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Spiked and \mathcal{PT} -symmetrized decadic potentials supporting elementary N-plets of bound states

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Abstract. We show that the potential wells $V(x) = x^{10} + ax^8 + bx^6 + cx^4 + dx^2 + f/x^2$ with a central spike possess arbitrary finite multiplets of elementary exact bound states. Their strong asymptotic growth implies an ambiguity in their \mathcal{PT} symmetrically generalized quantization (via complex boundary conditions) but the three eligible methods coincide at our exceptional solutions.

1. Introduction

Realistic calculations in quantum physics and field theory are often guided by a parallel study of a simplified quantum mechanical model in one dimension. A typical example may be found in [1], where a self-interacting scalar field theory is being modified in a non-perturbative manner. It is emphasized there that one has to pay due attention, not only to the interaction potential V(x) itself, but also to the boundary conditions imposed upon solutions in infinity.

In general, the latter conditions are not unique. One of the most transparent explicit examples of their ambiguity has been offered by Bender and Turbiner [2]. In essence, they considered a partially solvable sextic potential $V(x) = x^6 - 3x^2$ and its zero-energy ground-state wavefunction $\psi(x) = \exp(-x^4/4)$. In this model it is obvious that once you start working in the whole complex plane, $x = \varrho e^{\varphi} \in \mathbb{C}$, the asymptotic normalizability of the wavefunction keeps satisfied not only on the real line but, in general, within the four different asymptotic wedges defined by the elementary equation $\operatorname{Re}(-x^4) < 0$. This gives the admissible angles $\varphi \in S_k$, k = 1, 2, 3, 4 lying within the four separate intervals:

$$S_1 = (-\pi/8, \pi/8)$$
 $S_2 = (3\pi/8, 5\pi/8)$ $S_3 = (7\pi/8, 9\pi/8)$ $S_4 = (11\pi/8, 13\pi/8).$ (1)

Schematically, the situation is depicted in figure 1. One imagines that the eligible *complex* physical coordinates can be arbitrary curves with ends which do not enter the 'forbidden' asymptotic domains. Thus, the current real line starts at $\varphi_L \in S_3$ in the left infinity and ends at $\varphi_R \in S_1$. Its slightly bizarre 'Wick-rotated' alternative $S_4 + S_2$ has also been discussed in the literature as a weird example of a system whose real spectrum is not bounded below [3]. The elementary zero-energy bound state itself is *shared* by both these non-equivalent spectra.

From a retrograde point of view the choice of the sextic V(x) proved unfortunate since its menu (1) is not yet rich enough. Further progress was only achieved 5 years later when Bender and Boettcher [4] came to the conclusion that a privileged role must be played by the pairs of sectors with a mirror left–right symmetry. This symmetry keeps the trace of its

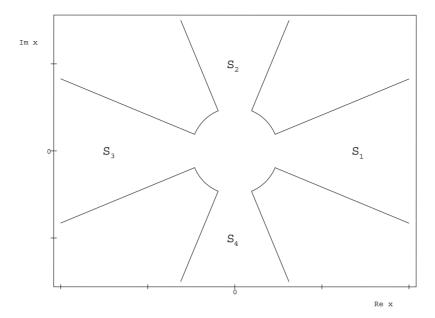


Figure 1. Permitted domain for sextic oscillators.

origin in field theory and is called \mathcal{PT} symmetry. In the quantum mechanical context the Hamiltonians H have to commute with the product of \mathcal{P} (parity) and \mathcal{T} (complex conjugation or time reflection) [5]. It is currently believed that this guarantees the reality of the spectrum for many non-Hermitian complex Hamiltonians [6].

