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Matching method and exact solvability of discrete $\mathcal{PT}$-symmetric square wells

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

E-mail: znojil@ujf.cas.cz

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Abstract
Discrete $\mathcal{PT}$-symmetric square wells are studied. Their wavefunctions are found to be proportional to classical Tshebyshev polynomials *of complex argument*. The compact secular equations for energies are derived giving *the real spectra* in certain intervals of non-Hermiticity strengths Z. It is amusing to note that although the known square well re-emerges in the usual continuum limit, a twice as rich, upside-down symmetric spectrum is exhibited by all its present discretized predecessors.

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1. Introduction

Undoubtedly, solvable models represent one of the most important and inspiring sources of insight in the physical properties of real quantum systems [1]. For illustration, one may recollect how the concept of the so-called shape-invariant analytic potentials $V(x)$ [2] opened the path towards a better understanding of supersymmetry [3]. Recently, a similar major progress in our understanding of some less standard structures admitted by the standard quantum mechanics [4] has been initiated by a few numerical as well as non-numerical analyses [5–7] of certain complex potentials exhibiting another interesting invariance property,

$$V(x) = [V(-x)]^*. \tag{1}$$

It has been argued [7] that the latter invariance may prove highly relevant in physics as it makes all the Hamiltonian $\mathcal{PT}$-symmetric, i.e. commuting with the product of parity $\mathcal{P}$ and complex conjugation $\mathcal{T}$ while, in its turn, the latter operator represents the time-reversal operation in the language of phenomenological considerations.

In the resulting slightly innovated formalism of quantization (called, for definiteness, $\mathcal{PT}$-symmetric quantum mechanics (PTSQM) [8, 9]), you admit that Hamiltonians need not necessarily be Hermitian in the usual trivial metric I in Hilbert space, $H \neq H^\dagger$. As an illustrative example, one may recollect the ordinary differential Schrödinger equation on a finite interval,

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right]\psi(x) = E\psi(x), \qquad \psi(\pm 1) = 0 \tag{2}$$

where PTSQM admits potentials $V(x)$ of equation (1) which are not real but merely 'parity plus time-reversal' symmetric.

One of the most immediate consequences of the invariance (1) replacing Hermiticity is that the corresponding Hamiltonian $H \neq H^\dagger$ admits the existence of complex eigenvalues $E_n \neq E_n^*$. In the language of experimental physics this simply means a potential *instability* of the whole system, a phenomenon truly encountered, e.g., in relativistic quantum mechanics [10] or in certain magnetohydrodynamical systems [11]. In the former case, the instability may either mean a complete collapse of the system or a mere controlled creation of the particle–antiparticle pairs [12]. An even less catastrophic scenario is encountered in experimental magnetohydrodynamics where the transitions to the unstable regime prove reversible as a rule [13].

The potential theoretical consequences of $\mathcal{PT}$-symmetry seem equally appealing at present. One of the reasons is that in equation (2) the coordinates x themselves may be *complex* and, hence, *manifestly* unobservable. This means that one gets quite close to the relativistic field theory where the corresponding analogue of x (namely, the field amplitude φ) is *also* an *auxiliary* (i.e. in principle, not necessarily observable) quantity [7, 14].

In a way inspired by the latter comment the *auxiliary* role of the *complex*, unobservable coordinate x may equally well be played by any other element x_k of any other unobservable set $\mathcal{D} \neq (-\infty, \infty)$. Without getting too deeply involved in this theoretical question, we decided to parallel the most popular strategy (where $\mathcal{D}$ is being specified as a suitable complex curve [6, 7]) and to try to treat the (admissible) replacement $(-\infty, \infty) \to \mathcal{D}$ as a *simplification*, *discretization* of the real axis.

Our present paper summarizes a few of our most interesting results. Firstly, we set the scene in section 2 where we list some supplementary motivations and show how we intend to construct our illustrative examples. In section 3 both the physical and mathematical background of our considerations are outlined in some necessary detail.

Up to the final brief summary of our results in section 7, the rest of our paper becomes more technical and it shows how our simplest discrete models can be solved and how their various generalizations can be treated and remain, in a current vague sense of the word, exactly solvable.

2. $\mathcal{PT}$-symmetry in quantum mechanics

2.1. Non-analytic Schrödinger equations

The admissibility of a complexification of spectra is a puzzling possibility which inspired qualitative analyses of many concrete models. For many analytic potentials $V(x)$ of an immediate physical interest, the constructive demonstrations of the stability (i.e. of the reality of the spectrum) have been performed by perturbative [15], quasi-classical [16] and purely numerical [17] methods.

At an early stage of development, the *non-analytic* solvable models have been considered conspicuous. Many of them—typically, potential $V(x) \sim |x|$ on the whole real line, solvable in terms of Airy functions by the matching method—happened to exhibit instabilities (i.e. complex energies) at *all* the non-vanishing values of the corresponding coupling constants [8].

This caused a certain delay of return to some of the most elementary exactly solvable piecewise-constant $\mathcal{PT}$-symmetric potentials in equation (2). Still, their later studies [18, 19] clarified that their spectrum of bound states may remain real in a fairly large domain of their coupling constants (cf also [20, 21]). In [22] it has been proved that our $\mathcal{PT}$-symmetric Schrödinger equation (2) possesses *solely* the discrete spectrum of *real* energies $E = E_n, n = 0, 1, \ldots$ for *all* the complex potentials which are 'not too strong':

$$\|V\|_\infty < \frac{3}{8}\pi^2 \approx 3.701. \tag{3}$$

At the same time, the possible emergence of the instabilities at all the non-zero couplings has been confirmed for certain piecewise-constant $\mathcal{PT}$-symmetric potentials acting on the complex, curved contours [23].

