

Non-Hermitian matrix description of the \mathcal{PT} -symmetric anharmonic oscillators

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Abstract. The \mathcal{PT} -symmetric differential Schrödinger equation $H\psi = E\psi$ with the operator $H = H(x) = p^2 + ax^4 + i\beta x^3 + cx^2 + i\delta x \equiv H^*(-x)$ on $L_2(-\infty, \infty)$ is studied. At $a > 0$ it is rearranged as a linear algebraic diagonalization. With rigorous proof, our non-variational construction of bound states offers an infinite-dimensional analogue to the recent finite-dimensional quasi-exact solution available at the less common $a < 0$.

1. Introduction

The study of the general parity-breaking anharmonic oscillators

$$V(x) = ax^4 + bx^3 + cx^2 + dx \quad (1)$$

has a colourful and inspiring history [1]. Its latest turn came with the recent letter by Bender and Boettcher [2] who discovered that after a partial restoration of symmetry in the complex plane,

$$V(x) = V^*(-x) \quad (2)$$

these potentials may become solvable quasi-exactly [3]. The extensive numerical experiments indicate that all the spectrum of energies E in the similar potentials is real, bounded and discrete. According to the conjecture by Daniel Bessis [4] this puzzling observation might be a straightforward mathematical consequence of the ‘weakened hermiticity’ (2). With motivations ranging from field theory [5] and nuclear structure [6] up to solid state physics [7] this hypothesis finds its further support in a few explicit analytic [8] and numerical [9] constructions and semi-classical [10] or perturbative [11] arguments as well as in several available rigorous mathematical proofs [12].

In the particular model (1) the condition (2) means that the couplings a and c remain real while their partners $b = i\beta$ and $d = i\delta$ are purely imaginary. The attention of paper [2] was solely paid to the *negative* values of the asymptotically dominant coupling a because of the related finite-dimensional reducibility and subsequent partial solvability of the bound state problem at certain special couplings and energies. In the present paper we intend to complement and complete the latter study by a parallel analysis of its ‘less solvable’ alternative with $a > 0$. One has to imagine that in spite of the manifest non-hermiticity of the related Hamiltonian the procedure of quantization may be kept equally well defined at any sign of a [13]. Extensive discussions of this point date back to the well known Dyson argument ([14]; cf the very recent summary in [15]). The same or similar formalism covers even the limiting case with vanishing $a = 0$ at any complex $b \neq 0$ [16].

The main reason for the conventional $a > 0$ is the simplicity of its physical interpretation. In an unquantized world the minus sign of a would mean that the particle can disappear and return from infinity in a finite time. In comparison, the asymptotically real and growing $V(x)$ admits a more immediate intuitive understanding. Its choice weakens the impact of the unusual invariance (2) which, in certain applications, mimicks the combined effect of parity and time reversal \mathcal{PT} [10]. With $a > 0$ we also get a closer contact with the already existing calculations [17] and with the resummations of perturbation series, say, in terms of the so-called Hill determinants [18, 19] or analytic [20] and matrix [21] continued fractions. The new, non-Hermitian options $\beta \neq 0$ and $\delta \neq 0$ open new perspectives.

We intend to show that the positivity of a which excludes the quasi-exact solvability need not contradict an efficient linear algebraic description of bound states. We shall rewrite the differential Schrödinger equation in an equivalent matrix form. Although its dimension remains infinite, its structure and derivation will parallel its Hermitian Hill-determinant predecessors characterized globally by a loss of their hermiticity (*pars pro toto*, the reader may consult the review [22]). For our present non-Hermitian interaction (1) + (2) such a loss is much less harmful.