In the very special class of these models $V(x) = x^2(ix)^{2\delta}$ the complex plane is to be cut upwards in order to keep the picture unique. Bender and Boettcher [4] started from the smallest exponents δ and picked up the lower sectors

$$S_L = (-3\Delta - \pi/2, -\Delta - \pi/2)$$
 $S_R = (\Delta - \pi/2, 3\Delta - \pi/2)$

with the half-width $\Delta = \pi/(4+2\delta)$. Of course, for any $\delta > 1/2$ there emerges an alternative pair of sectors

$$S_{L2} = (-5\Delta - \pi/2, -3\Delta - \pi/2)$$
 $S_{R2} = (3\Delta - \pi/2, 5\Delta - \pi/2)$

which has been used by Buslaev and Grecchi [7] in their study of asymptotically quartic potentials. In general, the latter possibility remains compatible with the current real coordinates in the interval of $\delta \in (1, 3)$.

For all the asymptotically power-law models the ambiguity of quantization is an interesting phenomenon. Numerically, this has been documented by several studies which made use of the limiting transition $\delta \to \infty$ [8] or of the absence of the cut at $\delta = 1, 2, \ldots$ [9]. An even simpler form of the δ dependence takes place at the positive integers $Z = 1 + \delta/2$ in the potentials $V(x) = x^{4Z-2} + \mathcal{O}(x^{4Z-3})$ since, asymptotically, their wavefunctions $\psi(x) \approx \exp(-x^{2Z}/2Z)$ are symmetric on the real line.

There appear the two new \mathcal{PT} symmetric pairs of sectors (S_L, S_R) at each odd value of the integer Z. Thus, the $\delta=4$ and Z=3 decadic oscillator is the first model with an ambiguity of this type. This is illustrated in figure 2 where the single left–right pair of the asymptotic boundary conditions of figure 1 is replaced by the triple choice. All three angles $\varphi_L \in S_{Lj}$ and $\varphi_R \in S_{Rj}$ with j=1,2 or 3 are equally compatible with the normalizability of the exponential

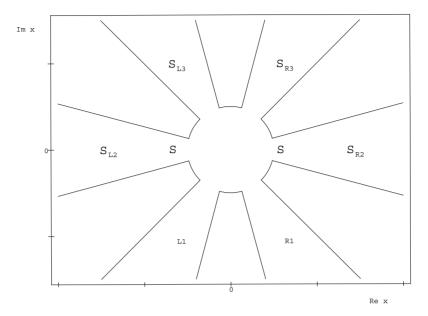


Figure 2. Permitted domain for decadic oscillators.

 $\psi(x) \approx \exp(-x^6/6)$. With this motivation we shall consider here all the decadic polynomial potentials complemented by a central spike:

$$V(r) = r^{10} + ar^8 + br^6 + cr^4 + dr^2 + f/r^2.$$
 (2)

These forces contain as many as five independent coupling constants and their real forms have been studied by several authors in the literature [10]. Here, we shall reconsider these 'spiked decadic' interactions within the generalized quantum mechanics of Bender $et\ al\ [5]$. It in effect weakens the current Hermiticity of the Hamiltonian to its mere \mathcal{PT} symmetry. For this reason one can construct more solutions in principle. We shall see below that such an expectation is well founded, indeed.

2. Decadic oscillators

The results of the study of Hermitian Hamiltonians with interactions (2) were summarized by Ushveridze in section 2.4 of his monograph [11] on the partially (so-called quasi-exactly) solvable models. This summary implies that the Hermitian decadic force lies somewhere in between the numerous purely numerical models (for which 'it seems absolutely unrealistic to find an exact solution' [11]) and quasi-exactly solvable models in the narrower sense (where one requires the algebraic solvability for a multiplet of K states at any pre-determined integer K).

The latter category (say, type-I QES) already lies quite close to the harmonic and other completely solvable models. Its properties are best exemplified by the standard Hermitian sextic model (cf equation (1.4.13) and related discussion in [11]). The former extreme, without any solvability, is usually illustrated by the Hermitian quartic oscillator (cf section 1.3 in [11]). In this comparison, the 'intermediate' decadic models (e.g. equation (2.4.5) in Ushveridze's book) admit merely a few (K) exact bound states with a strongly limited multiplicity $K \leq 5$ [10]. Such a property (let us call it QES of type II) is entirely trivial and can be easily illustrated for the first few K [12].