2.2. *Runge–Kutta option*

The indefiniteness of conclusions of the above observations inspired the present extension of the study of the piecewise-constant potentials towards the models which are defined over a mere *discrete*, equidistant lattice of points

$$x_0 = -1, \qquad x_k = x_{k-1} + h = -1 + kh, \qquad h = \frac{2}{N}, \qquad k = 1, 2, \ldots, N. \tag{4}$$

These models possessing $\mathcal{PT}$-symmetry and real spectra will be characterized by the *variability* of the number $N+1$ of grid points in (4). We believe that in this perspective our understanding of the generic $\mathcal{PT}$-symmetric models may acquire a new dimension, returning us to the usual differential-equation framework in the $N \to \infty$ limit.

One of the most natural possibilities of the discretization of the differential equation (2) is given by the well-known Runge–Kutta recipe [24]:

$$-\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2} + V(x_k)\psi(x_k) = E\psi(x_k). \tag{5}$$

Using the standard boundary conditions

$$\psi(x_0) = \psi(x_N) = 0,$$

we shall employ here just the piecewise-constant, purely imaginary antisymmetric potentials of [18, 21]:

$$V(x) = \begin{cases} +\mathrm{i}Z_n & x \in (-\ell_n, -\ell_{n-1}), \\ -\mathrm{i}Z_n & x \in (\ell_{n-1}, \ell_n), \end{cases} \qquad n = 1, 2, \ldots, q+1. \tag{6}$$

Their discontinuities lie at the matching points $\ell_0 = 0 < \ell_1 < \cdots < \ell_{q+1} = 1$ so that at $q = 0$ we have to solve the discrete Schrödinger bound-state problem

$$-\frac{\psi(x_{k+1}) - 2\psi(x_k) + \psi(x_{k-1})}{h^2} - \mathrm{i}\,\mathrm{sign}(x_k) Z\psi(x_k) = E\psi(x_k), \qquad q = 0, \tag{7}$$

etc. It is worth noting that the first nontrivial $N = 4$ version of equation (7) coincides with Weigert's matrix model

$$\begin{pmatrix} 2 + \frac{1}{4}\mathrm{i}Z & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 - \frac{1}{4}\mathrm{i}Z \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \gamma \\ \beta_0 \end{pmatrix} = \frac{1}{4}E \begin{pmatrix} \alpha_0 \\ \gamma \\ \beta_0 \end{pmatrix}, \tag{8}$$

studied in [25], in more detail, as 'the simplest nontrivial' Runge–Kutta discretization of the $\mathcal{PT}$-symmetric square well of [18].

3. Physics and mathematics behind the discrete Schrödinger equations

3.1. The definition of the physical metric

In the light of reviews [4, 9], the $\mathcal{PT}$-symmetric Hamiltonians are not compatible with the standard 'Dirac's' metric I in Hilbert space (indeed, we have $H \neq H^\dagger$). A construction of an appropriate (i.e. of a Hamiltonian-dependent) generalization $\Theta \neq I$ of the metric is necessary for a correct probabilistic interpretation of the measurements. This means that our Hamiltonian must only be Hermitian (or, more precisely, self-adjoint) with respect to the generalized metric:

$$H^\dagger = \Theta H \Theta^{-1}, \qquad I \neq \Theta = \Theta^\dagger > 0. \tag{9}$$

All the physical contents of our models must be derived from the new metric of course. For this reason, it makes sense to avoid confusion by calling equation (9) with $\Theta \neq I$ a 'quasi-Hermiticity' condition [4].

One can note that almost exclusively, standard textbooks train our 'quantum intuition' on the representations of the Hilbert space where the metric remains trivial. This means that all the nonstandard PTSQM considerations profit enormously from any construction of a sufficiently flexible class of solvable models. In such a setting our present finite-dimensional $\mathcal{PT}$-symmetric models may play the role of a guide towards the interpretation, especially due to their facilitated connection with the continuous $N \to \infty$ limit.

A parallel reason for the attention paid here to the discretized systems lies in the well-known difficulty of the problem of the efficient construction of $\Theta \neq I$ for a given $H \neq H^\dagger$. Using the Dirac-inspired 'brabraket' compact notation of [26] and employing the biorthogonal basis composed of the left and right eigenstates of our non-Hermitian Hamiltonian H, we may recollect (cf e.g., [27]) that the knowledge of the spectral representation of the Hamiltonian,

$$H = \sum_n |n\rangle \frac{E_n}{\langle\langle n|n\rangle} \langle\langle n|,$$

almost immediately leads to the parallel multiparametric formula

$$\Theta = \sum_n |n\rangle\rangle \theta_n \langle\langle n|, \qquad \theta_n > 0, \tag{10}$$

which specifies the correct metric as a (non-unique, parameter-sequence-dependent) solution of the operator (9). Thus, we can employ this formula and construct Θ, more or less comfortably, for the majority of the exactly solvable models of the form (2) [28]. This is in contrast with the situation where one must construct the states $|n\rangle\rangle$ by some approximative method. This would make formula (10) practically useless. Complicated computations would be needed which, typically, search for Θ in the form of a product where the parity $\mathcal{P}$ is multiplied by a charge $\mathcal{C}$ (from the left [9]) or by a quasi-parity $\mathcal{Q}$ (from the right [29]).

3.2. Matching method

Let us recollect that the $N = \infty$ continuous-limit models (6) are exactly solvable at any $q \geqslant 0$ and that their practical solution remains feasible and transparent at $q = 0$ [18], $q = 1$ [30] and $q = 3$ [31] at least. The solvability in a closed form also characterizes the parallel modifications of these models characterized by the periodic boundary conditions [32].