2. Non-terminating recurrences at $a > 0$

Forces (1) with the ‘weak’ symmetry (2) enter the differential Schrödinger equation

$$\left(-\frac{d^2}{dx^2} + ax^4 + i\beta x^3 + cx^2 + i\delta x \right) \psi(x) = E\psi(x) \quad x \in (-\infty, \infty) \quad (3)$$

which has the two independent asymptotic solutions

$$\psi^{(\pm)}(x) = \exp \left[u \frac{x^3}{3} + v \frac{x^2}{2} + \mathcal{O}(x) \right] \quad u = \pm\sqrt{a} \neq 0 \quad v = i\frac{\beta}{2u}. \quad (4)$$

This explains the difference between $a < 0$ and $a > 0$. In the former case we may move the real axis downwards in the complex plane, $x = r - i\eta$, $\eta > 0$, $r \in (-\infty, \infty)$. Whenever we pick up $\eta > -\beta/4\sqrt{|a|}$, we discover that the asymptotic solution $\psi^{(-)}(x)$ remains integrable at *both* ends of the real axis r . Some of the (necessarily, analytic) bound states $\psi^{(exact)}(x)$ may (and do) acquire an elementary form of an exponential-times-polynomial product for $a < 0$ [2].

Let us now consider a positive coupling $a > 0$ and rescale its value to $a = 1$ for simplicity. The general solution of our Schrödinger equation (3) will have the form $\psi^{(gen)}(x) = \mu_{\pm}\psi^{(+)}(x) + \nu_{\pm}\psi^{(-)}(x)$. It may only be made compatible with the required asymptotic decrease near $x \rightarrow \pm\infty$ by the sign-of- x -dependent choice of its parameters,

$$\begin{aligned} \psi^{(phys)}(x) &= \nu_{+}\psi^{(-)}(x) & x \gg 1, \\ \psi^{(phys)}(x) &= \mu_{-}\psi^{(+)}(x) & x \ll -1. \end{aligned} \quad (5)$$

In contrast to the preceding case, the exact solution cannot be constructed as a product of an exponential with a polynomial any more. One has to resort to the next eligible possibility, say,

$$\psi^{(ansatz)}(x) = e^{-sx^2} \sum_{n=0}^{\infty} h_n(ix)^n. \quad (6)$$

This is a manifestly \mathcal{PT} -invariant infinite-series ansatz. Abbreviating $ix = y$ we derive the recurrences

$$A_n h_{n+2} + C_n h_n + \delta h_{n-1} + \theta h_{n-2} - \beta h_{n-3} + h_{n-4} = 0. \quad (7)$$

All its coefficients are real: $A_n = (n + 1)(n + 2)$, $C_n = 4sn + 2s - E$ and $\theta = 4s^2 - c$. By construction, the set (7) is equivalent to our differential equation (3). At all the tentative energies E it defines the coefficients h_n from an input pair h_0 and h_1 . We have to determine these parameters via a fit of (6) to the appropriate boundary conditions

$$\psi^{(ansatz)}(X_R) = 0 = \psi^{(ansatz)}(-X_L) \quad X_R \gg 1 \quad X_L \gg 1. \quad (8)$$

In comparison with the other numerical methods of solution of the bound state problems with symmetry (2) [9] such a recurrently specified recipe does not seem any superior, especially since it requires a cumbersome numerical limiting transition $X_{R,L} \rightarrow \infty$. A deeper insight and simplifications are asked for.

3. The asymptotics of coefficients h_n at $n \gg 1$

Recurrences (7) form a linear difference equation of the sixth order. One may recall the standard theory of its solution [23] as well as its immediate application to quartic oscillators [24, 25]. At the large indices n , the sextuplet of the independent asymptotic solutions h_n acquires the general Birkhoff form as presented, say, in [26]. All these solutions decrease as $h_n \sim \mathcal{O}(n^{-n/3})$ at least. For our present purposes, they may easily be re-derived as follows.

Firstly, in the leading-order approximation, we replace equation (7) by the mere two-term dominant relation between h_{n+2} and h_{n-4} . This inspires us to change variables $h_n \rightarrow g_n$ and we rewrite all the six independent solutions in the same compact form:

$$h_n(p) = \frac{\lambda^n(p)g_n(p)}{(3^{1/3})^n \Gamma(1 + n/3)} \quad p = 1, 2, \dots, 6. \quad (9)$$

The p -dependent complex parameter $\lambda(p) = \exp[i(2p - 1)\pi/6]$ characterizes the dominant n -dependence of the separate solutions while the new functions or coefficients $g_n = g_n(p)$ vary more slowly with n .