2.1. PT-symmetric regularization

The best illustration of the influence of the replacement of Hermiticity by the mere \mathcal{PT} symmetry of the Hamiltonian is provided by the popular quartic oscillators. In [13] these potentials were shown to belong to type I of the QES category. Obviously, \mathcal{PT} symmetry plays a crucial role in such an improvement of solvability.

The picture will be completed in what follows. We are going to demonstrate that a \mathcal{PT} symmetrization of equation (2) still leads to the maximal type-I form of the QES property. We shall see that, for the complexified decadic oscillators, the integer K may be chosen arbitrarily large. It is worth noting that the same enhanced solvability, admitting the arbitrarily large multiplets, remains freely applicable in any spatial dimension D.

In a preparatory step of the explicit constructions let us remind the reader that in any (= ℓ th) partial-wave projection the *D*-dimensional differential Schrödinger equation with a virtually arbitrary *regular* central potential is

$$\left[-\frac{d^2}{dr^2} + \frac{L(L+1)}{r^2} + V(r) \right] \psi(r) = E\psi(r) \qquad L = \ell + \frac{(D-3)}{2}.$$
 (3)

In a more general perspective, we can add a centrifugal-like spike to the regular force. This is known to preserve the exact solvability of the spiked harmonic oscillator [14]. In a close parallel, we do not need to change the notation too much, re-defining only the angular momenta L = L(f) in such a way that

$$L(L+1) = f + \left(\ell + \frac{D-3}{2}\right) \left(\ell + \frac{D-1}{2}\right). \tag{4}$$

As a consequence, equation (3) may be assigned a pair of independent solutions with the well known behaviour near the central singularity $\sim 1/r^2$:

$$\psi_1(r) \sim r^{-L(f)}$$
 $\psi_2(r) \sim r^{L(f)+1}$

In such a setting the 'forgotten possibility' of a suitable ansatz lies in the *simultaneous* use of both these solutions in the (complex) vicinity of the origin:

$$\psi(r) \sim C_1 r^{-L} [1 + \mathcal{O}(r^2)] + C_2 r^{L+1} [1 + \mathcal{O}(r^2)]. \tag{5}$$

A similar idea is slightly counterintuitive but it has already been used in several papers on the quartic oscillators with $\delta=1$. In 1993, Buslaev and Grecchi [7] paved the way by the mathematically rigorous example of the introduction of the complex coordinates for a problem of the present type. They achieved a regularization of the centrifugal spike by a constant imaginary shift of the real axis:

$$r = r(x) = x - i\varepsilon$$
 $x \in (-\infty, \infty)$ $\varepsilon > 0.$ (6)

This makes the centrifugal spikes smooth and fully regular at all x:

$$\frac{L(L+1)}{(x-\mathrm{i}\varepsilon)^2} = \frac{L(L+1)(x+\mathrm{i}\varepsilon)^2}{(x^2+\varepsilon^2)^2} = -\frac{L(L+1)}{\varepsilon^2} + \mathcal{O}(x^2).$$

A longer discussion of some consequences of this type of \mathcal{PT} -symmetric regularization has been provided by Znojil [14]. There, both the even and odd wavefunctions of the exactly solvable harmonic oscillator and other models were assigned their separate analytic continuations to the complex x. In accord with expectations, the spectrum of the energies remained real.

In this paper we shall try to follow the same pattern and imagine that the *two-term* ansatz (5) may remain compatible with the *single* Taylor-series expansion of $\psi(r)$ (say, in powers of r^2) whenever the ratio r^{L+1}/r^{-L} is itself equal to an integer power of r^2 . In other words, under a

suitable convention L+1 > -L, our key assumption will be L+1/2 = M where M can only be a positive integer, $M=1,2,\ldots$

We shall see below that this type of constraint will lead to significant simplification of the solutions as well as to their easier interpretation. Indeed, the trivial choice of f=0 implies that $M=\ell-1+D/2=1$. This mimics the four-dimensional s-wave or two-dimensional p-wave situation since, in both cases, L=1/2. Similarly we arrive at the alternative choice between the six-dimensional s-wave, four-dimensional p-wave or two-dimensional d-wave Schrödinger equation at M=2, etc.

