlying mathematics. In the context of physics, our present choice of the discrete interaction operators $V$ finds its important motivation in the context of scattering. According to Refs. [24, 25] the very natural requirement of the causality and unitarity of the $S$–matrix seems to require the use of the weakly non-local interaction potentials of the present type.

Using the words of paper [19] we may formulate our present task as a “study [of] the effect of the appearance of isolated eigenvalues at the boundaries of the gaps in the essential spectrum”. In section 5, therefore, we shall turn attention to the construction of the spectra. The weakly non-local nature of our interaction potential $V$ will be shown to lead to a number of answers to the phenomenologically inspired qualitative questions.

In spite of an unusually flexible, $2J$–parametric tridiagonal-matrix form of our interactions $V$, the model may be claimed exactly solvable. Such a characteristic has two roots. Firstly, it reflects the facilitated nature of the matching of solutions in the models based on tridiagonal matrices [26]. Secondly, in a way described in section 6 a decisive and specific advantage of our model will be found in the possibility of conversion of the traditional polynomial-zero-search bound-state constructions into their closed-formula continued-fraction alternatives, user-friendly and amenable to a straightforward geometric interpretation.

Our results will be briefly discussed and summarized in sections 7 and 8.
2 The model

2.1 The real and discrete version of $\mathcal{PT}$ symmetry

The doubly infinite discrete Laplacean

\[ H_0 = \begin{bmatrix} \ddots & 2 & -1 & \ddots & \vdots \\ \ddots & -1 & 2 & \ddots & \vdots \\ -1 & 2 & -1 & 2 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \\ \end{bmatrix} \]

(1)

can be interpreted as a quantum Hamiltonian of a free particle moving along the discrete real line, with the usual continuous coordinate $x \in (-\infty, \infty)$ replaced by the grid of points $x_n = n$ with, say, $n = \ldots, -1, 0$ to the left and $n = 1, 2, \ldots$ to the right from the partitioning line. As long as matrix (1) is real and symmetric, it may be treated as time-reversal symmetric. Formally, we write $H_0\mathcal{T} = \mathcal{T}H_0$. We may require that the time-reversal operator $\mathcal{T}$ performs the transposition (and, in general, also complex conjugation) of matrices [12].

In the spirit of review [4], the same Hamiltonian may be also perceived as parity-time-reversal symmetric, $H_0\mathcal{PT} = \mathcal{PT}H_0$. The real and symmetric matrix of parity may be chosen in the following antidiagonal matrix form

\[ \mathcal{P} = \begin{bmatrix} 1 & \ddots & \ddots & \ddots \\ \ddots & 1 & \ddots & \ddots \\ \ddots & \ddots & 1 & \ddots \\ \ddots & \ddots & \ddots & 1 \\ \end{bmatrix} \]

(2)

of a square root of the unit matrix.

In the increasingly popular $\mathcal{PT}$–symmetric quantum mechanics [1, 4], the discrete-matrix nature of the kinetic-energy operator (1) and of its non-Hermitian $\mathcal{PT}$–symmetric perturbations

\[ H = H_0 + V \neq H^\dagger, \quad H\mathcal{PT} = \mathcal{PT}H \]

(3)
played the key role, e.g., in the conceptual studies of the scattering [25, 27, 28]. These considerations were facilitated by the $\mathcal{PT}$–symmetric toy-model choices of various special
cases of the general real-matrix nearest-neighbor interaction

\[ V = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots \\
\ddots & 0 & b & \ddots \\
-b' & 0 & a & \ddots \\
-a' & 0 & b & \ddots \\
\ddots & \ddots & \ddots & \ddots 
\end{bmatrix}. \] (4)

In the light of the tridiagonal-matrix form of the kinetic-energy component (1) of Hamiltonians (3) the same, slightly non-local tridiagonality of the interaction could enrich the physics without making the calculations too complicated. The readers should also consult paper [29] in which we demonstrated, that, and why, the choice of the non-Hermitian tridiagonal real-matrix Hamiltonians leaves several technical aspects of the constructive model-building unexpectedly user-friendly and preferable.

In our present paper we shall study Hamiltonians (3) + (4), i.e., the doubly infinite matrices

\[ H = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & 2 & -1+b & \ddots & \ddots \\
-1-b' & 2 & -1+a & \ddots & \ddots \\
-1-a' & 2 & -1+b & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots 
\end{bmatrix}. \] (5)

in the bound-state dynamical regime. We shall assume that the parameters form a real 2J–plet \(a, a', b, b', \ldots, z, z'\), i.e., that the dynamics is controlled by the 2J independently variable real matrix elements of \(V\), with the outermost \(V_{-J,-J+1} = V_{J-2,J-1} = z\) and \(V_{1-J,-J} = V_{J-1,J-2} = -z'\), etc.

The choice of Eq. (5) could be generalized to the \(J \to \infty\) limit with infinitely many free parameters (in this respect see also section 6 below). Alternatively, the analogous \(PT\)–symmetric interaction Hamiltonians

\[
H = \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & 2 & -1 & \ddots & \ddots \\
-1 & 2 & -1 & \ddots & \ddots \\
-1 & 2 & -1 & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots 
\end{bmatrix}
+ \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & 0 & b & \ddots & \ddots \\
-b' & 0 & a & \ddots & \ddots \\
-a' & 0 & a & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots 
\end{bmatrix}
+ \begin{bmatrix}
\ddots & \ddots & \ddots & \ddots & \ddots \\
\ddots & 0 & b & \ddots & \ddots \\
-b' & 0 & a & \ddots & \ddots \\
-a' & 0 & a & \ddots & \ddots \\
\ddots & \ddots & \ddots & \ddots & \ddots 
\end{bmatrix}
\]
of the odd dimensions after truncation and of a different partitioning could have been considered as well. For the sake of brevity, nevertheless, the latter version of the doubly infinite Hamiltonians will not be studied in our present paper.

2.2 Boundary conditions

As long as \( J < \infty \) remains finite, our present Schrödinger equation

\[
H|\psi\rangle = E|\psi\rangle
\]

is a linear difference equation of the second order, with the two independent asymptotic solutions of the form

\[
|\psi\rangle_n = const \times \exp(n\alpha), \quad |n| \gg J \geq 1
\]

where \( \alpha \in \mathbb{C} \) is a suitable complex number related to the (in general, complex) energy by the formula \( 2 - E = 2 \cosh \alpha \). These expressions represent the formally exact solutions of Eq. (6) in the whole free-motion kinematical range, i.e., for \( n \leq J \) and/or for \( n \geq J - 1 \). Suitable boundary conditions must be added.