This confirms the linear independence of our six solutions but leaves their absolute values indistinguishable. In order to remove this degeneracy in size we reintroduce equation (7) in its amended, second-order asymptotic form

$$g_{n+2} - g_{n-4} = \frac{4s\lambda^4}{n^{1/3}}g_n - \frac{\beta\lambda}{n^{1/3}}g_{n-3} + \mathcal{O}\left(\frac{g_n}{n^{2/3}}\right). \quad (10)$$

With most of the components of the Stirling formula still hidden within the error term, the smallness of the ratio $1/n^{1/3}$ enables us to infer that

$$g_n = e^{\gamma n^{2/3} + \mathcal{O}(n^{1/3})} \quad n \gg 1. \quad (11)$$

The complex exponent $\gamma = \gamma(p) = s\lambda^4(p) - \beta\lambda(p)/4$ depends on p . An elementary trigonometry gives the explicit formulae

$$\begin{aligned} \operatorname{Re} \gamma(1) = \operatorname{Re} \gamma(6) &= -\frac{\sqrt{3}}{8}\beta - \frac{s}{2} & \operatorname{Re} \gamma(2) = \operatorname{Re} \gamma(5) &= s \\ \operatorname{Re} \gamma(3) = \operatorname{Re} \gamma(4) &= \frac{\sqrt{3}}{8}\beta - \frac{s}{2}. \end{aligned} \quad (12)$$

In combination with equation (9) this already implies that the radius of convergence of our Taylor series (6) is infinite. The function $\psi^{(ansatz)}(x)$ is unique and well defined at any complex x . Its shape is fully determined by the energy E and by a not yet specified choice of the two initial complex coefficients h_0 and h_1 .

The second important consequence of identities (12) is that whenever we satisfy the condition

$$s > \frac{|\beta|}{4\sqrt{3}} \quad (13)$$

the general solution $h_n = \sum_{p=1}^6 G_p h_n(p)$ will itself be asymptotically dominated by its two most quickly growing components,

$$h_n = G_2 h_n(2) + G_5 h_n(5) \quad n \gg 1. \quad (14)$$

In this sense we are free to set $G_1 = G_3 = G_4 = G_6 = 0$ in the asymptotic domain of $n \gg 1$. Each choice of the energy E and initial h_0 and h_1 will only generate a different, x - and n -independent pair of coefficients G_2 and G_5 .

4. The asymptotics of $\psi^{(ansatz)}(x)$ at $|x| \gg 1$

Equation (14) is a key to our forthcoming replacement of the numerically awkward boundary conditions (8) by the much more natural approximative truncation of recurrences (7). We shall parallel the Hermitian construction of [22] and try to bracket the exact energy between its upper and lower estimates with $E \neq E(\text{physical})$. Under such an assumption our infinite series $\psi^{(ansatz)}(x)$ as defined by equation (6) will *always* exhibit an exponential asymptotic growth as described quantitatively by equation (4) above. This means that we shall exempt the possible lucky guess of the exact energy in its *full* precision as *never* relevant in *any* step of our forthcoming considerations. Such a very formal point of view does not contradict the underlying physical intuition since boundary conditions (8) are approximative. One has to move to the limit $X_{R,L} \rightarrow \infty$ in principle.

The most important immediate consequence of our 'bracketing' interpretation of boundary conditions is that at the large absolute values of the coordinate $|x| \gg 1$ the first N exponentially small components $\mathcal{O}(e^{-sx^2})$ may safely be ignored as irrelevant. We may also insert (9) and (14) in $\psi^{(ansatz)}(x) \sim \exp(-sx^2) \sum_{n=N+1}^{\infty} h_n(ix)^n$ with $N \gg 1$ and get

$$\psi^{(ansatz)}(x) \sim e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{G_2 \lambda^n(2) g_n(2) + G_5 \lambda^n(5) g_n(5)}{(3^{1/3})^n \Gamma(1+n/3)} (ix)^n \quad |x| \gg 1.$$

The validity of this formula is a strict consequence of the specific constraint (13) imposed (say, from now on) upon the admissible quasi-variational parameter s .