2.2. Correct asymptotics and recurrences

In 1998, Bender and Boettcher [13] discovered the partial solvability of the \mathcal{PT} -symmetrized quartic polynomial oscillators. In the present language this means that they just employed the ansatz of the type (5) at the particular L=0. This has been accompanied by the asymptotically bent choice of the complex integration path $r \to r(x) \in \mathbb{C}$. In a way inspired by [7] the latter construction has been extended to all L in our recent remark [15].

It is amusing to summarize that, except for the pioneering sextic study [2] and its harmonic-oscillator simplification [4, 14], virtually all the available papers on the (partially) solvable $\mathcal{P}\mathcal{T}$ -symmetric polynomial potentials pay exclusive attention to the asymmetric models $V(r) \neq V(-r)$ of degree two [16] and four [7, 13, 15]. In this way all of them avoid the ambiguity problem but necessitate the complex couplings and acquire the counterintuitive property Im $V(t) \neq 0$, even on the real axis of coordinates t.

The unpleasant asymmetries disappear within the decadic model (2) which is such that V(r) = V(-r). Its asymptotic growth is also steeper than in the current solvable models [17]. In what follows, we are going to show that this model represents, in fact, the 'missing' last item in a list of all the quasi-exactly solvable polynomial models. The first step towards this not quite predictable result lies in the manifestly normalizable ansatz

$$\psi(r) = \exp\left(-\frac{r^6}{6} - \alpha \frac{r^4}{4} - \beta \frac{r^2}{2}\right) \sum_{n=0}^{N-1} h_n r^{2n-L}.$$
 (7)

The insertion of this formula converts our differential Schrödinger equation (3) into the *finite* set of recurrences:

$$A_n h_{n+1} + B_n h_n + C_n h_{n-1} + D_n h_{n-2} = 0$$
 $n = 0, 1, ..., N.$ (8)

The use of the asymptotically optimal WKB-inspired parameters

$$a = 2\alpha$$
 $b = \alpha^2 + 2\beta$ $c = c(N) = 2\alpha\beta + 2M - 4N - 2$

enables us to simplify the coefficients significantly:

$$A_n = (2n+2)(2n+2-2M) \qquad B_n = E - \beta(4n+2-2M)$$

$$C_n = \beta^2 - d - \alpha(4n-2M) \qquad D_n = 4(N+1-n).$$
(9)

This is the concise, linear algebraic formulation of our present problem.

3. Terminating solutions

The centrifugal spike in equation (3) binds the integers M to its strength $f \neq 0$ in a way prescribed by formula (4). This means that certain non-vanishing spikes can emerge as the simple functions of the dimension and angular momentum:

$$f = M^2 - (\ell - 1 + D/2)^2$$
.

In particular, the most elementary choice of D = M = 1 and $\ell = 0$ implies that we just have to fix f = 3/4. This value is, by the way, precisely equal to a boundary of a certain mathematical regularity domain (cf our recent remark [18] for more details).

3.1. Sturmian multiplets of couplings at M = 1

We may notice that, in accord with our definitions (9), two coefficients vanish completely, $A_{-1} = 0$ and $D_{N+1} = 0$. This is vital for the consistency of our ansatz (7). The third consequence of our assumptions is $A_{M-1} = 0$ and has no obvious interpretation. Seemingly, it is redundant. Let us now pay more attention to its crucial and beneficial role.

Starting from the first nontrivial choice of M=1 we get simply $A_0=0$. In such a case we can fix E=0 and discover that the whole over-determined set of our recurrences (8) degenerates to the mere square-matrix recipe. As long as $C_n=C_n(d)=\beta^2-\alpha(4n-2M)-d$ we can write

$$\begin{pmatrix}
C_{1}(0) & B_{1} & A_{1} \\
D_{2} & C_{2}(0) & \ddots & \ddots \\
& \ddots & \ddots & B_{N-2} & A_{N-2} \\
& & D_{N-1} & C_{N-1}(0) & B_{N-1} \\
& & & D_{N} & C_{N}(0)
\end{pmatrix}
\begin{pmatrix}
h_{0} \\
h_{1} \\
h_{2} \\
\vdots \\
h_{N-1}
\end{pmatrix} = d \cdot \begin{pmatrix}
h_{0} \\
h_{1} \\
h_{2} \\
\vdots \\
h_{N-1}
\end{pmatrix}.$$
(10)

