Conditions for complex spectra in a class of $\mathcal{PT}$ symmetric potentials

Géza Lévali

Institute of Nuclear Research of the Hungarian Academy of Sciences, PO Box 51, H–4001 Debrecen, Hungary

Miloslav Znojil

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

Abstract

We study a wide class of solvable $\mathcal{PT}$ symmetric potentials in order to identify conditions under which these potentials have regular solutions with complex energy. Besides confirming previous findings for two potentials, most of our results are new. We demonstrate that the occurrence of conjugate energy pairs is a natural phenomenon for these potentials. We demonstrate that the present method can readily be extended to further potential classes.

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1 e-mail: levai@moon.atomki.hu
2 e-mail: znojil@ujf.cas.cz
1 Introduction

According to a rather elementary result of quantum mechanics, bound states in a real potential well have real eigenvalues, and the corresponding eigenfunctions are normalizable. Recently it was shown [1] that real energy eigenvalues can appear in one-dimensional complex (non-Hermitian) potentials if the Hamiltonian is $\mathcal{PT}$ symmetric, i.e. it is invariant under simultaneous space ($\mathcal{P}$) and time ($\mathcal{T}$) reflection. The kinetic energy term $(2m)^{-1}p^2$ is obviously invariant under this transformation, while for the potential term $V^*(-x) = V(x)$ is postulated.

The first $\mathcal{PT}$ invariant potentials have been studied using perturbation methods [2, 3] and numerical experiments. [4, 5, 6, 7] Later on, a number of solvable models have been identified, typically as the complexified versions of solvable problems of quantum mechanics. They included the complex square well [8, 9] and all the shape-invariant [10] (plus some Natanzon-class) [11] potentials. [12, 13, 14, 15, 16, 17] In these cases the existence of real energy eigenvalues has been confirmed, however, no consistent explanation has been given for this phenomenon. The reality of the spectra has been interpreted in terms of certain analytic, [3, 18] Lie-algebraic [19, 20] and perturbative [2, 21] arguments.

One has to note that in conventional (i.e. non-$\mathcal{PT}$ symmetric) quantum mechanics the energy eigenvalues in complex potentials are usually complex. The conditions for the energies Re($E$) < 0 and for the regularity of the corresponding state cease to come together, as it can be demonstrated in a simple solvable model [22]. It turned out that also the $\mathcal{PT}$ invariance of the potentials does not necessarily lead to the completely real spectrum, and complex-energy solutions have been constructed. Since in this case the Hamiltonian retains $\mathcal{PT}$ symmetry, while the wavefunctions do not, this phenomenon has been interpreted as the spontaneous breakdown of $\mathcal{PT}$ symmetry. Examples have been found in a quasi-exactly solvable potential [23] and among shape-invariant potentials with a strong non-Hermiticity. [24, 25]
These findings obviously raised the question whether it is possible to formulate some criteria for the appearance of complex-energy solutions in the generic $\mathcal{PT}$ symmetric potential. No general answer has been given to this question yet, rather the conditions varied in each case.

Motivated by the developments above, here we analyze a rather general family of $\mathcal{PT}$ symmetric solvable potentials to identify conditions under which these potentials support regular complex-energy solutions. We focus on potentials which, in conventional quantum mechanics, are called shape-invariant, and which contain the majority of the most well-known textbook examples. These potentials can easily be made $\mathcal{PT}$ symmetric by complexifying them after setting some of their parameters to imaginary values.

In this respect a particularly interesting parameter is an imaginary coordinate shift $x \to x + i\epsilon$. This transformation played a key role in converting most of the real potentials into $\mathcal{PT}$ symmetric ones, because it cancelled singularities (e.g. at the origin) which allowed the extension of radial and periodic problems to the full $x$ axis. In conventional quantum mechanics (real) coordinate shifts are usually irrelevant to the problem, as they do not influence the solutions and energy eigenvalues. In $\mathcal{PT}$ symmetric quantum mechanics, however, imaginary coordinate shifts have a special role. They can be interpreted in two ways. On the one hand, shifting potentials to lines parallel to the $x$ axis represent a special case of the procedure by which $\mathcal{PT}$ symmetric potentials are defined on various contours of the complex plane, along which the solutions are regular. On the other hand, however, for these relatively simple solvable cases the potential functions can be rewritten in such a way that the coordinate shift $\epsilon$ appears in the coupling coefficients, and the whole problem can still be though of as a potential defined on the $x$ axis.

