Discrete $\mathcal{PT}$–symmetric square-well oscillators

Miloslav Znojil

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

Abstract

Exact solvability of the discretized $N$–point version of the $\mathcal{PT}$–symmetric square-well model at all $N$ is pointed out. Its wave functions are found proportional to the classical Tshebyshev polynomials $U_k(\cos \theta)$ of a complex argument. A compact secular equation is derived giving the real spectrum of energies at all the non-Hermiticity strengths $Z \in (-Z_{\text{crit}}(N), Z_{\text{crit}}(N))$. In the limit $Z \to 0$ the model degenerates to a Hermitian Hückel Hamiltonian.

PACS 03.65.Ge, 02.60.Lj, 02.70.Bf, 31.15.Ct

\footnotetext[1]{e-mail: znojil@ujf.cas.cz}
1 Introduction

The essence of the concept of the so called PT—symmetric Quantum Mechanics [1] lies in a half-forgotten fact that although the operators of observables (say, Hamiltonians $H$) must be Hermitian (with respect to a metric $\Theta$ in Hilbert space), they are also allowed to be Hermitian with respect to a nontrivial metric,

$$H^\dagger = \Theta H \Theta^{-1}, \quad I \neq \Theta = \Theta^\dagger > 0.$$  \hfill (1)

In sufficient detail, the formal aspects of this idea were already well described in the review paper [2] showing that in nuclear physics a decisive simplification of certain Schrödinger equations may be achieved after a formal transition from the most common $\Theta_1 = I$ to another $\Theta_2 \neq I$.

Beyond the area of nuclear physics the feasibility of the necessary calculations represents a key technical challenge for $\Theta \neq I$. Fortunately, for some differential Hamiltonians $H = \hat{p}^2 + V(x)$, an unexpectedly satisfactory answer has been found in a factorization of $\Theta$, typically, into a product of parity $\mathcal{P}$ and the so called quasi-parity $\mathcal{Q}$ [3] or charge $\mathcal{C}$ [4]. In the other words, one requires that the observables are both PT—symmetric and CP—pseudo-Hermitian. This means that all our non-Hermitian observables must be compatible with eq. (1) and that they must also commute with certain operator $\mathcal{PT}$. In the terminology advocated by A. Mostafazadeh [5] the latter requirement should be generalized and re-interpreted as the so called $\mathcal{P}$—pseudo-Hermiticity relation

$$H^\dagger = \mathcal{P} H \mathcal{P}^{-1}, \quad I \neq \mathcal{P} = \mathcal{P}^\dagger.$$  \hfill (2)

In such a widely accepted scenario [6] our observables may remain manifestly non-Hermitian in the current sense, $H \neq H^\dagger$. Still, their spectra must remain real and the work with the underlying indefinite ‘pseudo-metric’ operators of generalized parity $\mathcal{P}$ should remain sufficiently easy.

In the light of these two requirements we feel particularly inspired here

- [a] by the rigorous Krein-space analysis [7] of the reality of spectra of quantum particles confined inside a one-dimensional $\mathcal{PT}$—symmetric box $V(x)$,
• [b] in context [a], by our older explicit construction [8] of bound states in one of the most elementary square-well forms of $V(x)$,

• [c] in context [b], by the very recent Weigert’s [9] three-by-three matrix discretization

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

(3)

of the oscillator of ref. [8].

In this general framework we intend to start from the $\mathcal{PT}$–symmetric ordinary differential Schrödinger equation

$$
\left[-\frac{d^2}{dx^2} + V(x)\right] \psi(x) = E \psi(x), \quad \psi(\pm 1) = 0, \quad V(x) = [V(-x)]^* \quad (4)
$$

and from the proof given in ref. [7] that the resulting spectrum of energies $E = E_n$, $n = 0, 1, \ldots$ is real and discrete for all the complex $\mathcal{PT}$–symmetric potentials $V(x)$ which are not too strong,

$$
\|V\|_\infty < \frac{3}{8} \pi^2 \approx 3.701. \quad (5)
$$

In the spirit of item [b] we shall only pay attention to one of the simplest piecewise constant and purely imaginary antisymmetric potentials

$$
V(x) = \begin{cases}
+ i Z & x \in (-1, 0), \\
- i Z & x \in (0, 1).
\end{cases}
$$

(6)

Along the lines of item [c] we shall introduce the Runge-Kutta discrete lattice of coordinates,

$$
x_0 = -1, \quad x_k = x_{k-1} + h = -1 + kh, \quad h = \frac{2}{N}, \quad k = 1, 2, \ldots, N
$$

and pay attention to the general discrete analogue

$$
- \frac{\psi(x_{k+1}) - 2 \psi(x_k) + \psi(x_{k-1})}{h^2} - i \text{sign}(x_k) Z \psi(x_k) = E \psi(x_k) \quad (7)
$$
of our differential Schrödinger equation (4) + (6). In combination with the boundary conditions

\[ \psi(x_0) = \psi(x_N) = 0, \]

this in fact represents a generalization of the Weigert’s \( N = 4 \) eq. (3) to all the integers \( N \).