2.2.1 Scattering states

The existence of the asymptotically traveling waves is possible under condition \( \text{Re} \alpha = 0 \), i.e., for the energies which belong to the continuous part of the spectrum of our Hamiltonians, i.e., for \( E \in (0, 4) \). In this dynamical regime a sample of the non-numerical construction of the experimentally relevant reflection and transmission coefficients may be found sampled, e.g., in Ref. [25].

2.2.2 Bound states

We shall exclusively pay attention to the bound state solutions of our Schrödinger Eq. (6) and, in particular, to the explicit constructive proofs of their existence. Once one requires that these solutions decrease at large \( |n| \gg J \), we have to split the discussion according to the sign of our discrete coordinate \( n \).

Along the negative discrete half-axis of \( n \) we only have to admit the exponentials (7) with \( \alpha = \varphi \) such that \( \text{Re} \varphi > 0 \). Having \( 2 - E = 2 \cosh \varphi \) this means that whenever the bound-state energy itself becomes real, it must be negative. In other words, our model does not admit the stable, unitarily evolving bound states embedded in the continuum.

Along the positive discrete half-axis of \( n \) we can only use exponentials (7) with an opposite sign in \( \alpha = -\varphi \). This enables us to postulate

\[
|\psi\rangle_n = \lambda \times \exp[(n + J)\varphi], \quad n \leq -J
\]
and

$$|\psi\rangle_n = \varrho \times \exp[(J - 1 - n)\varphi], \ n \geq J - 1.$$ \hspace{1cm} (9)

These relations guarantee the normalizability of the bound states, with the energy-representing parameter \(\varphi\) still being complex in general, restricted only by the above-mentioned bound-state constraint of normalizability \(\text{Re} \ \varphi > 0\). A matching of the asymptotics to the remaining part of our Schrödinger equation must be performed.

### 3 Bound state in two-parametric \(V \ (J = 1)\)

#### 3.1 The matching of wave functions in the origin

About the first nontrivial \(J = 1\) Schrödinger equation

$$\begin{bmatrix}
\ddots & \ddots & \ddots \\
\ddots & 2 - E & -1 \\
-1 & 2 - E & -1 + a \\
-1 - a' & 2 - E & -1 \\
-1 & 2 - E & \ddots \\
& \ddots & \ddots \\
\end{bmatrix} \begin{bmatrix}
|\psi\rangle_{-2} \\
|\psi\rangle_{-1} \\
|\psi\rangle_0 \\
|\psi\rangle_1 \\
|\psi\rangle_1 \\
\end{bmatrix} = 0$$ \hspace{1cm} (10)

we may say that up to the respective constant multiplier the bound-state eigenvectors are already known from the asymptotic analysis,

$$\ldots, \ |\psi\rangle_{-2} = \lambda \exp(-\varphi), \ |\psi\rangle_{-1} = \lambda, \ |\psi\rangle_0 = \varrho, \ |\psi\rangle_1 = \varrho \exp(-\varphi), \ldots \text{ } \text{ } (11)$$

This means that their matching will be mediated by the two innermost rows of system (10),

$$\begin{bmatrix}
-1 & 2 \cosh \varphi & -1 + a & 0 \\
0 & -1 - a' & 2 \cosh \varphi & -1 \\
\end{bmatrix} \begin{bmatrix}
|\psi\rangle_{-2} \\
|\psi\rangle_{-1} \\
|\psi\rangle_0 \\
|\psi\rangle_1 \\
\end{bmatrix} = 0$$

i.e.,

$$\begin{bmatrix}
-1 & 2 \cosh \varphi & -1 + a & 0 \\
0 & -1 - a' & 2 \cosh \varphi & -1 \\
\end{bmatrix} \begin{bmatrix}
\lambda \exp(-\varphi) \\
\lambda \\
\varrho \\
\varrho \exp(-\varphi) \\
\end{bmatrix} = 0$$

i.e.,

$$\begin{bmatrix}
\exp \varphi & -1 + a \\
-1 - a' & \exp \varphi \\
\end{bmatrix} \begin{bmatrix}
\lambda \\
\varrho \\
\end{bmatrix} = 0.$$  \hspace{1cm} (12)

This relation has a nontrivial solution iff the determinant vanishes,

$$\exp 2 \varphi - (-1 + a)(-1 - a') = 0.$$
3.2 Bound-state-supporting parameters

Figure 1: The thick-curve boundary of the doubly-connected domain $\mathcal{D}(a,a')$ supporting the bound state in the $a - a'$ plane at $J = 1$. The fixed-energy submanifolds are sampled by the thinner hyperbolic curves.

The analysis of solutions of the $J = 1$ toy-model Eq. (12) is entirely elementary. It implies that in the two-dimensional plane of parameters $a$ and $a'$ the boundary $\partial \mathcal{D}(a,a')$ of the doubly connected domain $\mathcal{D}(a,a')$ of the existence of a bound state will coincide with the hyperbolic curve $a = a'/(1 + a')$ (cf. Fig. 1). As long as the free parameters $a$ and $a'$ are real, we may abbreviate $(1 - a)(1 + a') = 1 + u(a,a')$ and have the following obvious result.

**Lemma 1** At $J = 1$ the bound state exists iff $u(a,a') > 0$.

In the $a - a'$ plane only the two lines with $a = 1$ or $a' = -1$ are singular. After their exclusion the bound state is found to exist either for $a' > -1$ and $a < a'/(1 + a')$ (i.e., under a hyperbolic-curve maximum of $a$) or for $a' < -1$ and $a > a'/(1 + a')$ (i.e., above a hyperbolic-curve minimum of $a$). In the definition of the Hamiltonian it would make sense to simplify the hyperbolic-curve geometry of the critical-parameter boundaries in the $a - a'$ plane and to replace the $a - a'$ plane, say, by the $u - a'$ plane (in which the energies would not depend on $a'$) or by the $a - u$ plane (in which the energies would not depend on $a$). We shall see below that the same type of reparametrization may be also recommended at any higher number of parameters $2J > 2$.