It would be highly desirable to extend the available exact solution of discrete Weigert's 'minimal' finite-dimensional model (8) with $q = 0$ and $N = 4$ to some higher integers N and/or q. A key purpose of our present paper is to show that such extensions are feasible, indeed, once we adapt the matching method, so efficient in its standard differential-equation form, to the needs of difference equations.

In the next section our constructive considerations will start from one of the most straightforward $N > 4$ generalizations

$$
\left(\begin{array}{cccc|c|cccc}
\mathrm{i}\xi - F & -1 & & & & & & & \\
-1 & \mathrm{i}\xi - F & \ddots & & & & & & \\
 & \ddots & \ddots & -1 & & & & & \\
 & & -1 & \mathrm{i}\xi - F & -1 & & & & \\
\hline
 & & & -1 & -F & -1 & & & \\
\hline
 & & & & -1 & -\mathrm{i}\xi - F & \ddots & & \\
 & & & & & \ddots & \ddots & -1 & \\
 & & & & & & -1 & -\mathrm{i}\xi - F &
\end{array}\right)
\left(\begin{array}{c}
\alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \\ \hline \gamma \\ \hline \beta_n \\ \vdots \\ \beta_0
\end{array}\right) = 0 \qquad (11)
$$

of Weigert's model represented by the $(N - 1 = 2n + 3)$-dimensional matrix transcription of our difference Schrödinger equation (7) with the rescaled energy eigenvalues $F = Eh^2 - 2$ and with the rescaled strength $\xi = Zh^2$ of the non-Hermiticity.

We shall see that such a matrix reformulation of the matching recipe proves solvable in a closed form at all $n = 0, 1, \ldots$. In the Hermitian context of quantum chemistry, we just arrive at the well-known Hückel's solvable models in the limit $Z \to 0$ [33].

4. Finite-dimensional Schrödinger equation (11)

4.1. Closed solvability

Recollecting the definition of the classical Tshebyshev polynomials of the second kind [34],

$$
U_k(\cos\theta) = \frac{\sin(k+1)\theta}{\sin\theta}, \qquad k = 0, 1, \ldots,
$$

(cf a collection of their most relevant properties in appendix) and using the *real* elements $\gamma = \psi(0)$, $a_k = \operatorname{Re}\psi(x_{k+1})$ and $b_k = \operatorname{Im}\psi(x_{k+1})$, we are now prepared to formulate our first result.

Theorem 1. *Whenever the $\mathcal{PT}$-symmetry remains unbroken, closed solutions of equation (11) are defined by the formulae*

$$
\begin{aligned}
&\alpha_k = a_k + \mathrm{i}b_k, \qquad \beta_k = a_k - \mathrm{i}b_k \equiv \alpha_k^*, \\
&\alpha_k = (a + \mathrm{i}b)U_k\left(\frac{-F + \mathrm{i}\xi}{2}\right), \qquad k = 0, 1, \ldots, n
\end{aligned} \qquad (12)
$$

and

$$
\gamma = (a + \mathrm{i}b)U_{n+1}\left(\frac{-F + \mathrm{i}\xi}{2}\right) = (a - \mathrm{i}b)U_{n+1}\left(\frac{-F - \mathrm{i}\xi}{2}\right), \qquad (13)
$$

complemented by the self-consistency constraint

$$
F\gamma = -(a + \mathrm{i}b)U_n\left(\frac{-F + \mathrm{i}\xi}{2}\right) - (a - \mathrm{i}b)U_n\left(\frac{-F - \mathrm{i}\xi}{2}\right). \qquad (14)
$$

Proof. In the first step of our analysis, we get the relation $\beta_k = \alpha_k^*$ due to the $\mathcal{PT}$-symmetry of our eigenvectors. We then identify equation (11) with the three-term recurrences satisfied by the Tshebyshev polynomials (cf appendix) and verify formula (12) for eigenvectors by showing that it is compatible with the corresponding boundary conditions (at the smallest subscripts k). As long as all this reduces the full tridiagonal $(N-1)\times(N-1)$-dimensional matrix (11) to the mere three matching conditions,

$$\begin{pmatrix} -1 & \mathrm{i}\xi - F & -1 & 0 & 0 \\ 0 & -1 & -F & -1 & 0 \\ 0 & 0 & -1 & -\mathrm{i}\xi - F & -1 \end{pmatrix} \begin{bmatrix} U_{n-1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) \\ U_n\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) \\ \gamma \\ U_n\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b) \\ U_{n-1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b) \end{bmatrix} = 0, \tag{15}$$

it remains for us to show that the first and the third lines may be simplified to give equation (13) while the middle line defines the product (14). □

Remark. Without an assumption of an unbroken $\mathcal{PT}$-symmetry, one would have to admit that the eigenvalues F are complex. A more explicit illustration of what happens has been described, in the continuum limit, in [35].

Corollary. *A nontrivial solution always exists at $F = 0$.*

Proof. In a discussion of the consequence of theorem 1, one has to note that formula (14) forces us to distinguish between two regimes where $F = 0$ and $F \neq 0$, respectively. Once we set, tentatively, $F = 0$, it is easy to deduce from equation (13) that the parameter a must vanish for even $n = 0, 2, 4, \ldots$ (and we may normalize $b = 1$) while $b = 0$ and $a = 1$ for odd $n = 1, 3, 5, \ldots$. Thus, equation (13) degenerates to the mere definition of the last element γ of the eigenvector and we are left with the single secular equation (14) which acquires the following two alternative forms:

$$\begin{aligned} &U_n\left(\tfrac{1}{2}\mathrm{i}\xi\right) - U_n\left(\tfrac{1}{2}\mathrm{i}\xi\right) = 0, \qquad && n = 2m, \\ &U_n\left(\tfrac{1}{2}\mathrm{i}\xi\right) + U_n\left(-\tfrac{1}{2}\mathrm{i}\xi\right) = 0, \qquad && n = 2m+1. \end{aligned} \tag{16}$$

