COMPLEX POTENTIALS WITH REAL EIGENVALUES AND THE INVERSE PROBLEM

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Abstract. The existence of complex potentials with real eigenvalues rises two questions. The first one concerns the determination of the local real equivalent potentials. The second one underlines the fact that any even potential with respect to \( x \) in the one-dimensional \( (D = 1) \) space has at least two complex partners with the same spectrum. The present paper illustrates this situation with a few examples.

Key words: Quantum mechanics; bound states; complex \( \mathcal{P}\mathcal{T} \)-symmetric potentials.

1. INTRODUCTION

The advent and the use of non-Hermitian potentials have brought new insights in quantum mechanics. It offers the possibility to describe physical systems within the Schrödinger equation formalism in a more complex way than with usual Hermitian cases. Let us quote, for instance, the energy dependent potentials [1, 2]. They allow to account for relativistic effects or the influence of the medium on elementary interactions.

The complex potentials have been considered since a long time in scattering theory, to treat the flux absorption (among many textbooks, see, for instance, the earlier ones by Newton and by Jackson [3, 4]). However, the discovery of complex potentials with real eigenvalues has opened a new and rich domain of applications. It touches various domain of physics. Here, we simply refer the reader to the papers by Bender [5] and by Mihalache et al. [6, 7], which give good overviews of the situation. At the same time, this class of potentials brings questions concerning the determination of a potential from the data. This is the subject we want to discuss in the present paper by considering the inverse problem.

In a succession of papers, we have developed a method to determine a real potential from its discrete spectrum [8–10]. The accuracy of the answer depends on the number of known excited states. An exact and unique solution is reached as this number tends to infinity. In this limit, the determination is free from ambiguities.

However, the advent of complex potentials with real eigenvalues changes the situation with respect to the uniqueness of the potential. It brings interesting ques-
tions. The first one concerns the existence and determination of a real potential having the same spectrum as the complex one. Inversely, we may ask if a real potential has one or several complex partners with the same real eigenvalues.

It is the purpose of the present paper to investigate these two questions. The work is restricted to the one-dimensional ($D = 1$) space. A couple of $P\mathcal{T}$-symmetric potentials are studied in Sec. 2. In Sec. 3, we discuss the existence of complex partners to real potential. Conclusions are drawn in Sec. 4.

2. COMPLEX POTENTIALS WITH A REAL DISCRETE SPECTRUM

The existence of complex potentials with real eigenvalues has appeared on the scene about 20 years ago. It started with a conjecture by D. Bessis (see the note quoted by Bender and Boettcher [11]). It gave rise to numerous works, few of the earlier ones are listed in the references [12–18]. We recall the general reviews by Bender and and Mihalache et al. in Refs. [5–7].

In the case of a complex potential with real eigenvalues, the question arises of the real equivalent potential. To our knowledge, this problem has not retained attention. For simple cases, the answer is rather trivial, but it may be interesting to look at it in a general view.

We consider the Schrödinger equation

$$\left[ -\frac{d^2}{dx^2} + V(x) + iW(x) \right] \psi_n(x) = E_n \psi_n(x).$$

(1)

The conditions to ensure $E_n$ to be real have been studied in many papers. The first cases were found for potential invariant under $P\mathcal{T}$ transformation ( $x \rightarrow -x; i \rightarrow -i$). However the $P\mathcal{T}$ symmetry can be spontaneously broken, leading to complex energies. Moreover, it does not constitute a necessary condition, as shown by Cannata et al. [14], as well as by Ahmed [19].

Given the real eigenvalues $E_n$ of a complex potential, the determination of its real equivalent potential $U(x)$ follows the same rules as for the ordinary real case. A unique answer is obtained if the number of known eigenvalues tends to infinity. Another condition is the excitation energies,

$$\Delta(n) = E_n - E_0,$$

(2)

to be discrete values of a continuous function of $n$ (see Appendix).
2.1. ANALYTICAL CASES

It is convenient to quote a few analytical examples. The harmonic oscillator studied by Znojil [13] provides us with a trivial but illustrative case. Consider

\[ V(x) + iW(x) = x^2 - 2icx - c^2 + \frac{\alpha^2 - 1/4}{(x - ic)^2}, \]

with \( \alpha > 0 \). The eigenvalues are given by

\[ E_{q,n} = 4n + 2 - 2q\alpha. \]

Here \( q = \pm 1 \) is a parity index corresponding to the two sets of acceptable solutions. Obviously the real equivalent potential is a shifted harmonic oscillator.