**Corollary 2** There are no $J = 1$ bound states at $a = a'$.

The latter observation sounds elementary but it could be extended to all $J$, forming an important addendum to the minimally nonlocal non-Hermitian models of Ref. [27] with $a = a'$, $b = b'$, etc. These models were shown to support the scattering which may be made, not quite expectedly [24], causal and unitary in an ad hoc physical Hilbert space (cf. also Refs. [25], [27], [30] in this respect).
4 Matching conditions at \( J \geq 2 \)

4.1 The four-parametric \( V \) as a methodical guide \((J = 2)\)

At \( J = 2 \) the insertion of the available exact solutions

\[
\ldots, \quad |\psi\rangle_{-3} = \lambda \exp(-\varphi), \quad |\psi\rangle_{-2} = \lambda, \quad |\psi\rangle_1 = \varphi, \quad |\psi\rangle_2 = \varphi \exp(-\varphi), \quad \ldots \quad (13)
\]

reduces the complete Schrödinger equation to the four matching conditions

\[
\begin{bmatrix}
-1 & 2 \cosh \varphi & -1 + b \\
0 & -1 - b' & 2 \cosh \varphi \\
0 & 0 & -1 - a' \\
0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
0 \\
-1 + a \\
2 \cosh \varphi \\
-1 - b' \exp \varphi
\end{bmatrix}
\begin{bmatrix}
\lambda \\
|\psi\rangle_{-1} \\
|\psi\rangle_0 \\
\varphi \exp(-\varphi)
\end{bmatrix} = 0
\]

alias

\[
\begin{bmatrix}
\exp \varphi & -1 + b \\
-1 - b' & 2 \cosh \varphi \\
0 & -1 - a' \\
0 & 0
\end{bmatrix}
\begin{bmatrix}
0 \\
-1 + a \\
2 \cosh \varphi \\
-1 - b' \exp \varphi
\end{bmatrix}
\begin{bmatrix}
\lambda \\
|\psi\rangle_{-1} \\
|\psi\rangle_0 \\
\varphi \exp(-\varphi)
\end{bmatrix} = 0.
\]

Once we abbreviate

\[
(1 - a)(1 + a') = 1 + u, \quad (1 - b)(1 + b') = 1 + v
\]

and once we eliminate \( a = 1 - (1 + u)/(1 + a') \) and \( b = 1 - (1 + v)/(1 + b') \) and require that

\[
\exp 2 \varphi = x^2 = t > 1,
\]

an elementary algebra leads to the amazingly compact and exactly solvable secular equation

\[
t^2 - t(1 + u + 2v) + v^2 = 0
\]

alias

\[
(t - v)^2 = t(1 + u)
\]

alias

\[
(t - v) = \pm \sqrt{t(1 + u)}.
\]

With \( 1 + u > 0 \) and for \( t > v_{\text{minimal}} = -(1 + u)/4 \) we see that in Eq. (17) the left-hand-side straight line always intersects the right-hand-side parabola at the two real values of \( t > 0 \).

From Eq. (16) we may deduce, equivalently, that the right-hand-side straight line always intersects the left-hand-side parabola at the same two real values of \( t > 0 \). Naturally, only the roots with the property \( t > 1 \) correspond to the physical bound states.
Lemma 3  At \( J = 2 \) the ground state exists in the upper part of the \( u - v \) plane, viz., in the domain of \( u > u_{\text{min}}(v) \) bounded, from below, by the thick curve \( u_{\text{min}}(v) \) of Fig. 2.

Proof. The larger root
\[
t_+ = \frac{1}{2} \left[ 1 + u + 2v + \sqrt{(1 + u + 4v)(1 + u)} \right]
\]
of the quadratic algebraic Eq. (15) remains real to the right from the line “A” of Fig. 2 (which is decisive for \( v < -1 \)) and above the line “D” (which is decisive for \( v > 1 \)). The parabolic segment of the boundary represents the restriction \( t_+ > 1 \).

\[\square\]

Lemma 4  The \( J = 2 \) model can also support the first excited state. The two-dimensional parametric subdomain of its existence is doubly connected. As a subdomain of the domain of Lemma 3 it shares its lower bound but lies below the parabolic curve “B” of Fig. 2.

Proof. The smaller root
\[
t_+ = \frac{1}{2} \left[ 1 + u + 2v - \sqrt{(1 + u + 4v)(1 + u)} \right]
\]
can only become bigger than one when its square-root part is sufficiently small. The opposite side of the parabolic boundary becomes allowed, therefore.

\[\square\]

The first excited state can only exist at \( v \not\in (-1, 1) \); either for \( u \in (-1, u_{\text{max}}^{(+)}(v)) \) at positive \( v > 1 \), or for positive \( u > 3 \) in an interval of \( u \in (u_{\text{min}}^{(-)}(v), u_{\text{max}}^{(-)}(v)) \) at negative \( v < -1 \). These observations may be checked in Fig. 2.
4.2 General effective secular determinants (any $J \geq 2$)

The general $J \geq 2$ matching condition has the $2J$-dimensional matrix form

$$
\begin{bmatrix}
\exp \varphi & -1 + z & 0 & \ldots & 0 \\
-1 - z' & 2 \cosh \varphi & -1 + y & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
\vdots & \ddots & -1 - a' & 2 \cosh \varphi & -1 + b & \ddots & \vdots \\
0 & \ddots & \ddots & \ddots & 0 \\
0 & \ldots & \ldots & 0 & -1 - z' & \exp \varphi
\end{bmatrix}
\begin{bmatrix}
\lambda \\
|\psi\rangle_{-J+1} \\
\vdots \\
|\psi\rangle_{-1} \\
|\psi\rangle_{0} \\
\vdots \\
|\psi\rangle_{J-2} \\
0
\end{bmatrix} = 0.
$$

This equation is, in effect, the Feshbach’s [31] model-space reduction of our initial doubly infinite Schrödinger equation. In general, the energy-dependence of the Feshbach’s effective Hamiltonian would be complicated. In order to be able to proceed, one has to return to the further few nontrivial algebraic-manipulation experiments with the model.

5 The six-parametric solutions ($J = 3$)

One may expect that the evaluation of the secular determinant of Eq. (18) and the search for its bound-state-energy zeros might proceed along the same lines as in the previous example with $J = 2$, in principle at least. In practice, the prospect of the non-numerical solution of Eq. (18) seems less encouraging. Even the very evaluation of the secular determinant of Eq. (18) would be hardly feasible without a standard symbolic manipulation software.

5.1 The change of variables

At the first sight, even the use of a computer algebra does not seem too promising. A preliminary naive test may be performed to show that the length of the typical results (say, of a formula for the secular determinant at any $J \geq 3$) already requires too many printed pages for being of any use. One must return again to the heuristic experiments, still at the not too large integers $J$.

The construction of the two-dimensional domains of the physical parameters and of their boundaries (cf. Fig. 2) as well as the proofs of Lemmas 3 and 4 at $J = 2$ were too elementary. They relied heavily upon the availability of the explicit formulae for the bound-state energies. Such a naive approach fails to work even at the next choice of $J = 3$. As expected, the evaluation of the $J = 3$ secular determinant of Eq. (18) (containing seven
variables) was already hardly feasible by pen and pencil. Even the symbolic-manipulation software did not help too much. We had to conclude that the use of the computer merely transfers the difficulty from the feasibility of the evaluation to the readability of the formula. The “exact” secular polynomial seemed too long for offering any insight. We imagined that before any transition to the higher $J \geq 3$ the naive approach to the construction of the bound states via matching (18) had to be thoroughly reanalyzed and amended.

