

**Anomalous doublets of states  
in a  $\mathcal{PT}$  symmetric quantum model**

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Abstract

We complexify one of the Natanzon's exactly solvable potentials in  $\mathcal{PT}$  symmetric manner and discover that it supports the pairs of bound states with the same number of nodal zeros. This could indicate that the Sturm Liouville oscillation theorem does not admit an immediate generalization.

## I. FRAMEWORK: $\mathcal{PT}$ SYMMETRIC QUANTUM MECHANICS

Bound states in a smooth *real* potential  $V(x) \geq 0$  are most easily interpreted in the language of Sturm–Liouville theory [1]. Its oscillation theorems imply that the  $N$ -th bound state  $\psi_N(x)$  possesses  $N$  nodal zeros. Even the standard boundary conditions may be understood as the presence of an *additional* pair of zeros which are located at both ends of the interval of coordinates  $\mathcal{J} = (-\infty, \infty)$  in one dimension or of the radial axis  $\mathcal{J} = (0, \infty)$  in three dimensions.

A non-standard, additional constraint is only necessary for some strongly singular forces [2]. Unfortunately, the latter, mathematically rigorous requirement of the elimination of the irregular solutions may prove fairly counterintuitive and, for this reason, it is often being forgotten in practice. For illustration, we may recollect the paper on supersymmetry [3] which describes a singular map of the shifted harmonic oscillator. This example (attributed to A. Khare in Acknowledgements) is marred by a subtle violation of the boundary condition in the origin. A very similar inconsistency appears in the “conditionally exact” model by A. de Souza Dutra [4], in some phenomenological studies in quantum chemistry [5] etc.

An extensive clarification of the latter point may be found elsewhere [6]. In order to avoid similar misunderstandings, the underlying mathematics can be significantly simplified via analytic continuation (or even re-formulation) of the physical boundary conditions [7]. This is an innovative idea which proved unexpectedly fruitful. Recently, one of its more specific versions became a cornerstone of the so called  $\mathcal{PT}$  symmetric approach to quantum mechanics [8].

The latter formalism dispenses with the Hermiticity of the Hamiltonian  $H$  and keeps only a weaker requirement of the commutativity of  $H$  with the product of parity ( $\mathcal{P}x = -x$ ) and complex conjugation ( $\mathcal{T}i = -i$  which mimics the time reversal). The singular Schrödinger equations may be then regularized in the way which preserves the reality of the spectrum. Such a  $\mathcal{PT}$  symmetric non-Hermitization can be applied

easily to many solvable potentials, e.g., via a constant complex shift of the coordinate axis [9],

$$r = r(t) = t - i\varepsilon, \quad t \in (-\infty, \infty), \quad \varepsilon > 0. \quad (1.1)$$

This enables us, in essence,

- to work, more easily, with the analytic wave functions  $\psi(r)$  which prove available within the whole complex plane of  $r$ ,
- to return, whenever necessary, to the Hermitian Hamiltonian by means of the limiting transition  $\varepsilon \rightarrow 0$  and/or of a suitable selection of the additional constraints.

Both the one-dimensional and three-dimensional exactly solvable harmonic oscillators  $V^{(E)}(r) = \ell(\ell + 1)/r^2 + r^2$  with parity  $\ell = -1, 0$  or angular momentum  $\ell = 0, 1, \dots$ , respectively, become suddenly tractable on equal footing (details may be found in ref. [10]). In the three-body context of the so called Calogero's exactly solvable model [11], the same singular harmonic-oscillator-like differential equation and the same limiting transition  $\varepsilon \rightarrow 0$  reproduce the correct Hermitian solutions in spite of the utterly different physical origin and meaning of the singular term [12]. Via a modified transition to the Hermitian limit, another solvable model is revealed [13].

One can summarize that the  $\mathcal{PT}$  symmetric quantum mechanics offers a new approach to the explicit construction of bound states. It will be applied here to the potential

$$V(\xi) = \frac{3/4}{(1 - e^{2i\xi})^2} + \frac{2i\beta \exp(2i\xi)}{\sqrt{1 - e^{2i\xi}}} - \frac{C}{1 - e^{2i\xi}} \quad (1.2)$$

with certain unusual features. Already Singh and Devi [14] have noticed that it does not belong to the family of the shape invariant potentials. Dutt et al [15] emphasized

that this is the only existing nontrivial example of the conditionally exactly solvable potential. We have recently shown [16] that this exactly solvable potential of the Natanzon class [17] possesses a natural supersymmetric interpretation and offers a nontrivial opportunity of the rigorous study of its solutions near the singularity. The latter point proved in fact also the main motivation of our continuing interest in this example.