We use a simple method based on variable transformations to derive the potentials mentioned above. This method was found especially suited to the analysis of the $\mathcal{PT}$ symmetrized versions of some shape-invariant potentials, partly because
the imaginary coordinate shift appears in it in a natural way. [17]

2 Derivation of the potentials by variable transformation

Our procedure is a variable transformation \( x \rightarrow z(x) \), which takes the Schrödinger equation

\[
\frac{d^2 \psi}{dx^2} + (E - V(x))\psi(x) = 0 \tag{1}
\]

into the second-order differential equation

\[
\frac{d^2 F}{dz^2} + Q(z)\frac{dF}{dz} + R(z)F(z) = 0 \tag{2}
\]

with known solutions. Typically, \( F(z) \) is a special function of mathematical physics. Selecting \( F(z) \) (and with it, the \( Q(z) \) and \( R(z) \) functions too), and introducing the \( z(x) \) re-scaling one can define a solvable potential,

\[
E - V(x) = \frac{z''(x)}{2z'(x)} - \frac{3}{4} \left( \frac{z''(x)}{z'(x)} \right)^2 + (z'(x))^2 \left( R(z(x)) - \frac{1}{2} \frac{dQ(z)}{dz} - \frac{1}{4} Q^2(z(x)) \right). \tag{3}
\]

The solutions can then be expressed in terms of \( Q(z) \) and \( R(z) \) defining the special function \( F(z) \), and the \( z(x) \) function controlling the variable transformation:

\[
\psi(x) \sim (z'(x))^{-\frac{i}{2}} \exp \left( \frac{1}{2} \int^{z(x)} Q(z)dz \right) F(z(x)). \tag{4}
\]

This old method [26] has been applied in a systematic search for shape-invariant potentials in the Hermitian context in Ref. [27] where the \( F(z) \) special function was chosen as an orthogonal (viz., Jacobi, generalized Laguerre and Hermite) polynomial. The \( z(x) \) function governing the variable transformation was then determined from the direct integration of a first-order differential equation obtained from the condition that some term on the right-hand side of Eq. [3] has to account for the constant
(energy) term on its left-hand side. This requirement leads to a first-order differential equation for \( z \) of the type

\[
\left( \frac{dz}{dx} \right)^2 \phi(z) = C,
\]

where \( \phi(z) \) is a function of \( z \) originating from \( Q(z) \) and \( R(z) \). Its general solution is given by

\[
\int \phi^{1/2}(z)dz = C^{1/2}x + \delta,
\]

where, in contrast to Hermitian problems, the constant of integration plays a special role for \( \mathcal{PT} \) symmetric systems as the imaginary coordinate shift. \[17\] However, similarly to the Hermitian case, this coordinate shift has no effect on the energy eigenvalues. A further important implication of this method is that the transformation properties of the \( z(x) \) function under the \( \mathcal{PT} \) operation can easily be established, which facilitates the enforcement of \( \mathcal{PT} \) symmetry on the potential \( V(x) \) in Eq. (3).

In this way whole classes of potentials can be treated on an equal footing.

Here we specify the method for the Jacobi and the generalized Laguerre polynomials by choosing \( Q(z) = (\beta - \alpha)(1 - z^2)^{-1} - (\alpha + \beta + 2)z(1 - z^2)^{-1} \), \( R(z) = n(n + \alpha + \beta + 1)(1 - z^2)^{-1} \) and \( Q(z) = -1 + (\alpha + 1)/z \), \( R(z) = n/z \), respectively. In what follows we occasionally make reference to the a previous study in which conditions have been derived for having real spectra of the same \( \mathcal{PT} \) symmetric potentials. \[17\].