These conditions are satisfied identically at any $m = 0, 1, \ldots$. Thus, our tentative 'guess of the energy' was correct and $F = 0$ is always an eigenvalue. □

Remark. In spite of the non-Hermiticity of the Hamiltonian, the $F = 0$ eigenvalue is 'robust' [30] and remains real at *all* the real couplings $Z \in (-\infty, \infty)$. The spectrum remains symmetric with respect to this 'middle point' (note that $F = 0$ corresponds to the energy $E = E_{n+2} = 2/h^2 = N^2/2 = 2(n+2)^2$). The existence of such a 'central' eigenvalue is not in contradiction with the differential-equation results of [22]. Indeed, this level moves up with dimension N and disappears in infinity in the limit $N \to \infty$. We may conclude that in this sense a 'richer' structure is exhibited by the spectrum at the finite dimensions.

4.2. *Properties of the 'fragile' $F \neq 0$ solutions*

Whenever $F \neq 0$ we may treat equation (13) not only as the condition of vanishing of the imaginary part of γ,

$$U_{n+1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) = U_{n+1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b), \tag{17}$$

but also as an explicit definition of the non-vanishing left-hand-side quantity $F\gamma$ in equation (14). Its insertion simplifies the latter relation

$$T_{n+1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) = -T_{n+1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b), \tag{18}$$

where $T_k(z)$ denotes the kth Tshebyshev polynomial of the first kind.

One of the latter two relations defines the normalization vector $(a, b) = (a_0, b_0)$ while their ratio gives

$$T_{n+1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)U_{n+1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)+T_{n+1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)U_{n+1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)=0. \tag{19}$$

This represents our final secular equation which defines, in an implicit manner, the energies F as functions of the couplings ξ.

An efficient numerical treatment of the latter eigenvalue problem may be based on the reparametrization

$$\frac{-F+\mathrm{i}\xi}{2}=\cos\varphi, \qquad \operatorname{Re}\varphi=\alpha, \qquad \operatorname{Im}\varphi=\beta, \tag{20}$$

i.e.

$$\tfrac{1}{2}F=-\cos\alpha\cosh\beta, \qquad \tfrac{1}{2}\xi=-\sin\alpha\sinh\beta \tag{21}$$

and, in the opposite direction,

$$\cos\alpha=-\frac{1}{2\cosh\beta}F, \qquad \sinh\beta=\frac{1}{2\sqrt{2}}\sqrt{F^2+\xi^2-4+\sqrt{(F^2+\xi^2-4)^2+16\xi^2}}.$$

This change of variables transforms equation (19) into the trigonometric secular equation

$$\operatorname{Re}\frac{\sin[(n+1)\varphi]\cos[(n+1)\varphi^*]}{\sin\varphi}=0. \tag{22}$$

Its roots must be determined, in general, numerically.

Lemma. *In the domain with negative $\beta < 0$, the roots of equation (22) have $\alpha \in (0, \pi/2)$ at the negative $F < 0$ and $\alpha \in (\pi/2, \pi)$ at the positive $F > 0$.*

Proof. The constant value of the coupling $\xi > 0$ is mapped upon a downwards-oriented half-oval in the α–β plane. Its top lies at $\alpha = \pi/4$ while its two asymptotes $\alpha = 0$ and $\alpha = \pi/2$ are reached in the limit $\beta \to -\infty$. In such a representation, the 'robust' and ξ-independent energy level $F = 0$ lies on the top of the half-oval while its decreasing and increasing neighbours are found displaced to the left and right, respectively, along the half-oval downwards. □

Remark. At the first few lowest dimensions $N - 1 = 2n + 3$, the roots of equation (22) may be written in a closed form,

$$F_0=0, \qquad F_\pm=\pm\sqrt{2-\xi^2}, \qquad n=0,$$

$$F_0=0, \qquad F_{\pm,\pm}=\pm\sqrt{2-\xi^2\pm\sqrt{1-4\xi^2}}, \qquad n=1,$$

etc. This enables us to determine the respective critical values $Z = Z_{\text{crit}}(N)$, i.e. the exact $Z_{\text{crit}}(4) = 4\sqrt{2} \approx 5.66$ at $n = 0$ and $Z_{\text{crit}}(6) = 9/2 = 4.50$ at $n = 1$ followed by the numerically calculated values $Z_{\text{crit}}(8) = 4.463$ at $n = 2$, $Z_{\text{crit}}(10) = 4.461$ at $n = 3$, $Z_{\text{crit}}(12) = 4.463$ at $n = 4$, etc. These results do not contradict the expected $n \to \infty$ limit as derived in [35], $Z_{\text{crit}}(\infty) = 4.475$ (cf figure 1).

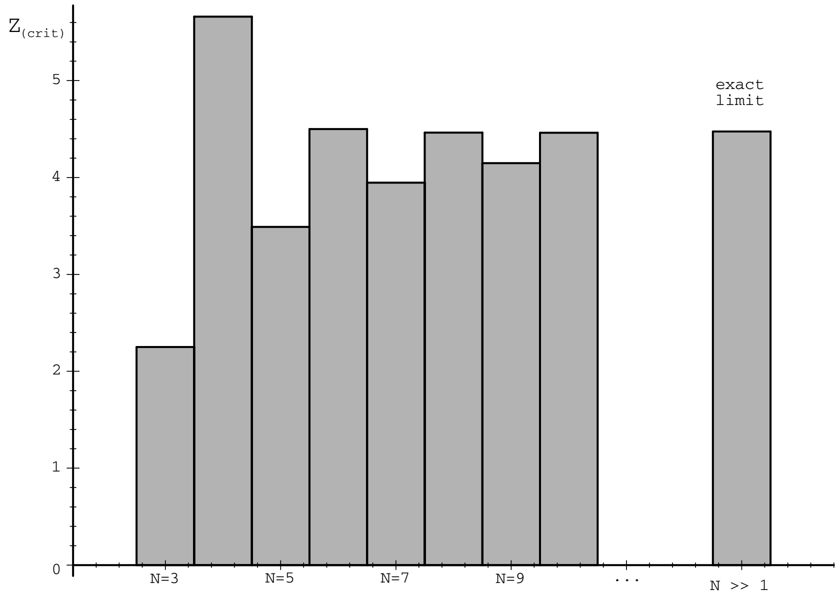

Figure 1. Numerical values and convergence of the critical couplings $Z_{\rm crit} = Z_{\rm crit}(N)$.