## II. THE METHOD: A CHANGE OF COORDINATES

In a way which dates back to the work of Liouville [18] one can change variables in the Schrödinger equation

$$\left[ -\frac{d^2}{dr^2} + V^{(E)}(r) \right] \psi^{(E)}(r) = E^{(E)} \psi^{(E)}(r) \quad (2.1)$$

using the recipe

$$r \rightarrow \xi = \xi(r), \quad \psi^{(E)}(r) \rightarrow \psi^{(D)}(\xi) = \sqrt{\xi'[r(\xi)]} \cdot \psi^{(E)}[r(\xi)]. \quad (2.2)$$

This generates the new differential equation of the similar form,

$$\left[ -\frac{d^2}{d\xi^2} + V^{(D)}(\xi) \right] \psi^{(D)}(\xi) = E^{(D)} \psi^{(D)}(\xi). \quad (2.3)$$

The explicit relationship between the two respective potentials is determined by the identity which is easily derived,

$$V^{(E)}(r) - E^{(E)} = [\xi'(r)]^2 \{ V^{(D)}(\xi) - E^{(D)} \} + \frac{3}{4} \left[ \frac{\xi''(r)}{\xi'(r)} \right]^2 - \frac{1}{2} \left[ \frac{\xi'''(r)}{\xi'(r)} \right]. \quad (2.4)$$

Once you postulate the solvability of the original equation (2.1) in terms of some known polynomials, it is possible to construct another exactly solvable equation by the suitable choice of the re-parametrization  $\xi(r)$ . Its special cases which mediate all the mutual canonical transformations between the *real* shape invariant potentials were listed in review [19] (cf., in particular, Figure 5.1 there).



Once we switch our attention to the non-Hermitian examples and retain the split of the shape invariant models into the Laguerre-solvable and Jacobi-solvable subsets (cf. Figure 5.1 of ref. [19] once more), we can easily parallel many of the above transformations. For the Laguerre-solvable subset, all the details may be found in refs. [20] and [21]. In a less exhaustive manner, the Jacobi-solvable shape invariant  $\mathcal{PT}$  symmetric family has been described in refs. [9] and [22]. One of the most striking features of some of the complexified changes of variables lies in the characteristic bent shape of the integration contours  $\xi$ . For illustration, let us recollect the implicit definition

$$\sinh r = -ie^{i\xi} \quad (2.5)$$

of the Hulthén-force generating function  $\xi = \xi(r)$  as employed in ref. [22]. Its straight-line input  $r = r_{(t)} = t - i\varepsilon$  with  $\varepsilon > 0$  becomes strongly deformed after the transition to  $\xi = \xi(r) = \xi(r_{(t)})$ .

In more detail, the left path could also inessentially be deformed, for the sake of simplicity, in such a way that  $\varepsilon = \varepsilon(t) \rightarrow 0$  for  $|t| \rightarrow \infty$ . This asymptotically modified contour of  $r = r_{(t)}$  avoids the upwards-running cut and comfortably coincides with the real line at both its asymptotic ends. It remains parametrized by  $t \in (-\infty, \infty)$  and defines the right-hand side bent curve  $\xi = \Omega - iZ$  via the pair of the real implicit equations

$$\begin{aligned} \sinh t \cos \varepsilon(t) &= e^Z \sin \Omega, \\ \cosh t \sin \varepsilon(t) &= e^Z \cos \Omega. \end{aligned}$$

Their explicit solution

$$\begin{aligned} \Omega_{(t)} &= \arctan \left[ \frac{\tanh t}{\tan \varepsilon(t)} \right] \in \left( \Omega_{(-\infty)}, \Omega_{(\infty)} \right) \equiv \left( -\frac{\pi}{2} + \varepsilon(-\infty), \frac{\pi}{2} - \varepsilon(\infty) \right), \\ Z_{(t)} &= \frac{1}{2} \ln \left[ \sinh^2 t + \sin^2 \varepsilon(t) \right] \end{aligned}$$

shows that the new curve  $\xi = \xi(t) = \Omega_{(t)} - iZ_{(t)}$  is arch-shaped and symmetric. It starts in a left imaginary minus infinity (at  $Z_{(-\infty)} \gg 1$ ) and ends in its right parallel

(with  $\Omega_{(\infty)} = \pi/2 - \varepsilon(\infty)$  and  $Z_{(\infty)} \gg 1$ ). Its top  $Z_{(0)} = \ln \sin \varepsilon < 0$  at  $t = \Omega_{(0)} = 0$  moves upwards in an inverse proportion to the decrease of the original shift  $\varepsilon(0) \rightarrow 0$ .