2.1 The PI potential family

The generic form of the shape-invariant PI type potentials (which are known as type A potentials elsewhere \[28, 27\]) and their energy spectrum is

\[
E - V(x) = C \left( n + \frac{\alpha + \beta + 1}{2} \right)^2 + \frac{C}{1 - z^2(x)} \left[ \frac{1}{4} - \left( \frac{\alpha + \beta}{2} \right)^2 - \left( \frac{\alpha - \beta}{2} \right)^2 \right] - \frac{2Cz(x)}{1 - z^2(x)} \left( \frac{\alpha + \beta}{2} \right) \left( \frac{\alpha - \beta}{2} \right).
\]
This is obtained from (3) by substituting the appropriate form of $Q(z)$ and $R(z)$ and setting $\phi(z) = (1 - z^2)^{-1/2}$ in (3). As discussed in, [17] the four different solutions $z(x)$ of (6) are obtained as hyperbolic and trigonometric functions and are either invariant under the $\mathcal{PT}$ operation, or change their sign. The six PI type $\mathcal{PT}$ symmetric potentials and the energy eigenvalues are listed in the first six lines of Table 1, along with the conditions under which the eigenvalues are complex and the corresponding solutions are regular. These potentials are obtained from (7) by setting $z(x)$ and $C$ to $i \sinh(ax + i\epsilon)$, $\cosh(ax + i\epsilon)$, $\cosh(2ax + i\epsilon)$, $\cos(ax + i\epsilon)$, $\cos(2ax + i\epsilon)$, $\sin(ax + i\epsilon)$ and $C = -a^2, -a^2, -4a^2, a^2, 4a^2, a^2$.

Let us discuss the details with the example of the potential appearing in the first line,

$$V(x) = -\left(\frac{\alpha^2 + \beta^2}{2} - \frac{1}{4}\right) \frac{a^2}{\cosh^2(ax + i\epsilon)} - ia^2 \left(\frac{\alpha^2 - \beta^2}{2}\right) \frac{\sinh(ax + i\epsilon)}{\cosh^2(ax + i\epsilon)}.$$  \hspace{1cm} (8)

(It Table 1 we used $a = 1$ everywhere for simplicity.) This potential remains non-singular in the limit $\epsilon \to 0$. Specifying the generic form of the solution (4) for this case we find that it is regular for $x \to \pm \infty$ (i.e. $|z| \to \infty$) if $n < -\frac{1}{2}[\text{Re}(\alpha + \beta) + 1]$ holds, while regularity for $x \to 0$ ($z \to \pm 1$) requires $\epsilon \neq \frac{\pi}{2} \pm k\pi$. Combining these with the conditions $\alpha^* = \pm \alpha, \beta^* = \pm \beta$ securing $\mathcal{PT}$ symmetry of the potential [17] and the requirement of having complex energy eigenvalues we find that to satisfy all these criteria, either $\alpha$ or $\beta$ has to be imaginary, and also we need $\epsilon \neq \frac{\pi}{2} \pm k\pi$, as displayed in Table 1.

This potential has also been analyzed in [24] for the special case of $\epsilon = 0$. There it is underlined that complex energies appear if $|V_2| > V_1 + \frac{1}{4}$ holds, where $V_1$ and $V_2$ are the coefficients of the real and the imaginary parts of the potential. This agrees with our results (for $\epsilon = 0$), according to which either $\alpha$ or $\beta$ has to be imaginary, since $-|V_2| + V_1 + \frac{1}{4}$ equals to the square of the imaginary parameter (i.e. $\alpha^2$ or $\beta^2$) and is always negative. If both $\alpha$ and $\beta$ are imaginary, then the solutions become irregular for $|z| \to \infty$, while if both of them are real, then the energy eigenvalues become real.
For \( \epsilon \neq 0 \) the two potential terms both become complex, so the decomposition of the potential into real and imaginary component is less trivial. We only note that for \( \epsilon = \frac{\pi}{2} \pm k\pi \) the potential becomes the real version of the singular generalized Pöschl–Teller potential, corresponding to the case denoted with PI(cosh(ax + i\epsilon)), setting \( \epsilon = 0 \).