5. The role of the integers *N* and *q*

5.1. *Closed solvability at the odd* $N = 2n + 3$

In comparison with [25], a 'one-step easier' discretization of equation (2) emerges at $q = 0$ and at the odd $N = 3$, with two energy roots. A non-equivalent discrete alternative to equation (11) could then read, in the same notation,

$$\left(\begin{array}{cccc|cccc} {\rm i}\xi - F & -1 & & & & & & \\ -1 & {\rm i}\xi - F & \ddots & & & & & \\ & \ddots & \ddots & -1 & & & & \\ & & -1 & {\rm i}\xi - F & -1 & & & \\ \hline & & & -1 & -{\rm i}\xi - F & \ddots & & \\ & & & & \ddots & \ddots & -1 & \\ & & & & & -1 & -{\rm i}\xi - F & \end{array} \right) \left(\begin{array}{c} \alpha_0 \\ \alpha_1 \\ \vdots \\ \alpha_n \\ \hline \alpha_n^* \\ \vdots \\ \alpha_0^* \end{array} \right) = 0. \qquad (23)$$

This leads to the following alternative result.

Theorem 2. *Whenever the $\mathcal{PT}$-symmetry remains unbroken, closed solutions of equation (23) are defined by formulae (12) accompanied by the alternative matching condition*

$$(a + {\rm i}b)U_{n+1}\left(\frac{-F + {\rm i}\xi}{2}\right) = (a - {\rm i}b)U_n\left(\frac{-F - {\rm i}\xi}{2}\right) \qquad (24)$$

and by the odd-N counterpart of equation (19)

$$U_n\left(\frac{-F + {\rm i}\xi}{2}\right)U_n\left(\frac{-F - {\rm i}\xi}{2}\right) = U_{n+1}\left(\frac{-F + {\rm i}\xi}{2}\right)U_{n+1}\left(\frac{-F - {\rm i}\xi}{2}\right). \qquad (25)$$

Proof. Definition (12) of the eigenvectors remains unchanged, but the matching condition generated by the subproblem

$$\begin{pmatrix} -1 & \mathrm{i}\xi - F & -1 & 0 \\ 0 & -1 & -\mathrm{i}\xi - F & -1 \end{pmatrix} \begin{bmatrix} U_{n-1}\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) \\ U_n\left(\frac{-F+\mathrm{i}\xi}{2}\right)(a+\mathrm{i}b) \\ U_n\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b) \\ U_{n-1}\left(\frac{-F-\mathrm{i}\xi}{2}\right)(a-\mathrm{i}b) \end{bmatrix} = 0 \tag{26}$$

is just one, $\alpha_{n+1} = \alpha_n^*$. The ratio of this equation to its Hermitian conjugate eliminates all the normalization ambiguities and leads to the secular equation (25). □

Remark. The secular equation (25) is an implicit definition of the $N = 2n + 3$ energy levels $F = F(\xi)$. It possesses the compact analytic solutions at the first few values of n of course:

$$F_{\pm} = \pm\sqrt{1-\xi^2}, \qquad n = 0,$$
$$F_{\pm,\pm} = \pm\tfrac{1}{2}\sqrt{6 - 4\xi^2 \pm 2\sqrt{5-16\xi^2}}, \qquad n = 1$$

The respective elementary expressions for the critical constants

$$Z_{\mathrm{crit}}(3) = \frac{9}{4} = 2.25, \qquad n = 0,$$
$$Z_{\mathrm{crit}}(5) = \frac{25\sqrt{5}}{16} \approx 3.49, \qquad n = 1$$

are followed by the complex Cardano representation of the real $Z_{\mathrm{crit}}(7) = 3.946$ at $n = 2$. At $n > 2$ one switches to a purely numerical algorithm giving $Z_{\mathrm{crit}}(9) = 4.148$ at $n = 3$, etc. In comparison with the parallel results derived at even N in section 4, we note that the numerical convergence towards $n = \infty$ is perceivably slower and from the opposite side at odd N (cf figure 1).

5.2. Models with more matching points

New features of the spectrum emerge when we choose $q > 0$ in equation (6). In the light of the differential-equation results [30, 31], one may expect the existence of the so-called robust levels at $q \geqslant 1$ and $N < \infty$. By definition, they remain real at the arbitrarily large coupling constants Z_k. *A priori*, the position of these levels may be expected to be controlled by both the parameters Z_k and ℓ_k.

Obviously, the interpretation of the discretization becomes facilitated when we choose the discontinuities at the simple rational numbers ℓ_k. It is interesting to note, marginally, that their choice simplifies even the trigonometric secular determinants in many differential-equation models. Nevertheless, in our present context it is much more important that the choice of the simplest ℓ_k at $q \geqslant 1$ enables us to continue working with the not too large matrix dimensions $N - 1$.