At $J = 3$ the first success in our methodical experiments came with the $(J = 2)$—inspired tentative change of parametrization

\[(1-a)(1+a') = 1 + u, \quad (1-b)(1+b') = 1 + v, \quad (1-c)(1+c') = 1 + w\] (19)

followed by the elimination

\[a = 1 - (1+u)/(1+a'), \quad b = 1 - (1+v)/(1+b'), \quad c = 1 - (1+w)/(1+c').\]

The trick worked and shortened the formulae (say, for the secular determinants) back to a tractable size. This encouraged us to prolong the series of reparametrizations (19),

\[(1-d)(1+d') = 1+y, \quad (1-e)(1+e') = 1+z, \quad (1-f)(1+f') = 1+m, \quad (1-g)(1+g') = 1+n\]

etc (where, as the famous Littlewood’s joke says, “e need not be equal to 2.718...”).

5.2 The emergence of the ground state from continuum

At $J = 3$ the Feshbach’s effective secular determinant remained almost polynomial not only in the energy variable $x = \exp \varphi > 1$ but also in its square $t = \exp 2 \varphi > 1$. The determinant appeared to be a sum of a polynomial and of a single, utterly elementary inverse-power term $w^2/t$. As long as $t > 1$, the latter term may be considered nonsingular. After a pre-multiplication by $t$ the secular equation acquires the quartic polynomial form

\[t^4 - (1 + u + 2v + 2w)t^3 + (2uw + (v + w)^2)t^2 + (w^2(1-u) + 2vw)t + w^2 = 0.\] (20)

A surprise emerged when we checked the behavior of this equation near the origin of the three-dimensional space of the new, reduced parameters $u$, $v$ and $w$.

**Lemma 5** For the sufficiently small, $O(\lambda)$ parameters $u$, $v$ and $w$ there exists a unique non-small, $O(1)$ energy root

\[t_0 = 1 + u + 2v + 2w + O(\lambda^2).\] (21)

This means that inside the half-space with $u + 2v + 2w > 0$ (i.e., in particular, in the positive-parameter quadrant with $u > 0$, $v > 0$ and $w > 0$) there exists a physical bound state which emerges from the continuum, with $E_0 = -(u + 2v + 2w)^2 + O(\lambda^3)$. 

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Proof. Up to quadratically small corrections Eq. (20) reads \[ t^4 = (1 + u + 2v + 2w) t^3. \] This implies that as many as three of the roots remain small (i.e., unphysical, much smaller than one). Thus, we get \[ \varphi_0 = u + 2v + 2w + \mathcal{O}(\lambda^2). \] □

In the light of our numerous symbolic-manipulation experiments the same conclusion seems to remain valid at any number \( J \) of the “reduced” parameters \( u, v, \ldots \).

**Conjecture 6** At any integer \( J \) there exists a physical bound state which emerges from the continuum in the positive-parameter vicinity of the origin \( u = 0, v = 0, \ldots \).

Figure 3: Graphical proof, via Eq. (24), of the existence of the two excites states at \( J = 3 \), \( u = 17, v = 6 \) and \( w = 5 \).

### 5.3 The emergence of the excited states from continuum

The choice of \( J = 3 \) leads to the quartic-polynomial secular Eq. (20). Apparently, this is the ultimate special case of our Hamiltonian (9) from which one could extract the set of the energy roots as functions of the couplings in closed form, in principle at least. Naturally, it is necessary to add that the concrete form of the available exact formulae for \( E_n(u, v, w) \) is very complicated and makes them practically useless. Fortunately, our “last exactly solvable” secular Eq. (20) has a special form which may be pre-factorized,

\[ t^2 (t - v - w)^2 - t (1 + u) (t - w)^2 - 2w t (t - v - w) + w^2 = 0, \quad J = 3 \tag{22} \]

and, in the next step,

\[ [t(t - v - w) - w]^2 = t(1 + u)(t - w)^2, \quad J = 3. \tag{23} \]

This enables us to replace it by its simpler, square-rooted equivalent version

\[ [t(t - v - w) - w] = \pm(t - w)\sqrt{t(1 + u)}. \tag{24} \]
Such an equation is already much more transparent: its right-hand-side may be visualized as a loop while the left-hand side is a parabola. Thus, a graphical solution of this version of secular equation becomes elementary. It may be found sampled in Fig. 8 which represents, at the preselected triplet of parameters, a graphical proof of the existence of the first two excited bound states with negative energies, i.e., below the continuum.

In the picture the left-hand-side parabola intersects the right-hand-side loop at the three small circles (the fourth, rightmost, ground-state intersection is out of the range of the picture). The thinner vertical line marks the left boundary of the interval of admissible \( t \in (1, \infty) \). Thus, the leftmost intersection is spurious, not representing a bound state. It would yield a purely imaginary \( \phi \) and an unphysical wave function solution, incompatible with the physical Dirichlet’s asymptotic boundary conditions.

6 Multiparametric solutions \((J \geq 3)\)

6.1 Sturmians as exact solutions

The inspection of formulae (17) (where \( J = 2 \)) and (24) (where \( J = 3 \)) inspired us to make use of the following ansatz,

\[
\sqrt{(1 + u)}t = \pm f_J(t, v, w, \ldots), \quad J = 2, 3, \ldots.
\]

The hypothesis was based on the first three already available formulæ,

\[
f_1(t) = t, \quad f_2(t, v) = t - v, \quad f_3(t, v, w) = \frac{t^2 - (v + w) t - w}{t - w}.
\]

The structure of these formulæ can be extrapolated to all of the higher values of \( J \). We verified that the right-hand-side functions have the form of the ratio of two polynomials,

\[
f_J(t, v, w, \ldots) = \frac{t^{J-1} - c_1 t^{J-2} + \ldots}{t^{J-2} - d_1 t^{J-3} + \ldots}.
\]

This observation led us to the conclusion that

- it makes sense to keep using ansatz (25) + (27) and to treat the formula as the basic form of the solution of our present bound-state problem.

- it makes sense to abandon the traditional recipe in which the energies are sought as functions of the couplings. It seems optimal to replace this strategy by the formally equivalent but technically simpler approach in which the given-energy bound states are called “Sturmians” [32].
Once we decided to select the innermost coupling \( u_n \) as a quantity to be sought for, we may treat it as a function \( u_n(t, v, w, \ldots) \) of the remaining couplings and of the freely variable energy parameter \( t \in (1, \infty) \). The resulting implicit-function picture of the quantum system will have the advantage of circumventing the complicated search for the energy roots \( t_n \). In other words, the hypothesis of the Sturmian bound-state solvability provides an explicit definition of the bound states at all \( J \).