The conditions are rather similar to the other type PI potentials, with the exception that for the trigonometric potentials the regularity requirement of the solutions \( \psi_n(x) \) at \( |z| \to \infty \) is irrelevant, and therefore the principal quantum number \( n \) can take any number, i.e. these potentials have infinite bound states. It has to be noted that further analysis of the boundary conditions is necessary if these trigonometric potentials are \textit{defined} to be periodic by extending them to the full \( x \) axis. \[6, 29\]

### 2.2 The PII potential family

The PII (or type E \[28, 27\]) potentials are obtained in a similar way, taking \( \phi(z) = (1 - z^2)^{-1} \) in (5). The four \( \mathcal{PT} \) symmetric potentials belonging to this class are again characterized by \( z(x) \) functions of the hyperbolic or trigonometric type, which are either invariant under the \( \mathcal{PT} \) operation or change sign. The generic form of the potential and the energy spectrum for this class is

\[
E - V(x) = -C \left[ \left( \frac{\alpha + \beta}{2} \right)^2 + \left( \frac{\alpha - \beta}{2} \right)^2 \right] - 2C \left( \frac{\alpha + \beta}{2} \right) \left( \frac{\alpha - \beta}{2} \right) z(x) + C \left( n + \frac{\alpha + \beta}{2} \right) \left( n + \frac{\alpha + \beta}{2} + 1 \right) (1 - z^2(x)) \,.
\]

With a parameter transformation \( s = n + (\alpha + \beta)/2 \) and \( \Lambda = \frac{\alpha - \beta}{2} \frac{\alpha + \beta}{2} \) the dependence on \( n \) can be shifted to the constant (energy) term, leading to the potential function

\[
V(x) = -Cs(s + 1)(1 - z^2(x)) - 2C\Lambda z(x) \,.
\]

and the \( E = -C[(s - n)^2 + \Lambda^2(s - n)^{-2}] \) energy formula. The four \( \mathcal{PT} \) symmetric PII type potentials are again displayed in lines seven to ten in Table 1. These are
obtained from \([10]\) by choosing \(z(x) = \tanh(ax + i\epsilon), \coth(ax + i\epsilon), -i\cot(ax + i\epsilon), i\tan(ax + i\epsilon); C = a^2, a^2, -a^2, -a^2;\) and \(\Lambda = i\lambda, i\lambda, -\lambda\) and \(\lambda\).

As an example, let us analyse in more detail the hyperbolic Rosen–Morse potential obtained for \(z(x) = \tanh(ax + i\epsilon),\)

\[
V(x) = -a^2 \frac{s(s + 1)}{\cosh^2(ax + i\epsilon)} - 2i\lambda a^2 \tanh(ax + i\epsilon).
\]

(11)

(We used \(a = 1\) in Table 1 for these potentials too, for simplicity.) This potential is \(\mathcal{PT}\) invariant, if \(\lambda\) is real, and \(s\) is either real or it is complex, with Re\((s) = -1/2\). [17]

From Table 1 we then read that complex energies can appear only in this latter case, i.e. if \(s = -\frac{1}{2} + i\sigma\). However, this contradicts the regularity requirement for the solutions at \(z \to \pm 1\), which allows regular solutions only for real values of \(s\), therefore we conclude that this potential cannot support complex-energy solutions. This is not surprising, at least for \(\epsilon = 0\), since then \(s(s + 1) = -\sigma^2 - \frac{1}{4}\), i.e. the first (real) term of the potential is repulsive. For \(\epsilon \neq 0\) the situation is less clear, in a way similar to the PI type potentials.

With the exception of the above two examples, the potentials in Table 1 have singularities, and they can be regularized only with the use of the non-vanishing imaginary coordinate shift \(i\epsilon\). Otherwise, the detailed discussion is rather similar for these potentials, except that the requirements are again more relaxed for the trigonometric potentials, so complex-energy solutions are possible in those cases.