### III. PAIRS OF STATES WITH THE SAME $N$

In a search for a “new” solvable model  $V^{(D)}(\xi)$ , let us start from the complexified Schrödinger equation (2.1) defined on a complex contour  $r = r(t) = t - i\varepsilon(t)$ . We shall apply the change of the complex contours (2.5) to the complexified Eckart potential

$$V^{(E)}(r) = \frac{A(A-1)}{\sinh^2 r} - 2i\beta \frac{\cosh r}{\sinh r}, \quad \beta > 0. \quad (3.1)$$

Although our result will coincide (not surprisingly) with the above-mentioned shape-non-invariant potential (1.2), the mapping itself will be shown to exhibit certain very unusual and unexpected features.

In a preparatory step, the exact solvability of such a model may be most easily demonstrated via an auxiliary re-parametrization suggested in ref. [22],

$$\psi^{(E)}(r) = (y-1)^u (y+1)^v \varphi\left(\frac{1-y}{2}\right), \quad y = y(r) = \frac{\cosh r}{\sinh r} = 1 - 2z$$

with

$$4v^2 = 2i\beta - E, \quad 4u^2 = -2i\beta - E.$$

This leads to the new differential equation

$$z(1-z)\varphi''(z) + [c - (a+b+1)z]\varphi'(z) - ab\varphi(z) = 0 \quad (3.2)$$

which is completely solvable in terms of the Gauss hypergeometric series,

$$\varphi(z) = C_1 \cdot {}_2F_1(a, b; c; z) + C_2 \cdot z^{1-c} {}_2F_1(a+1-c, b+1-c; 2-c; z) \quad (3.3)$$

where

$$c = 1 + 2u, \quad a + b = 2u + 2v + 1, \quad ab = (u+v)(u+v+1) + A(1-A).$$

All the freedom of parameters becomes fixed by the boundary conditions  $\psi(\pm\infty) = 0$  which give  $b = -N$  and  $a = b \pm (2A - 1)$ . Jacobi polynomials  $P^{(\alpha,\beta)}(x)$  [23] enter the elementary formula for the wave functions,

$$\psi^{(E)}(r) = \left(\frac{1}{\sinh r}\right)^{u+v} e^{(v-u)r} \cdot P_N^{(u/2,v/2)}(\coth r). \quad (3.4)$$

These solutions remain normalizable if and only if

$$a = 2A - N - 1, \quad u + v = A - N - 1 > 0, \quad u - v = -i \frac{\beta}{A - N - 1}. \quad (3.5)$$

The model possesses  $N_{max} < A - 1$  bound states with the energies

$$E^{(E)} = -(A - N - 1)^2 + \frac{\beta^2}{(A - N - 1)^2}, \quad N = 0, 1, \dots, N_{max}. \quad (3.6)$$

We are prepared to transform this solution into its partner of eq. (2.3). It suffices to change variables via eq. (2.5). This replaces the Eckart problem (2.1) by the new Schrödinger equation (2.3). The implicit definition (2.4) of the new potential  $V^{(D)}(\xi)$  acquires a more explicit form

$$\begin{aligned} V^{(D)}(r) - E^{(D)} &= \frac{3}{4 \cosh^4 r} - \frac{1}{\cosh^2 r} \left[ N(N+1) + (2N+1)\delta_N + 1 + \frac{\beta^2}{\delta_N^2} \right] + \\ &+ \left( \frac{\beta^2}{\delta_N^2} - \delta_N^2 \right) + 2i\beta \frac{\sinh r}{\cosh r}, \quad \delta_N = A - N - 1 > 0. \end{aligned} \quad (3.7)$$

In the domain of the large  $|r| \gg 1$  this formula is dominated by the last two terms. Only the very last one depends on the sign of  $\text{Re } r$  so that the coupling  $\beta$  must be independent of  $N$  (we do not wish to have a state-dependent potential). We then determine (i.e., strictly speaking, remove the shift-ambiguity of) the energy  $E^{(D)}$  by the convenient requirement that  $V^{(D)}(\pm\infty)$  vanishes at  $\beta = 0$ . The other two asymptotically smaller components of  $V^{(D)}(\xi)$  are of the first and second order in  $1/\cosh^2 r(\xi)$ . Both of them must be also independent of  $N$  of course. In the first order this gives the strict rule

$$N^2 + N + 1 + (2N + 1)\delta + \beta^2/\delta^2 = \text{constant} (= C). \quad (3.8)$$

In the second order, the coefficient is equal to 3/4 and the condition remains trivial. We just confirmed that the replacement of  $r$  by  $r(\xi)$  transforms the Eckart potential (3.1) into its exactly solvable descendant (1.2), indeed.