5.2.1. $\ell = 1/2$ and $N = 6$. For the $q = 1$ interaction model (6) with $\ell_1 = 1/2$,

$$V(x) = \begin{cases} +\mathrm{i}Z \\ 0 \\ -\mathrm{i}Z \end{cases} \quad \text{for} \quad x \in \begin{cases} \left(-1, -\frac{1}{2}\right), \\ \left(-\frac{1}{2}, \frac{1}{2}\right), \\ \left(\frac{1}{2}, 1\right) \end{cases} \tag{27}$$

we may start from its discretization (5) with the most elementary choice of $N = 6$,

$$\left(\begin{array}{c|ccc|c} i\xi - F & -1 & & & \\ \hline -1 & -F & -1 & & \\ & -1 & -F & -1 & \\ & & -1 & -F & -1 \\ \hline & & & -1 & -i\xi - F \end{array}\right)\left(\begin{array}{c} \alpha_0 \\ \hline \gamma_0 \\ \gamma \\ \gamma_0^* \\ \hline \alpha_0^* \end{array}\right) = 0. \tag{28}$$

This equation determines the following five eigenvalues:

$$F_0 = 0, \qquad F_{\pm,\pm} = \pm\tfrac{1}{2}\sqrt{8 - 2\xi^2 \pm 2\sqrt{4+\xi^4}}.$$

Besides the constant and ξ-independent level $F_0 = 0$, one can show that the two 'external' levels

$$F_{\pm,+} = \pm\sqrt{3}\left[1 - \frac{1}{12}\xi^2 + \frac{5}{288}\xi^4 + \frac{5}{3456}\xi^6 + O(\xi^8)\right]$$

remain robustly real for all the values of ξ and never complexify,

$$F_{\pm,+} = \pm\sqrt{2}\left[1 + \frac{1}{4}y^2 - \frac{1}{32}y^4 - \frac{31}{128}y^6 + O(y^8)\right], \qquad y = 1/\xi.$$

They are complemented by the fragile pair of levels $F_{\pm,-}$ which coincides with $F_0 = 0$ at the critical value of $\xi_{\mathrm{crit}} = \sqrt{3/2} \approx 1.2247$ and complexify beyond this 'exceptional' point.

5.2.2. $\ell = 1/2$ and $N = 8$ and more. The $N = 8$ calculations lead to the observation that the two outmost energy levels as well as the 'middle' $F = 0$ level remain robust and real at all the real ξ. At the critical value of $\xi_{\mathrm{crit}} = 0.845\,479\,352$, we observe the confluence and subsequent complexification of both the remaining (i.e. positive and negative) energy pairs at the respective two numerical values of $F_{\mathrm{crit}} = \pm 1.051\,672\,18$. With the further growth of ξ the quantity Re F^2 becomes negative beyond $\xi_{\mathrm{zero}} = 3.222\,215\,2046$, with the purely imaginary crossing point $F_{\mathrm{zero}} = \pm 2.146\,638\,195\,\mathrm{i}$.

At $N = 10$ the secular algebraic equation for the energy-level characteristics $y = F^2$ has the following four roots in the Hermitian limit with $\xi = 0$:

$$y_{a,\pm} = \tfrac{5}{2} \pm \tfrac{1}{2}\sqrt{5}, \qquad y_{b,\pm} = \tfrac{3}{2} \pm \tfrac{1}{2}\sqrt{5}.$$

Numerically, one finds that the real quadruplet

$$0.517\,357\,1919,\ 1.810\,807\,242,\ 1.810\,964\,520,\ 3.356\,678\,112$$

of these values gives the single roots $F = \pm 0.719\,275\,4632$ and $F = \pm 1.832\,123\,935$ and the double roots $F = \pm 1.345\,662\,380$ at $\xi_{\mathrm{subcrit}} = 0.502\,092\,09$. In parallel, the complex quadruplet

$$0.517\,357\,1921,\ 1.810\,885\,878 \pm 0.000\,052\,688\,897\,24\mathrm{i},\ 3.356\,678\,117$$

emerges numerically at the upper estimate of the critical coupling strength $\xi_{\mathrm{supercrit}} = 0.502\,092\,091$.

Similar observations have also been made at $N = 12$ and $N = 14$ and all of them are parallel and reproduce the qualitative features as observed in [30] in the $N \to \infty$ continuum limit.

6. The role of the shift-parameter ℓ

6.1. Suppressing the non-Hermiticity using $\ell = 5/8$

In order to illustrate the emergence of a pair of the robust levels, let us reconsider the $q = 1$ interaction model (6) and employ a larger shift $\ell_1 = 5/8$. In the resulting potential

$$V(x) = \begin{cases} +\mathrm{i}Z \\ 0 \\ -\mathrm{i}Z \end{cases} \quad \text{for} \quad x \in \begin{cases} \left(-1, -\frac{5}{8}\right), \\ \left(-\frac{5}{8}, \frac{5}{8}\right), \\ \left(\frac{5}{8}, 1\right) \end{cases} \tag{29}$$

the non-Hermiticity is weakened at a fixed coupling Z. We get the matrix analogue of problem (28) from the discretized equation (5) with $N = 8$,

$$\left(\begin{array}{c|ccccc|c} \mathrm{i}\xi - F & -1 & & & & & \\ \hline -1 & -F & -1 & & & & \\ & -1 & -F & -1 & & & \\ & & -1 & -F & -1 & & \\ & & & -1 & -F & -1 & \\ & & & & -1 & -F & -1 \\ \hline & & & & & -1 & -\mathrm{i}\xi - F \end{array} \right) \left(\begin{array}{c} \alpha_0 \\ \hline \gamma_1 \\ \gamma_0 \\ \gamma \\ \gamma_0^* \\ \gamma_1^* \\ \hline \alpha_0^* \end{array} \right) = 0. \tag{30}$$