2.3 The LI potential family

Potentials related to the generalized Laguerre polynomials are obtained by setting \(Q(z) = -1 + (\alpha + 1)/z\) and \(R(z) = n/z\). Setting \(\phi(z) = z^{-1/2}\) in (3), the type LI potential, i.e. the harmonic oscillator is obtained (which is referred to as the type C family elsewhere. [28, 27]) The \(\mathcal{PT}\) symmetric version of this problem is obtained using the complex \(z(x) = \frac{C}{4}(x + i\epsilon)^2\) function. (We note that due to the particular form of the solutions [14], the imaginary coordinate shifts do not lead to normalizable
states for the other two shape-invariant potentials related to the generalized Laguerre polynomials, the LII (or type F [28, 27]) Coulomb and the LII (or type B [28, 27]) Morse potentials, so these have to be defined on more sophisticated contours of the complex plane. [15, 16])

The \( \mathcal{PT} \) symmetric harmonic oscillator is then obtained from the current version of (3) as

\[
E - V(x) = C\left(n + \frac{\alpha + 1}{2}\right) - \frac{C}{4} z(x) - \frac{C}{4z(x)} \left(\alpha^2 - \frac{1}{2}\right),
\]

if \( \alpha \) is real or imaginary. [17] Using the notation \( C = 2\omega \) one gets the familiar form of the potential displayed in the last line of Table 1. Its solutions are necessarily regular asymptotically (for \(|z| \to \infty\)) and also at \( x \to 0 \), if \( \epsilon \neq 0 \) holds. Complex-energy solutions emerge if \( \alpha \) is imaginary, provided that the singularity of the potential is cancelled by taking \( \epsilon \neq 0 \). This induces a finite and attractive centrifugal term with complex angular momentum. This again agrees with the findings of Refs. [14, 25]

3 Conclusions

In conclusion, we have reviewed a wide class of \( \mathcal{PT} \) symmetric potentials and specified conditions under which they can support complex-energy solutions. For this we had to combine various requirements for the potential parameters. In some cases these requirements contradict each other, so no such potentials can exist. Our results agree with those of Ref. [25] for the harmonic oscillator, and contain the findings of Ref. [24] as a special case. All our other results are new.

A general feature of the present potential class is that the functional form of the potentials depends on the squares of the potential parameters which can take on imaginary values (i.e. \( \alpha, \beta, i\sigma \)), therefore the potentials are insensitive to the sign of this parameter. However, this sign appears explicitly in the energy formulae as the sign of the imaginary component of the energy, thus the occurrence of complex
conjugate energy pairs is a necessity. From the structure of the energy formulae it is apparent that depending on the potential parameters, the energy eigenvalues of these potentials either all real or complex, so they practically do not occur together at the same time. It can be noted, however, that it might be possible to make a single energy eigenvalue real by “fine tuning” the potential parameters such that the principal quantum number \( n \) is cancelled by the real part of the potential parameters and the numerical constants.

Further systematic studies of the same potentials can be planned to find real spectra in complex potentials that do not fulfill \( \mathcal{PT} \) symmetry. Such potentials have been sought, \(^8, \, 30\) and the present method seems rather appropriate for such purposes. As a further possibility, a similar study of \( \mathcal{PT} \) symmetric potential defined on bent contours of the complex \( x \) plane represents a challenging task.

We note that the present formalism is applicable to potentials beyond the shape-invariant class. In particular, some “implicit” potentials belonging to the Natanzon class \(^1\) can be made \( \mathcal{PT} \) symmetric, \(^17\) and the conditions for real- or complex-energy regular solutions can be derived. As an example we mention the potential in Ref. \(^31\), which had been introduced as conditionally exactly solvable. Later it was shown that it is just an element of the exactly solvable Natanzon potential class. \(^32\) The energy eigenvalues of this potential are obtained from a cubic algebraic equation. The complexified \( \mathcal{PT} \) symmetric version of this potential has been studied, \(^33\) and in the present context the interpretation of the complex roots of the cubic equation seems a rather intriguing question.