During the re-construction of the potential  $V^{(D)}(\xi)$ , energies  $E_N^{(D)}$  and wave functions  $\psi_N^{(D)}(\xi)$  the auxiliary,  $N$ -dependent value of  $\delta = \delta_N = A - N - 1 > 0$  is to be determined as a root of the cubic equation (3.8). In Hermitian setting, the correct account of the physical boundary conditions makes this root unique [16]. In the generalized,  $\mathcal{PT}$  symmetric setting, the exceptional boundary condition in the origin becomes redundant. This is the reason why we have chosen our particular example. *A priori*, one may expect that the choice of the root  $\delta_N$  could be ambiguous.

In the light of our present construction, the latter expectation proves fulfilled. At the sufficiently large values of  $C \geq C_{min} > 0$  there exist three real roots  $\delta_N$ . Only one of them (viz., the negative one) can be eliminated as violating the asymptotic physical boundary conditions (i.e., the normalizability of the wave function). In contrast to the Hermitian case, two of the roots  $\delta = \delta^{(\pm)} = \delta_N^{(\pm)}(\beta, C) > 0$  of our cubic eq. (3.8) remain equally acceptable. At any number of nodal zeros  $N$ , each of them defines a separate energy level,

$$E = E_N^{(D)(\pm)} = \left( \delta_N^{(\pm)} + N + \frac{1}{2} \right)^2 + \frac{3}{4} - C. \quad (3.9)$$

The related  $\mathcal{PT}$  symmetric wave functions

$$\psi = \psi_N^{(D)}(\xi) = \sqrt{\xi' [r(\xi)]} \cdot \psi_N^{(E)} [r(\xi)]$$

are proportional to the same Jacobi polynomials as above,

$$\psi = e^{-i\delta\xi} \left[ 1 - e^{-2i\xi} \right]^{1/2} \left[ \sqrt{e^{2i\xi} - 1} - e^{i\xi} \right]^{i\beta/\delta} P_N^{([\delta-i\beta/\delta]/4, [\delta+i\beta/\delta]/4)} \left( \sqrt{1 - e^{-2i\xi}} \right).$$

This is the core of our present message. In the  $|t| \gg 1$  asymptotic regions we have  $\xi \approx -iZ \pm \pi/2$  with  $Z \gg 1$ . This re-confirms that both our series of wave functions  $\psi^{(\pm)}$  are asymptotically vanishing as  $\exp(-\delta^{(\pm)}Z)$ . For both the roots  $\delta = \delta_N^{(\pm)} > 0$ , they are safely normalizable.



## IV. DISCUSSION

The use of the commutativity  $[H, \mathcal{PT}] = 0$  complies with our intuitive expectations in the numerical setting [24] and in perturbation theory [25], in the WKB approximation [26] and in the supersymmetric context [27] as well as in the phenomenologically oriented field-theoretical studies [28]. In contrast, our present results form a paradox since the change of variables mediates an utterly unusual *one-to-two* correspondence between the two complex potentials. For the force  $V^{(D)}(\xi)$  this gives the two parallel series of bound states which must be distinguished by an additional, parity-type quantum number  $q = \pm 1$ . The nodal count  $N$  itself does not suffice to characterize the energy levels (3.9). This is a puzzling situation since we see no obvious reason for the introduction of  $q$ . One has to assume the existence of some unknown, hidden symmetry in our problem (2.3), but it is still necessary to accept the fact that this symmetry has to break down during an apparently innocent change (2.5) of the coordinates.

We can summarize that our above conclusions are to be added to the list of the “oddities” which emerge in  $\mathcal{PT}$  symmetric quantum mechanics due to its weaker boundary conditions. Let us just remind the reader that this is not in fact an isolated paradox. Our traditional intuition has already had really hard times with the unavoided level crossings in ref. [10], with the decrease of the energy with  $N$  in ref. [20], with the high excitations caused by a weak potential in refs. [29] etc. Thus, just another item is provided by our present example.

We may formulate our tentative conclusion that the  $\mathcal{PT}$  symmetric deformations of the integration paths can in fact destroy the (*a priori*, plausible) similarity between the complex and ordinary parity. One of the most important implications is that any future appropriate generalization of the Hermitian Sturm–Liouville oscillation theorems will be necessarily not entirely trivial. Also the closely related concept of the completeness of states [30] must be dealt with an exceptional care in any future

development of the  $\mathcal{PT}$  symmetric quantum mechanics. We might point out that the similar words of warning have been recently issued also on the purely numerical basis [31].

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