## 2 Models with the even \( N = 2n + 4 \)

Let us recollect that the continuous \( N = \infty \) model (6) is exactly solvable [8]. The solvability in closed form also characterizes its modifications with periodic boundary conditions and/or more discontinuities [10]. In this context, the exact solvability of the following \( (N - 1) \)-dimensional matrix generalization

\[
\begin{pmatrix}
i\xi - F & -1 & & & \\
-1 & i\xi - F & \ddots & & \\
& \ddots & \ddots & -1 & \\
& & -1 & i\xi - F & -1 \\
-1 & -F & -1 & & \\
& & -1 & -i\xi - F & \ddots \\
& & & \ddots & \ddots \\
& & & & -1 & -i\xi - F
\end{pmatrix}
\begin{pmatrix}
\alpha_0 \\
\alpha_1 \\
\vdots \\
\alpha_n \\
\gamma \\
\beta_n \\
\vdots \\
\beta_0
\end{pmatrix}
= 0 \quad (8)
\]

of the three-dimensional Weigert’s model (3) with the re-scaled energy eigenvalues \( F = E h^2 - 2 \) and with the re-scaled strength \( \xi = Z h^2 \) of the non-Hermiticity would not be too surprising.

In the first step of our analysis, due to the \( \mathcal{PT} \)-symmetry of our problem we may set

\[ \alpha_k = a_k + i b_k, \quad \beta_k = a_k - i b_k \equiv \alpha_k^*, \quad k = 0, 1, \ldots, n \]

with some real elements \( \gamma = \psi(0), a_k = \text{Re} \psi(x_{k+1}) \) and \( b_k = \text{Im} \psi(x_{k+1}) \). Once we recollect the definition of the classical Tshebyshev polynomials of the second kind
we immediately obtain the wave functions in closed form,

\[ \alpha_k = U_k \left( \frac{-F + i\xi}{2} \right) (a + ib), \quad k = 0, 1, \ldots, n. \]  

(9)

This reduces the full tridiagonal \((N-1) \times (N-1)\)-dimensional matrix eq. (8) to the mere three matching conditions,

\[
\begin{pmatrix}
-1 & i\xi - F & -1 & 0 & 0 \\
0 & -1 & -F & -1 & 0 \\
0 & 0 & -1 & -i\xi - F & -1 \\
\end{pmatrix}
\begin{pmatrix}
U_{n-1} \left( \frac{-F + i\xi}{2} \right) (a + ib) \\
U_n \left( \frac{-F + i\xi}{2} \right) (a + ib) \\
\gamma \\
U_n \left( \frac{-F - i\xi}{2} \right) (a - ib) \\
U_{n-1} \left( \frac{-F - i\xi}{2} \right) (a - ib)
\end{pmatrix} = 0. \tag{10}
\]

The first and the third lines may be simplified to give

\[ \gamma = U_{n+1} \left( \frac{-F + i\xi}{2} \right) (a + ib) = U_{n+1} \left( \frac{-F - i\xi}{2} \right) (a - ib). \tag{11} \]

The middle line defines the product

\[ F \gamma = -U_n \left( \frac{-F + i\xi}{2} \right) (a + ib) - U_n \left( \frac{-F - i\xi}{2} \right) (a - ib). \tag{12} \]

This forces us to separate the \( F = 0 \) case as exceptional.