One of the main practical consequences of such an innovated approach may be seen in the reduction of the solution of the matching condition (25) to the search for intersections between the right-hand-side curve \( f_J(t, v, w, \ldots) \) with the left-hand-side parabola \( \pm \sqrt{(1 + u)t} \). In this presentation the width of the parabola is exclusively controlled by the innermost coupling \( u > -1 \) while the factorized rational function

\[
f_J(t, v, w, \ldots) = \prod_{k=1}^{J-1} \frac{(t - \beta_k)}{J-2} \prod_{m=1}^{J-1} \frac{(t - \gamma_m)}{J-2}
\]

has the growing asymptotes \( f_J(t, v, w, \ldots) \sim t + \mathcal{O}(1) \) and (in general, complex) poles at the values of \( t = \gamma_m \) with \( m = 1, 2, \ldots, J-2 \).

In the most elementary scenario all of the latter positions of the singularities \( \gamma_m \) and zeros \( \beta_k \) may be assumed real. The global shape of the function \( f_J(t, \ldots) \) will be then determined by the distribution of the \( J-1 \) zeros of the numerator among the \( J-1 \) intervals \((-\infty, \gamma_1), (\gamma_1, \gamma_2), \ldots, (\gamma_{J-2}, \infty)\).

The menu of the possible intersection patterns with the \( u \)-dependent parabola may be then illustrated at \( J = 3 \), with just two intervals \((-\infty, \gamma_1) \) (=“left”, \( L \)) and \( (\gamma_1, \infty) \) (=“right”, \( R \)). Then, with both of the zeros of the numerator in \( L \), we will receive a hyperbolic curve of \( f_3(t) \) composed of its \( \cap \)-shaped branch to the left and of its \( \cup \)-shaped branch to the right. Next, for both of the zeros of the numerator in \( R \), the shape of the \( v \)- and \( w \)-dependent hyperbola \( f_3(t) \) (and, hence, also the discussion of its possible real intersections with the \( u \)-dependent parabola) will remain qualitatively the same.

A different intersection pattern will only be encountered in the third possible case with \( \beta_1 \in L \) and \( \beta_2 \in R \). In this case the hyperbolic curve \( f_3(t) \) with its two asymptotes \( f_3(t) \sim t \) and \( f_3(t) \sim -1/(t - \gamma_1) \) will represent a map of either \( L \) or \( R \) on the whole real axis so that one will always have to deal with the four real intersections. Thus, the classification of the whole bound-state spectrum will be restricted to the identification of the “physical” intersections such that \( t > 1 \) (cf. Eq. (14)).

At the larger counts of parameters \( J > 3 \) the discussion will remain qualitatively the same. In every interval of \( t \in (\gamma_m, \gamma_{m+1}) \) one merely has to distinguish between the occurrence of the odd number of the zeros \( \beta_k \) (leading to the asymptotically \( \cap \)-shaped or \( \cup \)-shaped forms of \( f_J(t) \)) and the occurrence of the even number of the zeros \( \beta_k \) leading to the map of the interval on the whole real axis, i.e., to the guarantee of the existence of at least two real intersections with the \( u \)-dependent parabola in the interval.
6.2 Partial fraction expansions

The main encouragement of our present study of multiparametric interactions \cite{1} originated from the \( J = 3 \) formula \cite{24} which became amazingly elementary in its partial-fraction-expanded version

\[
f_3(t, v, w) = t - v - \frac{(1 + v)w}{t - w}.
\]  

(29)

One of the immediate consequences of this expansion is the simplified classification of the shapes of \( f_3(t, v, w) \). This function has the form of the \( \bigcap \bigcup \) -shaped hyperbola iff \( (1 + v)w < 0 \). \textit{Vice versa}, the / + /-shaped two-growing-curves hyperbola (i.e., a guarantee of the existence of the four intersections with the \( u \)-dependent parabola) takes place at \( (1 + v)w > 0 \) (naturally, the spike disappears at \( (1 + v)w = 0 \)).

The latter observations combine the algebraic reduction of formulae with an enhancement of an intuitive insight and graphical classifications of the curve-intersections and of the related alternative dynamical scenarios. This is a decisive final simplification of the discussion which could be also achieved at the higher parameter counts \( J > 3 \). The test has been performed in the eight-parametric model. Using the computer-assisted symbolic manipulations we revealed that near \( t = 0 \) the secular determinant exhibits the singularity \( y^2/t^2 + \mathcal{O}(t^{-1}) \) (let us remind the readers that \( y = (1 - d)(1 + d' - 1) \). After its subsequent pre-multiplication by \( t^2 \) it is replaced by its regular version

\[
t^6 + (-1 - 2w - 2y - u - 2v)t^5 + (2wy + 4vy + 2uw + v^2 + 2uy + w^2 + 2vw + y^2)t^4 +
\]

\[
+ (-y^2u + y^2 - 2wvy - w^2u - 2wuy + 2wy + 2wy - 2y^2v - 2vy + 2vw + w^2)t^3 +
\]

\[
+ (2wy + y^2 + y^2v^2 - 2wvy - 2wvy - 2wvy - 2y^2u + w^2 + 2vy - y^2v) t^2 +
\]

\[
+ (-2y^2v + 2vy - y^2u + y^2) t + y^2 = 0.
\]

The factorization of this long equation for the \( u \)-coupling Sturmians is again found by the computer and leads to the final result of the form \cite{25},

\[
(-y - ty + tyv - t^2y - t^3 - tw - t^2w) = \pm \left(t^2 - (w + y) t - y \right) \sqrt{t(1 + u)}.
\]

(30)

This is to be re-read as the definition of \( f_4(t, v, w, y) \) in formula \cite{25}, i.e., as the definition of the Sturmian bound-state coupling \( u_n = u_n(t, v, w, y) \), i.e., as our ultimate closed-form description of the bound states.

6.3 Continued fractions

The evaluation of the partial-fraction expansion of \( f_4(t, v, w, y) \) was only rendered possible by the use of computer software but the computer provided the fairly elementary formula rather quickly,

\[
f_4(t, v, w, y) = t - v - \frac{y + tw + yv + tvw}{t^2 + (-y - w) t - y}.
\]
We noticed that it seems quite natural to apply the same partial-fraction expansion algorithm to the denominator. This led to the truly elementary finite-continued-fraction formula

$$f_4(t, v, w, y) = t - A_0 - \frac{B_1}{t - A_1 - \frac{B_2}{t - A_2}}$$

where $A_0 = A_0(v) = v$ was already determined at $J = 2$, where $B_1 = B_1(v, w) = (1 + v)w$ was already determined at $J = 3$ and where the determination of $A_1 = A_1(w, y) = w + y + y/w$ was new. The last two coefficient functions $\tilde{B}_2 = -(1 + w)y^2/w^2$ and $\tilde{A}_2 = -y/w$ are marked by the tildas. The reason is that the determination of these functions can only be completed on a higher level of calculations using $J = 5$ and $J = 6$. The ultimate, untilded formulae for

$$B_2 = B_2(w, y, z) = (1 + w)(y^2 - (1 + y)wz)/w^2$$

and

$$A_2 = A_2(w, y, z, m) = -\frac{y}{w} + z + \frac{yz - (1 + y)(1 + z)wm}{y^2 - wz(1 + y)}$$

have been evaluated using models with $J = 5$ and $J = 6$, therefore.