We see that a more or less routine diagonalization of a four-diagonal matrix determines, in principle, the N different eigencouplings $d = d_k$ with k = 1, 2, ..., N. These values may be found numerically at an arbitrary N. In other words, the whole problem becomes quasi-exactly solvable of type I. This is our first important result.

It makes sense to introduce a shifted coupling $F = d - \beta^2 + 2N\alpha$. For the first few smallest dimensions $N \ge 0$ this simplifies the formulae and leads to the transparent implicit definitions of the shifted couplings F(d, N):

$$F = 0 N = 1$$

$$F^{2} + 16\beta - 4\alpha^{2} = 0 N = 2$$

$$-F^{3} + (16\alpha^{2} - 64\beta)F + 256 = 0 N = 3$$

$$F^{4} + (160\beta - 40\alpha^{2})F^{2} - 1536F + 144\alpha^{4} - 1152\beta\alpha^{2} + 2304\beta^{2} = 0 N = 4$$

$$-F^{5} + (80\alpha^{2} - 320\beta)F^{3} + 5376F^{2} + (8192\beta\alpha^{2} - 1024\alpha^{4} - 16384\beta^{2})F$$

$$+196608\beta - 49152\alpha^{2} = 0 N = 5 \dots$$

We may summarize that, at M=1, our solutions remain purely non-numerical up to degree N=4. In a sufficiently broad part of the (α, β) plane (or, if you wish, of the (a, b) plane of the octic and sextic coupling constants) the multiplets of exact and elementary bound states exist and are numbered by their (real) quadratic couplings d_n at any value of the multiplicity N.

3.2. Multiplets of energies at M=2

We have seen that our M=1 multiplets have been formed by the so-called Sturmian solutions. The role of their energy was marginal and fixed to the single value E=0. Returning now back to our main story we have to move to the next integer M=2. This replaces the abovementioned choice of E=0 (i.e. in effect, of $B_0=0$) by the virtually equally efficient simplification

$$\det\begin{pmatrix} B_0 & A_0 \\ C_1 & B_1 \end{pmatrix} = 0$$

which leads immediately to the compact formula

$$d = d(E) = \frac{E^2}{4} \qquad M = 2.$$

The insertion of this energy-dependent harmonic strength d returns us back to the square-matrix

$$A_n = (2n+2)(2n-2)$$
 $B_n = E - \beta(4n-2)$ $C_n = \beta^2 - E^2/4 - \alpha(4n-4)$

secular equation (10). With its three innovated diagonals $A_n = (2n+2)(2n-2)$ $B_n = E - \beta(4n-2)$ $C_n = \beta^2 - E^2/4 - \alpha(4n-4)$ it defines the spectrum E_n in a very similar manner as above, i.e. as roots of a certain polynomial. We can display its first nontrivial sample:

$$-E^{5} - 2\beta E^{4} + (-48\alpha + 8\beta^{2})E^{3} + (-96\beta\alpha + 192 + 16\beta^{3})E^{2} + (-256\beta - 512\alpha^{2} + 192\beta^{2}\alpha - 16\beta^{4})E$$
$$-1024\beta\alpha^{2} - 1280\beta^{2} + 4096\alpha - 32\beta^{5} + 384\beta^{3}\alpha = 0$$
$$M = 2 \qquad N = 3.$$

Its roots are not non-numerical anymore but three of them remain manifestly real at $\alpha = \beta = 0$ where their form remains closed, $(E_1, E_2, E_3) = (0, 0, \sqrt[3]{192})$. The consequent and precise specification of the whole domain of the reality of these roots remains as numerical a task as, say, its parallel studied in [13].