2.1 The existence of a nontrivial solution at \( F = 0 \)

Once we set, tentatively, \( F = 0 \), it is easy to deduce from eq. (11) that the parameter \( a \) must vanish for the even \( n = 0, 2, 4, \ldots \) (and we may normalize \( b = 1 \)) while \( b = 0 \) and \( a = 1 \) for the odd \( n = 1, 3, 5, \ldots \). Thus, eq. (11) degenerates to the mere definition of the last element \( \gamma \) of the eigenvector and we are left with the single secular eq. (12) which acquires the following two alternative forms,

\[
\begin{align*}
U_n \left( \frac{1}{2} i\xi \right) - U_n \left( \frac{1}{2} i\xi \right) &= 0, \quad n = 2m, \\
U_n \left( \frac{1}{2} i\xi \right) + U_n \left( -\frac{1}{2} i\xi \right) &= 0, \quad n = 2m + 1.
\end{align*}
\tag{13}
\]
At any $m = 0, 1, \ldots$ these conditions are satisfied identically. We may conclude that our tentative “guess of the energy” was correct and that $F = 0$ is always the eigenvalue. It is remarkable that in spite of the non-Hermiticity of the Hamiltonian, this “robust” eigenvalue remains real at all the real couplings $Z \in (-\infty, \infty)$.

3 Closed secular equations for $N = 2n + 4$

Whenever $F \neq 0$ we may treat eq. (11) not only as the condition of vanishing of the imaginary part of $\gamma$, \[ U_{n+1} \left( \frac{-F + i\xi}{2} \right) (a + ib) = U_{n+1} \left( \frac{-F - i\xi}{2} \right) (a - ib) \] but also as an explicit definition of the non-vanishing left-hand-side quantity $F\gamma$ in eq. (12). Its insertion simplifies the latter relation, \[ T_{n+1} \left( \frac{-F + i\xi}{2} \right) (a + ib) = -T_{n+1} \left( \frac{-F - i\xi}{2} \right) (a - ib) \] where $T_k(z)$ denotes the $k-$th 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 \[ T_{n+1} \left( \frac{-F + i\xi}{2} \right) U_{n+1} \left( \frac{-F - i\xi}{2} \right) + T_{n+1} \left( \frac{-F - i\xi}{2} \right) U_{n+1} \left( \frac{-F + i\xi}{2} \right) = 0. \] This is our final secular equation which defines, in an implicit manner, the energies $F$ as functions of the couplings $\xi$.

An efficient numerical treatment of the latter eigenvalue problem may be based on the re-parametrization \[ \frac{-F + i\xi}{2} = \cos \varphi, \quad \text{Re} \varphi = \alpha, \quad \text{Im} \varphi = \beta \] i.e., \[ \frac{1}{2} F = -\cos \alpha \cosh \beta, \quad \frac{1}{2} \xi = -\sin \alpha \sinh \beta. \] In opposite direction, the inversion of this change of variables \[ \cos \alpha = -\frac{1}{2 \cosh \beta} F, \quad \sinh \beta = \frac{1}{2\sqrt{2}} \sqrt{F^2 + \xi^2 - 4 + \sqrt{(F^2 + \xi^2 - 4)^2 + 16\xi^2}}. \]
transforms eq. (16) into the compact and transparent trigonometric secular equation

\[ \text{Re} \frac{\sin[(n+1)\varphi] \cos[(n+1)\varphi^*]}{\sin \varphi} = 0. \]  \hspace{1cm} (19)

Its roots may be determined, numerically, as lying in the domain with negative \( \beta < 0 \) and with \( \alpha \in (0, \pi/2) \) for the negative \( F < 0 \) and with \( \alpha \in (\pi/2, \pi) \) for the positive \( F > 0 \). In this picture, the constant value of the coupling \( \xi > 0 \) is mapped upon a downwards-oriented half-oval in the \( \alpha - \beta \) plane with a top at \( \alpha = \pi/4 \). Its two asymptotes \( \alpha = 0 \) and \( \alpha = \pi/2 \) are reached in the limit \( \beta \to -\infty \).

In the new graphical representation the robust, \( \xi \)-independent energy level \( F = 0 \) lies on the top of the half-oval while its decreasing and increasing neighbors are found displaced to the left and right, respectively, along the half-oval downwards. At the first few lowest \( N = 2n+4 \) the coordinates of these eigenvalues remain non-numerical,

\[
F_0 = 0, \quad F_\pm = \pm \sqrt{2 - \xi^2}, \quad n = 0, \\
F_0 = 0, \quad F_{\pm,\pm} = \pm \sqrt{2 - \xi^2 \pm \sqrt{1 - 4\xi^2}}, \quad n = 1
\]

etc. The closed form of these definitions enables us to determine the closed form of the respective critical values at which the spectrum ceases to be real,

\[
Z_{\text{crit}}(4) = 4 \sqrt{2} \approx 5.66, \quad n = 0, \\
Z_{\text{crit}}(6) = 9/2 = 4.50, \quad n = 1,
\]

followed by the numerically calculated \( Z_{\text{crit}}(8) \approx 4.463 \) (at \( n = 2 \)), \( Z_{\text{crit}}(10) \approx 4.461 \) (at \( n = 3 \)), \( Z_{\text{crit}}(12) \approx 4.463 \) (at \( n = 4 \)) etc. These results do not contradict the expected \( n \to \infty \) limit \( Z_{\text{crit}}(\infty) \approx 4.475 \) derived in ref. [12].