An inspection of the explicit form of the secular determinant of this equation,

$$\mathcal{D} = [-F^6 - F^4(\xi^2 - 6) + F^2(4\xi^2 - 10) - 3\xi^2 + 4]F, \tag{31}$$

confirms that all of its seven roots remain real in the Hermitian $\xi \to 0$ limit,

$$F_0 = 0, \qquad F_{\pm,0} = \pm\sqrt{2}, \qquad F_{\pm,\pm} = \pm\sqrt{2 \pm \sqrt{2}}, \qquad \xi \to 0. \tag{32}$$

Moreover, in a way as illustrated in figure 2, only two roots $F_{\pm,-}$ merge and complexify beyond $\xi_{\text{crit}} \approx 1.154\,70$. In other words, as many as five of the roots remain real for $Z \gg 1$,

$$F_0 = 0, \qquad F_{\pm,0} = \pm 1, \qquad F_{\pm,+} = \pm\sqrt{3}, \qquad \xi \to \infty.$$

This observation parallels the similar results obtained in the continuous limit. All this also agrees with the *a priori* expectations, reflecting the weakened influence of the non-Hermitian part of the potential at the comparatively large shift $\ell = 5/8$.

6.2. Strengthening the non-Hermiticity using $\ell = 3/8$

The number of the robust levels may vary with the width ℓ of suppression of the imaginary interaction. Using a weaker suppression $\ell_1 = 3/8$, we may modify equation (29) accordingly and we get the precise $N = 8$ analogue,

$$\left(\begin{array}{c|ccccc|c} \mathrm{i}\xi - F & -1 & & & & & \\ -1 & \mathrm{i}\xi - F & -1 & & & & \\ \hline & -1 & -F & -1 & & & \\ & & -1 & -F & -1 & & \\ & & & -1 & -F & -1 & \\ \hline & & & & -1 & -\mathrm{i}\xi - F & -1 \\ & & & & & -1 & -\mathrm{i}\xi - F \end{array} \right) \left(\begin{array}{c} \alpha_0 \\ \alpha_1 \\ \hline \gamma_0 \\ \gamma \\ \gamma_0^* \\ \hline \alpha_1^* \\ \alpha_0^* \end{array} \right) = 0, \tag{33}$$

of problem (30). It is easy to evaluate the related secular determinant

$$\mathcal{D} = [-F^6 - F^4(2\xi^2 - 6) + F^2(-\xi^4 + 4\xi^2 - 10) + 2\xi^4 + \xi^2 + 4]F, \tag{34}$$

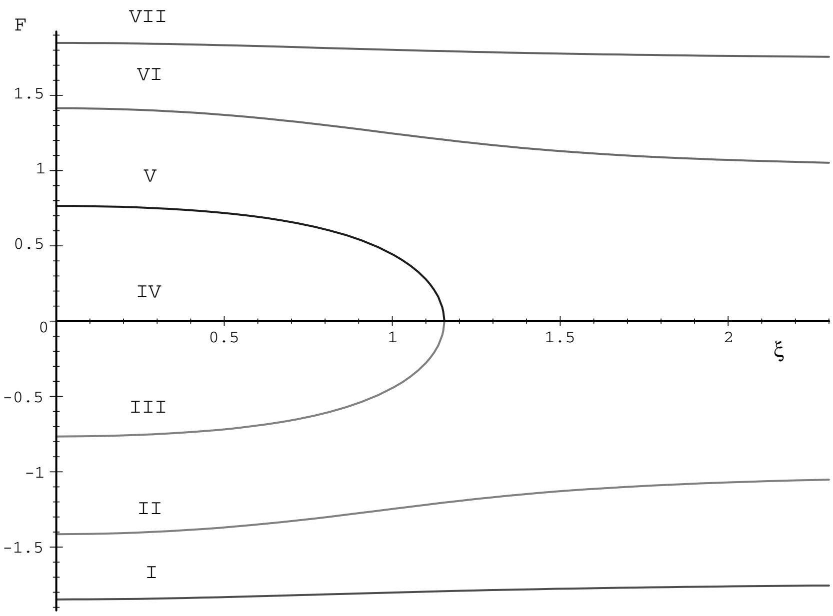

Figure 2. The ξ-dependence of the seven roots of the sample secular determinant (31).

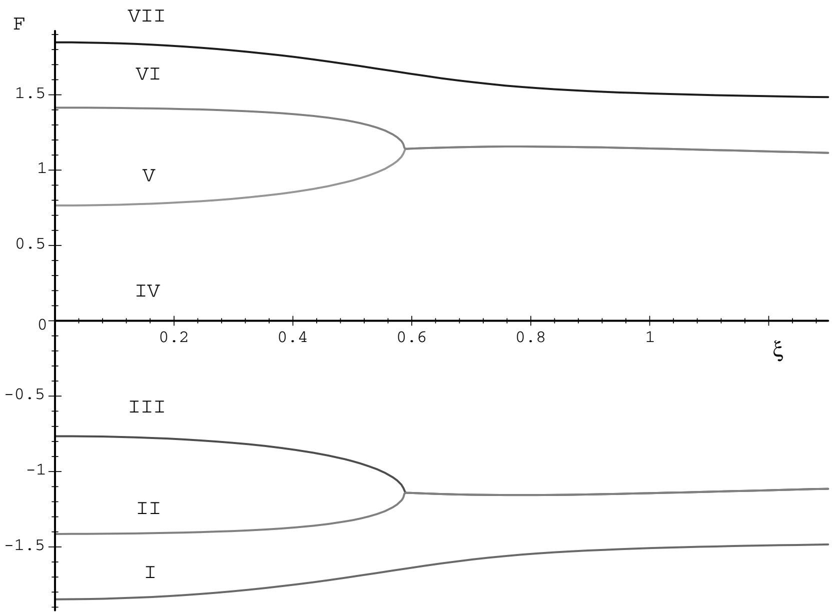

Figure 3. The ξ-dependence of the seven roots of the sample secular determinant (34).

which gives the same roots (32) in the weak non-Hermiticity-limit $\xi \to 0$. A change may be expected to emerge in the more non-Hermitian regime. Quantitatively, this change is being well illustrated by figure 3 where we see that merely two non-vanishing roots (namely, $F_{\pm,+} \to \pm\sqrt{2}$) remain robust and real at large $Z \to \infty$. We see that two complexifications take place at a certain finite coupling Z, i.e. at a unique critical point $\xi_{\text{crit}} \approx 0.587\,569\,1807$. In contrast to the previous case, we witness two *distinct* mergers of the eigenvalues $F_{\pm,0}$ with $F_{\pm,-}$ at the two different exceptional points $F_{\pm}^{\text{exc}} \approx \pm 1.140\,716\,421$.