Once we split $\psi^{(ansatz)}(x) = \psi^{(ansatz)}(G_2, G_5, x)$ into its two components

$$\begin{aligned} \psi^{(ansatz)}(G_2, 0, x) &\sim G_2 e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{(-x)^n \exp[\gamma(2)n^{2/3} + \mathcal{O}(n^{1/3})]}{(3^{1/3})^n \Gamma(1+n/3)} \\ \psi^{(ansatz)}(0, G_5, x) &\sim G_5 e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{x^n \exp[\gamma(5)n^{2/3} + \mathcal{O}(n^{1/3})]}{(3^{1/3})^n \Gamma(1+n/3)} \end{aligned}$$

we may apply the rule $e^z \sim (1+z/t)^t$, $t \gg 1$ in the error term and get

$$\frac{\psi^{(ansatz)}(G_2, 0, -y)}{\exp(-sy^2)} \sim G_2 \sum_{n=N+1}^{\infty} \frac{1}{(3^{1/3})^n \Gamma(1+n/3)} \left\{ y \cdot \left[1 + \mathcal{O}\left(\frac{1}{N^{1/3}}\right) \right] \right\}^n$$

and

$$\frac{\psi^{(ansatz)}(0, G_5, y)}{\exp(-sy^2)} \sim G_5 \sum_{n=N+1}^{\infty} \frac{1}{(3^{1/3})^n \Gamma(1+n/3)} \left\{ y \cdot \left[1 + \mathcal{O}\left(\frac{1}{N^{1/3}}\right) \right] \right\}^n.$$

This is valid at all the large arguments y . Along the *positive* semi-axis $y \gg 1$, both the right-hand-side summands are real and positive. They sum up to the same function $\exp[y^3/3 + \mathcal{O}(y^2)]$. This is a consequence of the approximation of the sum by an integral and its subsequent evaluation by means of the saddle-point method. The same trick was used by Hautot, in similar context, for the \mathcal{P} -symmetric and Hermitian anharmonic oscillators [27].

In contrast to the Hautot's resulting one-term estimates of ψ , the present asymmetric, \mathcal{PT} -invariant construction leads to the more general two-term asymptotic estimate

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_2 \exp[-x^3/3 + \mathcal{O}(x^2)] + G_5 \exp[x^3/3 + \mathcal{O}(x^2)] \quad |x| \gg 1.$$

As long as we deal with the holomorphic function of x , this estimate may be analytically continued off the real axis of x . Near both the ends of the real line and within the asymptotic wedges $|\text{Im } x|/|\text{Re } x| < \tan \pi/6$ we simply have the rules

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_2 \exp[-x^3/3 + \mathcal{O}(x^2)] \quad \text{Re } x < -X_L \ll -1 \quad (15)$$

and

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_5 \exp[x^3/3 + \mathcal{O}(x^2)] \quad 1 \ll X_R < \text{Re } x. \quad (16)$$

They are fully compatible with formula (5) since $a = 1$.

5. The matrix form of the Hamiltonian

Our complex differential Schrödinger equation (3) becomes asymptotically real, in the leading-order approximation at least. In a suitable normalization the wavefunctions $\psi^{(ansatz)}(x)$ may be made asymptotically real as well. Near infinity they will obey the standard Sturm–Liouville oscillation theorems [28]. In particular, after a small decrease of the tentative energy parameter $E > E(\text{physical})$ the asymptotic nodal zero X_R or $-X_L$ originating in one of our boundary conditions (8) will move towards infinity [29].