### 3.1 A real-matrix re-arrangement of eq. (8)

We may split eq. (8) in its real and imaginary parts and ‘glue’ them together in the following very natural pentadiagonal or, if you wish, block-tridiagonal eigenvalue
problem

\[
\begin{pmatrix}
-F & -\xi & -1 & 0 \\
\xi & -F & 0 & -1 \\
-1 & 0 & -F & -\xi \\
0 & -1 & \xi & -F
\end{pmatrix}
\begin{pmatrix}
a_0 \\
b_0 \\
a_1 \\
b_1 \\
\vdots \\
a_n \\
b_n \\
\gamma
\end{pmatrix}
= 0. \quad (20)
\]

This equation may be re-written in the partitioned-matrix notation,

\[
\begin{pmatrix}
X & -1 \\
-1 & X \\
\vdots & \vdots & \ddots & \ddots & \vdots & -1 \\
-1 & X & \bar{d} \\
2\bar{d}^T & -F
\end{pmatrix}
\begin{pmatrix}
\bar{c}_0 \\
\bar{c}_1 \\
\vdots \\
\bar{c}_n \\
\gamma
\end{pmatrix}
= 0. \quad (21)
\]

The obvious boldface two-by-two matrix elements degenerate, in an ‘odd’ anomalous last row and column, to an auxiliary vector \( \bar{d}^T = (1, 0) \).

A few comments are due. Firstly, all our wave-function components are now re-interpreted as proportional to the classical Tshebyshev polynomials \( U_k \) with a two-by-two matrix argument \( X \). Equation (21) leads to an alternative formula for the eigenvectors,

\[
\bar{c}_k = U_k \left( \frac{1}{2} X \right) \bar{c}_0, \quad X = \begin{pmatrix} -F & -\xi \\ \xi & -F \end{pmatrix}, \quad k = 0, 1, \ldots, n + 1. \quad (22)
\]

Secondly, once we introduce a complex angle \( \alpha \) we may parametrize \( F = -\varrho \cos \alpha \) and \( \xi = \varrho \sin \alpha \) using an optional, redundant parameter \( \varrho \). A peculiar feature of our matrices \( X \) is that their powers remain elementary in this representation,

\[
X^m = \varrho^m \begin{pmatrix} \cos m\alpha & -\sin m\alpha \\ \sin m\alpha & \cos m\alpha \end{pmatrix}.
\]
This means that all the formulae containing polynomials (22) remain amazingly transparent.

The existence of the explicit solutions (22) reduces eq. (21) to the two secular-equation constraints imposed upon the vector \( \mathbf{c}_{n+1} \). Of course, they are equivalent to our complex matching conditions as mentioned above.

4 Solutions at the odd \( N = 2n + 3 \)

Weigert [9] did not notice that a “one-step easier” discretization of eq. (4) emerges at the odd \( N = 2n + 3 \), with \( 2N + 2 \) energy roots at \( n \geq 0 \). An alternative to eq. (8) then reads, in the same notation,

\[
\begin{pmatrix}
  i\xi - F & -1 \\
  -1 & i\xi - F \\
  & \ddots & \ddots & -1 \\
  & & \ddots & \ddots & -1 \\
  & & & -1 & -i\xi - F \\
  -1 & -i\xi - F & \ddots & \ddots & -1 \\
  & \ddots & \ddots & \ddots & -1 \\
  & & & -1 & -i\xi - F
\end{pmatrix}
\begin{pmatrix}
  \alpha_0 \\
  \alpha_1 \\
  \vdots \\
  \alpha_n \\
  \alpha_n^* \\
  \alpha_0^*
\end{pmatrix}
= 0. \quad (23)
\]

Definition (9) of the eigenvectors remains unchanged but the matching condition is just one,

\[
\gamma = U_{n+1} \left( \frac{-F + i\xi}{2} \right) (a + ib) = U_n \left( \frac{-F - i\xi}{2} \right) (a - ib) . \quad (24)
\]