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Table 1: Solvable potentials with spontaneous $\mathcal{PT}$—symmetry breaking.

| $V(x)$                                                                 | $E_n$                                      | Complex-energy solutions                                                                 |
|-----------------------------------------------------------------------|--------------------------------------------|----------------------------------------------------------------------------------------|
| $-\frac{2(\alpha^2+\beta^2)-1}{4 \cosh^2(x+i\epsilon)} - \frac{(\alpha^2-\beta^2)\sinh(x+i\epsilon)}{2 \cosh(x+i\epsilon)}$ | $-\left(n + \frac{\alpha+\beta+1}{2}\right)^2$ | $\alpha$ or $\beta$ imaginary, $\epsilon \neq \frac{\pi}{2} \pm k\pi$                |
| $\frac{2(\alpha^2+\beta^2)-1}{4 \sinh^2(x+i\epsilon)} + \frac{(\alpha^2-\beta^2) \cosh(x+i\epsilon)}{2 \sinh(x+i\epsilon)}$ | $-\left(n + \frac{\alpha+\beta+1}{2}\right)^2$ | $\alpha$ or $\beta$ imaginary, $\epsilon \neq k\pi$                                   |
| $-\frac{4\beta^2-1}{4 \cosh^2(x+\frac{i}{2}\epsilon)} + \frac{4\alpha^2-1}{4 \sinh^2(x+\frac{i}{2}\epsilon)}$ | $-(2n + \alpha + \beta + 1)^2$ | $\alpha$ or $\beta$ imaginary, $\epsilon \neq k\pi$                                   |
| $\frac{2(\alpha^2+\beta^2)-1}{4 \sin^2(x+i\epsilon)} + \frac{(\alpha^2-\beta^2) \cos(x+i\epsilon)}{2 \sin^2(x+i\epsilon)}$ | $\left(n + \frac{\alpha+\beta+1}{2}\right)^2$ | $\alpha$ and/or $\beta$ imaginary, $\text{Im}(\alpha + \beta) \neq 0$, $\epsilon \neq 0$ |
| $\frac{4\beta^2-1}{4 \cos^2(x+\frac{i}{2}\epsilon)} + \frac{4\alpha^2-1}{4 \sin^2(x+\frac{i}{2}\epsilon)}$ | $(2n + \alpha + \beta + 1)^2$ | $\alpha$ and/or $\beta$ imaginary, $\text{Im}(\alpha + \beta) \neq 0$, $\epsilon \neq 0$ |
| $\frac{s(s+1)}{\cosh(x+i\epsilon)} - 2i\lambda \tanh(x+i\epsilon)$ | $-(s-n)^2 + \frac{\lambda^2}{(s-n)^2}$ | no such solutions                                                                      |
| $\frac{s(s+1)}{\sinh(x+i\epsilon)} - 2i\lambda \coth(x+i\epsilon)$ | $-(s-n)^2 + \frac{\lambda^2}{(s-n)^2}$ | no such solutions                                                                      |
| $\frac{s(s+1)}{\sin^2(x+i\epsilon)} - 2i\lambda \cot(x+i\epsilon)$ | $(s-n)^2 + \frac{\lambda^2}{(s-n)^2}$ | $s = -\frac{1}{2} + i\sigma$, $\epsilon \neq 0$                                        |
| $\frac{s(s+1)}{\cos^2(x+i\epsilon)} + 2i\lambda \tan(x+i\epsilon)$ | $(s-n)^2 + \frac{\lambda^2}{(s-n)^2}$ | $s = -\frac{1}{2} + i\sigma$, $\epsilon \neq 0$                                        |
| $\frac{\omega^2}{4} (x + i\epsilon)^2 + (\alpha^2 - \frac{1}{4}) \frac{1}{(x+i\epsilon)^2}$ | $2\omega(n + \frac{\alpha+1}{2})$ | $\alpha$ imaginary, $\epsilon \neq 0$                                               |