This may be rephrased as follows. At a more or less correct physical real pair $h_0 = \rho \cos \zeta$ and $h_1 = \rho \sin \zeta$ with $\zeta \in (0, 2\pi)$ and with the convenient normalization $\rho = 1$ a small change of the energy E somewhere near its correct physical value $E_0 \approx E(\text{physical})$ will cause a sudden change of the sign of the asymptotically growing exponentials (15) and (16) at some $\zeta_0 \approx \zeta(\text{physical})$. This may be re-read as a doublet of conditions:

$$G_2 = G_2(E_0, \zeta_0) = 0 \quad G_5 = G_5(E_0, \zeta_0) = 0. \quad (17)$$

In the limit $N \rightarrow \infty$ of vanishing corrections, these two requirements may be reinterpreted as a rigorous reincarnation of our original physical asymptotic boundary conditions (8). The conclusion has several important consequences. Firstly, at a fixed $N \gg 1$ we may define

$$f_p = G_p \frac{\lambda^N(p) \exp[\gamma(p)N^{2/3}]}{(3^{1/3})^N \Gamma(1 + N/3)} \quad p = 2, 5.$$

Functions $f_p = f_p(E, \zeta_0)$ differ from their sign-changing predecessors $G_p = G_p(E, \zeta_0)$ just by a constant factor near E_0 , $f_p(E, \zeta_0) \approx F_p \cdot (E - E_0)$. We may write

$$\begin{aligned} h_N &\approx (F_2 + F_5)(E - E_0) + \mathcal{O}[(E - E_0)^2] \\ (N + 3)^{1/3} h_{N+1} &\approx [F_2 \lambda(2) + F_5 \lambda(5)](E - E_0) + \mathcal{O}[(E - E_0)^2] \end{aligned}$$

due to equation (9). This formula connects the two functions G_2, G_5 with the two neighbouring Taylor coefficients $h_N = h_N(E_0, \zeta_0)$ and $h_{N+1} = h_{N+1}(E_0, \zeta_0)$ near the physical E_0 and ζ_0 by an easily invertible regular mapping. This means that the implicit algebraic boundary conditions (17) are strictly equivalent to the fully explicit requirements

$$h_N(E_0, \zeta_0) = 0 \quad h_{N+1}(E_0, \zeta_0) = 0 \quad N \gg 1. \quad (18)$$

Table 2. The growth of precision with dimension N .

N	Energies E_n							
	0	1	2	3	4	5	6	7
15	1.693 47	5.106	9.152	13.043	17.817	23.89	31.26	41.55
20	1.691 638	5.125 59	9.280 0	14.050	19.244	—	32.35	—
25	1.691 579	5.123 441	9.258 12	13.8689	18.7925	24.265	30.039	37.97
30	1.691 590	5.123 614	9.261 74	13.8826	18.8922	24.262	29.726	34.67
35	1.691 590	5.123 579	9.261 51	13.8793	18.8838	24.220	29.860	35.85

6.2. Determinantal formulae for the Taylor coefficients

With real h_0 and h_1 our wavefunctions $\psi^{(ansatz)}(x)$ are composed of the spacially symmetric real part and spacially antisymmetric imaginary part. Such a normalization fixes the phases of the complex constants G_2 and G_5 accordingly, i.e. via equation (14). This clarifies the structure of the asymptotics of the wavefunctions.

Polynomial approximants of the Taylor series (6) offer a reliable picture of $\psi(x)$ in a broad vicinity of the origin. We may recall recurrences (7) and reveal that the h_0 - and h_1 -dependence of any coefficient h_n is linear:

$$h_n = h_0\sigma_n + h_1\omega_n \quad \sigma_0 = \omega_1 = 1 \quad \sigma_1 = \omega_0 = 0.$$