The ratio between this equation and its Hermitian conjugate eliminates all the normalization ambiguities and leads to the odd-\( N \) counterpart of eq. (16),

\[
U_n \left( \frac{-F + i\xi}{2} \right) U_n \left( \frac{-F - i\xi}{2} \right) = U_{n+1} \left( \frac{-F + i\xi}{2} \right) U_{n+1} \left( \frac{-F - i\xi}{2} \right) . \quad (25)
\]

This secular equation is our final result. As an implicit definition of the \( N = 2n + 3 \) energy levels \( F = F(\xi) \) it possesses the compact non-numerical solutions at the first two values of \( n \) again,

\[
F_\pm = \pm \sqrt{1 - \xi^2}, \quad n = 0,
\]

\[
F_{\pm,\pm} = \pm \frac{1}{2} \sqrt{6 - 4\xi^2 \pm 2 \sqrt{3 - 16\xi^2}}, \quad n = 1.
\]
The respective elementary expressions for the critical constants

\[ Z_{\text{crit}}(3) = \frac{9}{4} = 2.25, \quad n = 0, \]
\[ Z_{\text{crit}}(5) = \frac{25\sqrt{5}}{16} \approx 3.49, \quad n = 1 \]

are followed by the complex Cardano representation of the real \( Z_{\text{crit}}(7) \approx 3.946 \) at \( n = 2 \). At \( n > 2 \) one switches to a purely numerical algorithm giving \( Z_{\text{crit}}(9) \approx 4.148 \) at \( n = 3 \) etc. In comparison with the parallel results sampled in section 3 at even \( N \) we notice a slowdown of the numerical convergence towards the \( n \to \infty \) limit.

**Acknowledgment**

Proportionally supported by NPI, IRP AV0Z10480505, and by GA AS, contract No. A 1048302.
References

[1] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80 (1998) 52 43;
   C. M. Bender, S. Boettcher and P. N. Meisinger, J. Math. Phys. 40 (1999) 2201.

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

[3] M. Znojil, Phys. Lett. A 259 (1999) 220;
   M. Znojil, math-ph/0104012.

[4] C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 89 (2002) 270401;
   C. M. Bender, Czech. J. Phys. 54 (2004) 1027.

[5] A. Mostafazadeh, J. Math. Phys. 43 (2002) 205 and 2814.

[6] R. Kretschmer and L. Szymanowski, quant-ph/0105054;
   P. Dorey, C. Dunning and R. Tateo, J. Phys. A: Math. Gen. 34 (2001) 5679;
   K. C. Shin, Commun. Math. Phys. 229 (2002) 543;
   F. Kleefeld, in “Hadron Physics, Effective Theories of Low Energy QCD”, AIP Conf. Proc. 660 (2003) 325;
   V. Jakubský, Czech. J. Phys. 54 (2004) 67;
   G. Scolarici, Czech. J. Phys. 54 (2004) 119;
   Q. Wang, Czech. J. Phys. 54 (2004) 143;
   A. Blasi, G. Scolarici and L. Solombrino, Czech. J. Phys. 54 (2004) 1055;
   H. B. Geyer, F. G. Scholz and I. Snyman, Czech. J. Phys. 54 (2004) 1069;
   W. D. Heiss, Czech. J. Phys. 54 (2004) 1091;
   E. Caliceti, Czech. J. Phys. 55 (2005) 1077;
   U. Günther and F. Stefani, Czech. J. Phys. 55 (2005) 1099;
   A. Mostafazadeh, Czech. J. Phys. 55 (2005) 1157.
[7] H. Langer and Ch. Tretter, Czech. J. Phys. 54 (2004) 1113.

[8] M. Znojil, Phys. Lett. A. 285 (2001) 7;
   M. Znojil, J. Math. Phys. 45 (2004) 4418.

[9] S. Weigert, Czech. J. Phys. 55 (2005) 1183.

[10] B. Bagchi, S. Mallik and C. Quesne, Mod. Phys. Lett. A17 (2002) 1651;
    M. Znojil, J. Phys. A: Math. Gen. 36 (2003) 7825;
    A. Mostafazadeh and A. Batal, J. Phys. A: Math. Gen. 37 (2004) 11645;
    V. Jakubský and M. Znojil, Czech. J. Phys. 54 (2004) 1101;
    M. Znojil, J. Math. Phys. 46 (2005) 062109;
    H. Bíla, V. Jakubský, M. Znojil, B. Bagchi, S. Mallik and C. Quesne, Czech. J.
    Phys. 55 (2005) 1075.

[11] G. Szegö, Orthogonal Polynomials, AMS, Providence, 1991.

[12] M. Znojil and G. Lévai, Mod. Phys. Lett. A 16 (2001) 2273.