7. Summary

A tentative weakening of the standard Hermiticity $H = H^{\dagger}$ to the mere $\mathcal{P}$-pseudo-Hermiticity of the Hamiltonian,

$$H^{\dagger} = \mathcal{P} H \mathcal{P}^{-1}, \tag{35}$$

employs only too often the ordinary differential Hamiltonian H and the parity operator $\mathcal{P}$ [7]. Here, we intended to emphasize that it is by far not the only possible scenario. For this reason, we replaced equation (2) by its discrete counterpart (5) and explained that its use may bring a few important advantages.

We feel satisfied by the fact that the purely formal application of the PTSQM recipe survives quite easily our present narrowing of one's attention to the very specific and *solvable* square-well models. We have shown that the use of various specific discrete versions of the Hamiltonians leads to very relevant formal simplifications emphasized throughout the text.

Within the dynamical region where our models possess the real spectrum, very close parallels were shown to emerge between the bound states for the standard continuous coordinate x [18, 30, 31] and for its present less standard discrete counterpart(s).

We have seen that in the discrete case it is particularly easy to complement the validity of the *auxiliary*, technical pseudo-Hermiticity condition (35) by the constructive solution of the *vital and essential* quasi-Hermiticity requirement (9) which is of key relevance in the context of physics.

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Appendix. Tshebyshev polynomials of scalars and matrices

A 'pedestrian's' way to the simultaneous work with the Tshebyshev's polynomials $Q_n(x)$ of the first kind (replace $Q_n(x) \to T_n(x)$) and of the second kind (replace $Q_n(x) \to U_n(x)$) leads through the 'universal' three-term recurrence relation

$$Q_{n+1}(x) - 2x Q_n(x) + Q_{n-1}(x) = 0, \tag{A.1}$$

complemented by the specific initial values,

$$\begin{aligned} &U_0(x) = 0, \qquad U_1(x) = \sqrt{1-x^2}, \quad \ldots \\ &T_0(x) = 1, \qquad T_1(x) = x, \quad \ldots. \end{aligned}$$

Many useful identities valid for these polynomials are available in the literature.

For complex arguments, an interesting situation emerges during a real-matrix rearrangement of equation (11). We may split equation (11) into real and imaginary parts and 'glue' them together in a pentadiagonal eigenvalue problem

$$\left(\begin{array}{cc|cc|cc|cc|c}
-F & -\xi & -1 & 0 & & & & & \\
\xi & -F & 0 & -1 & & & & & \\
\hline
-1 & 0 & -F & -\xi & \ddots & & & & \\
0 & -1 & \xi & -F & & \ddots & & & \\
\hline
 & & \ddots & & \ddots & \ddots & -1 & 0 & \\
 & & & \ddots & \ddots & \ddots & 0 & -1 & \\
\hline
 & & & & -1 & 0 & -F & -\xi & -1 \\
 & & & & 0 & -1 & \xi & -F & 0 \\
\hline
 & & & & & & -2 & 0 & -F
\end{array}\right)
\left(\begin{array}{c} a_0 \\ b_0 \\ \hline a_1 \\ b_1 \\ \hline \vdots \\ \vdots \\ \hline a_n \\ b_n \\ \hline \gamma \end{array}\right) = 0. \qquad \text{(A.2)}$$

It can be written in a partitioned form,

$$\begin{pmatrix}
\mathbf{X} & -\mathbf{1} & & & \\
-\mathbf{1} & \mathbf{X} & \ddots & & \\
 & \ddots & \ddots & -\mathbf{1} & \\
 & & -\mathbf{1} & \mathbf{X} & \vec{\mathbf{d}} \\
 & & & 2\vec{\mathbf{d}}^T & -F
\end{pmatrix}
\begin{pmatrix} \vec{\mathbf{c}}_0 \\ \vec{\mathbf{c}}_1 \\ \vdots \\ \vec{\mathbf{c}}_n \\ \gamma \end{pmatrix} = 0, \qquad \text{(A.3)}$$

with an 'odd' anomalous row and a column containing an auxiliary two-dimensional vector $[\vec{\mathbf{d}}^T = (1, 0)]$.

In the new context, all our wavefunctions are again proportional to the Tshebyshev polynomials,

$$\vec{\mathbf{c}}_\mathbf{k} = U_k\left(\frac{1}{2}\mathbf{X}\right)\vec{\mathbf{c}}_0, \qquad \mathbf{X} = \begin{pmatrix} -F & -\xi \\ \xi & -F \end{pmatrix}, \qquad \mathbf{k} = 0, 1, \ldots, n+1. \qquad \text{(A.4)}$$

The existence of the explicit solutions (A.4) (where polynomials U_k depend on a *two-by-two matrix* argument X) reduces equation (A.3) to the constraint imposed upon the two-dimensional real vector $\vec{\mathbf{c}}_{\mathbf{n+1}}$. Of course, this condition is equivalent to the complex matching as mentioned above.

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