In a compatibility check one may consider the limit $y \to 0$ in the new $J = 4$ continued fraction confirming the expected degeneracy to its $J = 3$ predecessor. Similarly, the limit $z \to 0$ returns the coefficient $B_2$ to its incomplete, reduced, tilded $J = 4$ version.

By induction one arrives at the general continued fraction formula

$$f_J(t, v, w, \ldots) = t - A_0 - \frac{B_1}{t - A_1 - \frac{B_2}{t - A_2 - \frac{B_3}{t - A_3 - \ddots}}}.$$

which is valid at all $J$. Whenever the integer $J$ remains finite, this continued fraction will terminate via the appearance of a tilded, vanishing value of the coefficient $\tilde{B}_{J-1} = 0$. In the opposite direction, the complete, untilded definition of the coefficients $B_k$ and $A_k$ will, in general, result from the routine evaluation and analysis of the secular determinants at $J = 2k + 1$ and $J = 2k + 2$, respectively.
7 Discussion

7.1 Quantum systems in the discrete-coordinate quasi-Hermitian representations

The study of quantum systems in their quasi-Hermitian and $\mathcal{PT}$−symmetric discrete representations usually originates from the needs of open-system studies [33] or of classical optics [34], especially in the light of the current quick developments of nanotechnologies [35]. Here we proceeded in a complementary direction of connecting these models with the simulations of the various forms of quantum phase transitions (cf., e.g., [36, 37]).

In the latter setting people feel most often inspired by the Bender’s and Boettcher’s [3] conjecture that beyond the scope of the conventional textbooks, the unitary evolution of quantum systems may still be described as generated by certain non-standard Hamiltonians $H$ with real spectra. In the language of our recent review [13], these operators $H$ are interpreted as self-adjoint in the (by assumption, overcomplicated) “standard” physical Hilbert space $\mathcal{H}^{(S)}$ (where one might write $H = H^\dagger$) but, at the same time, non-self-adjoint in a “friendlier” manifestly unphysical and auxiliary Hilbert space $\mathcal{H}^{(F)}$ (where we have, using the most conventional notation, $H \neq H^\dagger$).

There exist good reasons (cf., e.g., [24, 38] or [39]) why one should be very careful when leaving the safe mathematics of self-adjoint operators in $L^2(\mathbb{R})$ and when extending the study of the Schrödinger’s bound-state equations (with real spectra) to the models with the complex (e.g., $\mathcal{PT}$−symmetric [4] or, more generally, pseudo-Hermitian [12]) local interactions $V(x) \neq V^*(x)$. One of these reasons is that, by assumption, we have $H = T + V \neq H^\dagger$ in $L^2(\mathbb{R})$. Hence, the latter (and, certainly, maximally user-friendly) Hilbert space must be declared unphysical, i.e., in the present notation, we have $L^2(\mathbb{R}) \equiv \mathcal{H}^{(F)}$. Then, the theory (cf., e.g., its compact formulation in [13]) tells us that the physical requirement $H = H^\dagger$ of the self-adjointness in $\mathcal{H}^{(S)}$ finds its equivalent representation

$$H^\dagger \Theta = \Theta H, \quad \Theta = \Omega^\dagger \Omega \quad (33)$$

in $\mathcal{H}^{(F)}$, mediated by an introduction of an auxiliary metric operator $\Theta \neq I$.

Under certain additional subtler mathematical conditions the validity of the latter relation enables us return to the quantum theory of textbooks while calling the Hamiltonian itself, for the sake of clarity of the terminology, quasi-Hermitian [14]. In [13] the readers may also find an exhaustive explanation of the role and origin of the so called Dyson’s maps $\Omega$ and/or of the physical Hilbert-space metric operator $\Theta$ entering the formula. The mathematical meaning of this condition is, in principle, elementary [40]. Its appeal in physics was discovered by Dyson [41] and widely used in nuclear physics [14]. In essence, the relation just reflects the mathematical compatibility of a given non-Hermitian Hamiltonian $H$ (with real spectrum) with the natural physical requirement of its observability [12, 12].
In practice, the key problem is that for a given $H$, we must find at least one operator $\Theta$ which would satisfy Eq. (33). In paper [29] we showed that such a search remains exceptionally straightforward if and only if the matrix representation of $H$ is real and tridiagonal. This was, after all, one of the most important mathematical reasons for our present choice of model (5).

One should add that in the applied quantum mechanics one often encounters a conflict between the tractability and flexibility of the available phenomenological models. The exactly solvable ones are usually not too flexible, and vice versa. This may be also perceived as a supportive argument in favor of the discrete models. After the acceptance of new physics behind $\mathcal{PT}$–symmetric potentials [3] a widely welcome progress has recently been achieved in this field [43]. A perceivable extension of the menu of the eligible tractable Hamiltonians has been obtained. The common textbook self-adjoint versions of quantum models were complemented by a new class using non-Hermitian Hamiltonians.

As long as the precise range of the applicability of the theory using Hamiltonians $H = T + V \neq H^\dagger$ is not yet fully understood, the use of the discrete models has an advantage of not being directly exposed to the Trefethen’s [38] purely mathematical criticism (based mainly on the work with differential operators, cf. also [39]). Moreover, the discretization very well fits the otherwise rather counterintuitive bounded-operator preference as recommended, in reaction to the Dieudonné’s [40] slightly more abstract criticism, by nuclear physicists [14].

7.2 The physical appeal of quantum systems exhibiting phase transitions

The birth of quantum mechanics might have been dated by the resolution of the classical-physics paradox of the experimentally observed stability of the large number of the atoms and molecules. In the language of mathematics the explanation was provided by a sophisticated identification of the measured discrete quantities with the elements of the spectrum of the corresponding self-adjoint operator. Thus, typically, the predicted real values of the energy levels $E_n$, say, in hydrogen atom were shown obtainable, from a suitable self-adjoint Hamiltonian $\hbar \mathcal{H} = \hbar \mathcal{H}^\dagger$, as its eigenvalues. In the methodical setting it has been found useful to illustrate the theory via the one-dimensional Schrödinger equations with various real and local (and, often, exactly solvable [44]) confining potentials $V = V(x)$.