All three sequences h_n , σ_n and ω_n satisfy the same recurrences. As long as $\sigma_1 = 0$ and $\omega_0 = 0$ we may omit the second or first column from equation (19) in the latter two respective cases. In terms of the $(m + 1)$ -dimensional matrices

$$\Sigma_m = \begin{pmatrix} C_0 & A_0 & & & & & & & \\ \delta & 0 & A_1 & & & & & & \\ \vdots & C_2 & 0 & A_2 & & & & & \\ 1 & \vdots & C_3 & \ddots & \ddots & & & & \\ 0 & -\beta & \ddots & \ddots & 0 & A_{m-2} & & & \\ \vdots & 1 & \ddots & \delta & C_{m-1} & 0 & A_{m-1} & & \\ & & \ddots & \dots & \delta & C_m & 0 & & \end{pmatrix}$$

and

$$\Omega_m = \begin{pmatrix} 0 & A_0 & & & & & & & \\ C_1 & 0 & A_1 & & & & & & \\ \delta & C_2 & 0 & A_2 & & & & & \\ \vdots & \delta & C_3 & \ddots & \ddots & & & & \\ 1 & \vdots & \delta & \ddots & 0 & A_{m-2} & & & \\ & & \ddots & -\beta & \ddots & C_{m-1} & 0 & A_{m-1} & \\ & & & 1 & \dots & \delta & C_m & 0 & \end{pmatrix}$$

we may rewrite not only the recurrences themselves but also their unexpectedly compact solution

$$\sigma_{n+1} = (-1)^n \frac{\det \Sigma_{n-1}}{n!(n+1)!} \quad \omega_{n+1} = (-1)^n \frac{\det \Omega_{n-1}}{n!(n+1)!} \quad n = 1, 2, \dots \quad (20)$$

We need to know just the correct physical values of the three variable parameters (the norm $\rho = \sqrt{h_0^2 + h_1^2}$, the ratio $h_1/h_0 \equiv \tan \zeta$ and the physical energy E) in order to be able to define our physical wavefunction $\psi(x)$ completely in terms of these closed formulae.

6.3. Alternative ansätze and constructions

We have shown that the Taylor-series ansatz (6) mediates a useful transition from differential equation (3) to the difference equation (7), followed by its further replacement by our final matrix Schrödinger equation (19). In this context it is important to mention that our choice of the initial form of ansatz (6) is far from unique.

A nice example of an alternative expansion may be found in [31] where the Hill-determinant study of the symmetric potentials $V(x) = x^2 + \lambda u(x)$ with the non-polynomial anharmonicity $u(x) = x^2/(1 + gx^2)$ via the series of the form (6) has been rendered possible by the use of the Taylor series in powers of the 'adapted' variable $u(x)$. Sophisticated versions of the latter trick move the (complex) singularities off the physical domain of convergence and their active use in physics dates back to Jaffé [32] at least. They may even help us to deal with relativistic corrections [33] etc.

Unfortunately, an application of the changes of variables to asymmetric potentials is not without its specific difficulties. Efficient methods of their suppression have been suggested, therefore, in our older paper [34] and, recently, by Bay *et al* [25]. Most often, one employs the *two independent* separate ansätze (one for each half-axis) and matches the wavefunctions, say, in the origin.

In the latter comparison, the method of paper [25] is most straightforward. It is based simply on an introduction of the second free parameter (G or V in the original notation). Even from the very numerical point of view, the essence of the algorithm of Bay *et al* remains purely iterative, therefore.

The more algebraic method of [34] works directly with the matched, 'doubly infinite' sparse matrices. Although the algorithm itself is already fully algebraicized, its universality seems redundant for our present purposes. Indeed, the \mathcal{PT} -symmetric forces (1) are only composed of the real part which is spatially symmetric and of the non-vanishing imaginary part which is spatially antisymmetric. This additional information is well reflected and used by our present non-matching approach.

We summarize that we were able to preserve a maximal similarity of our 'new Hill determinants' to their current Hermitian predecessors (cf, e.g., [19]). Moreover, in a way completing the parallel studies of the other \mathcal{PT} symmetric potentials, the very specific form of their spatial asymmetry again proved 'extremely weak' from the purely methodical point of view. We reconfirmed that its simplifying role strongly resembles the role of the usual \mathcal{P} -symmetry (i.e. parity), so useful in many parts of the current textbook quantum mechanics.

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