3.3. More complicated multiplets at M = 3, etc.

Explicit formulae with the integers $M \ge 3$ become appreciably more complicated. For all the really large truncations $N \gg M$ they may remain useful. Their derivation would proceed along the same lines as before. One starts from the general pre-conditioning requirement

$$\det\begin{pmatrix} B_0 & A_0 \\ C_1 & B_1 & A_1 \\ D_2 & C_2 & \ddots & \ddots \\ & \ddots & \ddots & B_{M-2} & A_{M-2} \\ & D_{M-1} & C_{M-1} & B_{M-1} \end{pmatrix} = 0$$
(11)

The shape to be inserted in the presumably much larger main secular determinant.

and its solutions have to be inserted in the, presumably, much larger main secular determinant

$$\det\begin{pmatrix} C_{1} & B_{1} & A_{1} \\ D_{2} & C_{2} & \ddots & \ddots \\ & \ddots & \ddots & B_{N-2} & A_{N-2} \\ & & D_{N-1} & C_{N-1} & B_{N-1} \\ & & & D_{N} & C_{N} \end{pmatrix} = 0.$$
 (12)

The procedure only becomes inefficient at the larger integers M. In such a setting it would be more appropriate to treat both the 'small' and 'large' secular equations (11) and (12) on an equal footing as a mutually coupled algebraic system.

In the $M \approx N$ setting one suddenly loses the main advantage of our present construction, viz. its reducibility to the single secular equation. In practice, one also has to replace the insertions of E or d by the use of the so-called Gröbner bases. The algorithm determines both d and E at once and is routinely provided by languages such as MAPLE [19].

Although the generalized M > 3 formulae and calculations need not necessarily become hopelessly complicated (and, in fact, give nice results, e.g., in the $M \to \infty$ limit [20]) their use would definitely require another motivation. Once we get that far, we would have no reason for maintaining our main assumption (4). At any real quantity M = 2L + 1 (reflecting a free variability of the coupling f) we would only have to replace the 'small' dimension Min equation (11) by the overall truncation N itself.

4. Concluding remarks

Results of our explicit constructions share their transparent algebraic character: mathematically, one eliminates the auxiliary or 'redundant' root of 'the simple' condition (11) and ends up with the single 'effective-Hamiltonian-like' square-matrix eigenvalue problem (12). This is the main merit (and general feature) of the QES systems of type I. Indeed, once we return to the explicit Hermitian decadic N=2 construction of section 2.4 in [11], we discover that, in the same language, the main shortcoming of the type-II QES constructions lies precisely in the necessity of solving $several\ coupled$ eigenvalue problems at once.

Our present sample non-numerical constructions available at the first few smallest integers M parallel, in fact, many other quasi-exactly solvable models. In particular, the Sturmian constant-energy form of the elementary multiplets characterized already the very first quasi-exactly solvable (namely Coulomb plus harmonic) model as discovered by Hautot [21]. A more complicated relation between the couplings and energies characterizes, for example, the partially solvable anharmonicities $\sim (1 + gr^2)^{-1}$ revealed by Flessas [22] and explained algebraically [23].

In this paper the most elementary multiplets using auxiliary integer M=1 proved purely Sturmianic. Their spike-shaped short-range part of the interaction $\sim f$ is not arbitrary and can only vanish in even dimensions. Vice versa, the emergence of a spike for our s-wave multiplets in three dimensions is reminiscent of the so-called conditionally solvable models where the choice of f=3/4 is obligatory [18].

At any auxiliary M, in comparison with all the Hermitian QES-I systems related to certain tridiagonal matrix representations of Lie algebras [24], all the decadic examples are distinguished by the four-diagonal and N-dimensional secular determinants (12). In the Hermitian setting this 'four-diagonality' was, in fact, the main reason of the restricted type-II solvability. We have shown that only the appropriate complexification can move the decadic systems to a higher, type-I QES group. At present, this group which exhibits the appealing \mathcal{PT} symmetry already encompasses the asymptotically decreasing quartic forces of Bender $et\ al\ [13,15]$ and the Coulomb + harmonic model [16].

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