One of the weak points of the textbook theory may be seen in the necessity of an appropriate assignment of the self-adjoint Hamiltonian $\hbar$ to a quantum system in question. From a purely pragmatic perspective this assignment has two deep aspects. Firstly, in the context of phenomenology, the self-adjointness of $\hbar$ is a robust property which does not offer a suitable tool for the description of any finite-life or resonant quantum systems
which often occur in the nature and for which the energy levels should not be strictly real. Secondly, in opposite direction, the stability (i.e., the reality of the energy levels) may be guaranteed even when the Hamiltonian itself is not a self-adjoint operator. A number of the exactly solvable illustrative examples of the one-dimensional differential Schrödinger equation may be found, e.g., in Ref. [15].

The later option has been made popular by Bender and Boettcher [3] and it extends the practical applicability of quantum theory. In its final formulation the option led to an upgrade of quantum mechanics (cf., e.g., its reviews [4, 12]). In essence, the extended family of many new manifestly non-selfadjoint Hamiltonians (with real spectra) was found compatible with the standard quantum mechanics of textbooks (cf. [14]; a number of the related mathematical as well as historical comments may be also found in the most recent book [1, 45]).

In the literature, unfortunately, the opinions concerning the nontrivial applications of the new theory are not yet unified. Nevertheless, in all of the existing versions of the theory the existence of the nontrivial real boundaries $\partial D$ of applicability belong to the cornerstones of the theory. Their localization and toy-model descriptions belong to the most interesting challenges and subjects of the future research. Certainly their study is openings new ways towards our understanding of the phenomena of the loss of the quantum stability or observability.

### 7.3 Computer-capacity limitations of the constructions

In the case of our present $\mathcal{PT}$—symmetric toy model (5) the applicability of the symbolic manipulations yielding exact solutions encounters the two main limitations in practice. The first one lies in the quick growth of the number of the independently variable parameters. This is an obstacle which already made some of the formulae next to useless (i.e., too long for being displayed in print) as early as at $J = 3$.

The second difficulty concerns the hidden nature of the information carried by the long formulae. The picture only remains fully transparent at $J = 1$. In this case the physical parametric domain $\mathcal{D}(a, a')$ has been found to have a clear and elementary shape (cf. Fig. 1). Even the very next, $J = 2$ physical parametric domain $\mathcal{D}(a, a', b, b')$ already becomes four-dimensional, i.e., not too easily displayed.

One of the specific merits of our present class of models is that the latter difficulties may be softened. For example, after the discovery of the energy-preserving submanifolds (sampled by the two thin hyperbolic curves in Fig. 1), we were able to halve the $2J$—plet of the physical parameters to the mere $J$—plet. In Fig. 2 we displayed the reduced, two-dimensional physical domain $\mathcal{D}(u, v)$ also at $J = 2$.

Thanks to several further unexpected simplifications of the representation of the bound states we were able to extend the transparent graphical interpretation of the spectra to
the six-parametric model with $J = 3$ (cf. its sample in Fig. 3) and, in principle, also to the eight-parametric model with $J = 4$ (cf. Eq. (30)).

A quick increase of the time and memory requirements limited our present constructions of the Sturmians to not too large $J > 4$. Using a small PC we still managed to work with $J = 5$ and $J = 6$. We obtained the above-displayed closed and still comparatively compact formulae (31) and (32) for the entirely general continued-fraction coefficient functions $B_2$ and $A_2$.

Unfortunately, the next round of calculations with $J = 7$ and $J = 8$ already reached, at $J = 7$, the upper bounds of the reasonable length of the secular polynomial (cca 12 pages), of the reasonable calculation time (cca 15 minutes) and of the memory consumption (822 M). Even the printing of the function $f_7(t,v,\ldots)$ already requires a separation into its polynomial numerator

$$-t^6 + (w + m + y + n + z + v) t^5 +$$

$$+ (-my - nw - nv - yv - ny + m - vz + y - mv - mw - wz + w - nz + n + z) t^4 +$$

$$+ (-wz - 2 nw - vz + vnz + n - my + vny + y + z - 2 ny +$$

$$+ wnz - nz - 2 mw - mv + m + mvy - nv) t^3 +$$

$$+ (vnz - my + wnz + n - 2 nw + m + vny + z - 2 ny - nv - nz - mv - mw) t^2 +$$

$$+ (n - nv - nw - ny + m - nz) t + n$$

and denominator

$$t^5 + (-y - z - w - m - n) t^4 + (my + wz + ny - z + mw - y - m - n + nw + nz) t^3 +$$

$$+ (-m + my + mw - wnz - n + 2 ny + nw - z + nz) t^2 + (-m - n + nw + nz + ny) t - n.$$ 

Thus, we gave up the continuation of the process. We decided not to reconstruct the next pair of functions $B_3$ and $A_3$ because the completion of the analysis, straightforward as it is, would certainly exceed the capacity of our desktop computer.

### 7.4 Broader context: open-quantum-system connections

It is worth emphasizing that the results of the detailed mathematical analysis of the particular model (5) (which, in the light of this analysis, appeared to be exactly solvable) may be perceived as having a broader impact and relevance for non-Hermitian physics.

Let us, first of all, recall the general comments on physical contexts as given in Introduction. For the sake of definiteness we will now restrict our attention just to the domain of quantum physics. Moreover, let us pick up just the subdomain of the theory in which people study the models which are characterized by the presence of non-Hermitian quantum operators. In this subdomain one finds, e.g., the studies of open quantum systems [10][11]
with which our present text shares interest in a constructive approach to the coexistence of bound states with the scattering solutions.

It is probably necessary to emphasize that although the latter coexistence is being studied via different formalisms in the literature, it seems truly challenging to search for their shared mathematical features as well as phenomenological predictions.

On the purely formal level the most obvious meeting point between the two specific (viz., $\mathcal{PT}$—symmetric and open-system) approaches to the non-Hermitian quantum physics and phenomenology may be seen in the use of the Feshbach’s concept of the so called model space [31]. This means that a certain projection-operator-specified subspace of the complete Hilbert space is chosen as a starting point. In this subspace the exact Hamiltonian is replaced by its (often called “effective”, i.e., isospectral) reduction $H_{\text{eff}}$ as sampled here by Eq. (18).

Naturally, the results of the comparison can only have a qualitative character. Still, it is worth emphasizing that such a comparison seems nontrivial due to its consequences. First of all, let us recall the most important physical problem of the unitarity of the scattering process. For open systems this problem may be found clarified, e.g., in Ref. [46] where one works with the Hamiltonians describing, in general, unstable systems. For their genuine non-Hermitian Hamiltonians the spectrum of the energies is not real so that the experimentalists are allowed to speak about resonances. For theoreticians, the closeness of the concept to the $\mathcal{PT}$—symmetric models immediately emerges when one admits that the $\mathcal{PT}$—symmetry becomes spontaneously broken [4] so that at least some of the energies become complex.

From the point of view of the experiment the complementarity of the theoretical perspectives seems best clarified in the scattering dynamical regime. Indeed, in the $\mathcal{PT}$—symmetric context the paradoxes (cf. [24]) are being resolved by an effective “smearing” of the potentials [27]. In parallel, the phenomenological description of the open systems leads to a very similar emergence of the concept of the “smearing”. Its physical essence is slightly different - it is intimately connected to the Feshbach’s elimination and transfer of the scattering wave functions to a “reservoir” which is “infinitely extended”. But the outcome is similar: the fundamental phenomenon of an effective “smearing” appears very naturally.

It is not too surprising that many differences between the $\mathcal{PT}$—symmetric and open systems survive. In the latter case, for example, the complex part of the energy (which just characterizes an extent of the spontaneous breakdown of the $\mathcal{PT}$—symmetry in the former case) has an immediate measurable, experimental interpretation [47]. In addition, the imaginary part of the energy in the open system can be also related to the nonorthogonality of the resonance states [48]. At the same time, whenever one succeeds in avoiding the complicated dynamical regime of resonances (i.e., firstly, whenever the width of the
resonance happens to shrink to zero and, secondly, whenever the resonance leaves, simultaneously, the continuous part of the spectrum), the present class of models (5) enters the game. It offers an amazingly rich variety of possible dynamical scenarios. Their description uses a manifestly non-perturbative, simplified but still exact, non-numerical picture of the qualitative changes in the quantum evolution during which a stable bound state emerges below the continuum.

8 Summary

The current growth of interest in $\mathcal{PT}$–symmetric quantum systems may be characterized by the novelty of its potential physical contents as well as by the not entirely standard nature of the related mathematics. Both of these challenges motivated also our present choice of the family of Hamiltonians (5).

Our choice was inspired, first of all, by the role of the special cases of Hamiltonians (5) (with $a = a'$, etc) in the constructive disproof [27] of the Jones’ oversceptical conjecture [24] that the scattering by a generic local $\mathcal{PT}$–symmetric potential $V(x)$ cannot be unitary. For our present purposes it was important that the resolution of the problem (cf. also [23] and [25]) was provided by the replacement of the “unsuitable” local potentials (i.e., in our present discrete-coordinate approach, of the diagonal matrices $V$) by their “minimally non-local” (i.e., tridiagonal-matrix) generalizations as sampled by Eq. (4).

Another important physical reason for the study of the latter class of the “smeared” [27] alias “nearest-neighbor” interactions was found in their level-attraction role played, in particular, by their extremely non-Hermitian antisymmetric-matrix special cases (with $a = a'$, etc) in the models of quantum catastrophes [6]. In the latter case, the attention (cf., e.g., [49, 50] remained restricted to the confined motion (i.e., to the purely bound-state models) using not only finite $J < \infty$ but also the truncated, finite-dimensional kinetic energy operators (1). Hence, it was entirely natural for us to ask what would happen when the truncation of the discrete Laplacean (i.e., in effect, an external confining square-well-type potential) were removed.

A priori we expected that the doubly infinite $\mathcal{PT}$–symmetric toy-model matrices (5) could enrich the slowly developing classifications of quantum catastrophes [18] by a new, multiparametric class of models in which the scattering dynamical regime could coexist with the parallel (and, due to the non-Hermiticity of $H$, fragile) existence of bound states (cf. also [23] where more or less the same questions were addressed via perturbation theory).

Our expectations proved confirmed. We found that in our model the “birth” of the stable bound states at the lower boundary of the continuous spectrum may be rather easily controlled. Serendipitously, we also discovered that besides its appeal in physics, the model offers an unexpectedly long list of certain truly amazing formal merits.
• from the point of view of the Feshbach’s constructive recipe [31], the description of all of our $J \leq \infty$ models proved non-numerical and reducible to the study of the closed-form effective Hamiltonians $H_{eff}$ (cf. Eq. (15)).

• the energy-dependence of the latter operators is rather complicated in general. In our model it remained, in effect, elementary (i.e., basically, polynomial – see, e.g., the six-parametric secular Eq. (20) for illustration).

• a pleasant surprise appeared after our replacement of the search for the bound-state energies $E_n$ as functions of the “reduced” couplings $u, v, \ldots$, by the search for the “Sturmian” bound-state couplings $u_n$ as functions of the freely variable energy $E$ and of the remaining couplings $v, w, \ldots$. What was a truly unexpected byproduct of this change of perspective was the second-power-type factorization of polynomials leading to an enormous simplification of the formulae.

• once we moved to the higher integers $J$ we imagined that the ultimate, most natural version of the construction of the bound states can be based on the last important simplification of their localization using the continued-fraction re-arrangement of the recipe. In the light of this result one could even contemplate a transition to the models with $J = \infty$, in principle at least.

• the latter two forms of simplification made the bound-state localization amenable also to its deeply intuitive and transparent graphical (re-)interpretation. In this way our “benchmark-model” samples of the birth of the bound states from the continuum could acquire a new physical relevance as the prototypes of quantum catastrophes of a new, less usual type.

• for the growing integers $J$, the increase of the complexity of the formulae caused by the linear growth of the number of the independently variable parameters $u, v, \ldots$ proved at least partially compensated by the survival of their sufficiently efficient and quick tractability by the symbolic-manipulation software. The limitations of this approach only started emerging at the values of $J$ as high as $J = 8$. Still, one can hardly find too many solvable quantum models with such a large number of independently variable parameters.

• we should not forget to mention that the determination of the $2J$–dimensional physical-parameter domains $D(a, a', b, b', \ldots)$ and/or of their boundaries $\partial D$ (sampled, at $J = 1$, by Fig. 1) proved reducible to the mere $J$–dimensional physical-parameter domains $D(u, v, \ldots)$ as sampled, at $J = 2$, in Fig. 2. Let us add that this was one of the most unexpected discoveries concerning the potential physics and phenomenology behind the model. The feature may be also perceived, in retrospective,
as one of the most important non-mathematical, descriptive reasons of our interest in the model in question.

- last but not least, we must emphasize that the most basic role was played again by our acceptance of the enormously productive requirement of $\mathcal{PT}$ symmetry (cf. Eq. (3)), i.e., in our model, of the symmetry of our real matrix (5) with respect to its antidiagonal.

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