Similarly, extensions of the Pöschl-Teller potential have been solved by Ahmed and Znojil [13, 19], respectively. The eigenvalues follow the form of the Pöschl-Teller spectrum.

Let us consider also the Morse potential proposed by Ahmed [19]:

\[ V(x) + iW(x) = (a + ib)^2e^{-2x} - (2c + 1)(a + ib)e^{-x}. \]

This potential is not \( \mathcal{PT} \) symmetric, but it generates a real spectrum.

In the domain of coupling constants leading to bound states of real energy, the eigenvalues can be expressed by

\[ E_n \propto -[\lambda - 1 - n]^2, \quad n \leq \lambda - 1. \]

The connection to an equivalent real Pöschl-Teller potential is immediate.

Actually, this equivalence at the spectrum level has roots in the fact that both the Morse and Pöschl-Teller are representations of the \( \text{SO}(2,1) \) algebra, as shown by Wu and Alhassid [20, 21]. Considering the real case \( (b = 0) \), the solutions of the Morse potential lie in \( 0 \leq x \leq \infty \), while those of the Pöschl-Teller potential extend over the whole \( x \) axis. This situation suggests that every real potential with solutions on the positive \( x \) axis has for partner an even potential giving the same spectrum.

2.2. A QUALITATIVE DETERMINATION

The next example is provided us by the potential

\[ V(x) + iW(x) = e^{2ix} \]

studied by Cannata et al. [14]. These authors found two types of solutions with real eigenvalues. We discard here solutions corresponding to “perforated” spectra, as they don’t fulfill the continuity condition of the excitation energies. So we are left with the particular case

\[ E_n \propto -[n + \frac{1}{2}]^2. \]
It corresponds to a \( n(n+1) \) spectrum shifted by a constant. In the \( D \geq 2 \) such spectra arise from the attractive delta-shell potential \([22]\). It can be simulated numerically by

\[
U(r) = \epsilon_0 - \lim_{\alpha \to \infty} 2\lambda \sqrt{\frac{\alpha}{\pi}} e^{-\alpha(r-r_0)^2},
\]

where \( r \) is the radial coordinate. Here, \( \epsilon_0 \) is the necessary shift to bring the ground state energy equal to \( E_0 \), \( \alpha \) and \( \lambda \) are constants large enough to produce the desired number of bound states.

The problem is somewhat similar the one-dimensional space \((D = 1)\), except that an attractive excentred delta potential has at the most two bound states. Actually, the desired potential is expected to be rather flat, slightly decreasing up to a sharp hedge. Asymptotically, it should approach an infinite wall, characteristic of the \( E_n \propto n^2 \) spectrum. Consequently we have concentrated our effort towards the determination of a potential of the general form

\[
U(x) = \epsilon_0 - (1 + ax^\alpha) \frac{U_0}{1 + \exp\left(\frac{\left|\left|x \right|-x_0\right|}{p(x)}\right)^2}.
\]

This form contains five free parameters. A first run of fits has shown that it was appropriate to fix \( \alpha = 8 \) and \( U_0 = 500 \). This last value is sufficient to get the lower part of the spectrum. It must tend to \( \infty \) to obtain an infinite number of discrete states.

The slope of the exponential, \( p(x) \), could vary with \( x \). Here, we simply consider the possibility of a single change at a given co-ordinate. Note that this abrupt change in \( p(x) \) generates a discontinuity in the potential, which is unimportant at this stage of our investigations. Recovering a continuous potential would require more parameters and thus more tedious fits to the data. Thus we are left with either three or four parameters. They have been fitted on few of the lowest levels.

Without entering into details, we give here an example of potential fitting the first 14 levels to better than 0.6%. It corresponds to a weighted average of two forms, and reads

\[
U(x) = 0.70 \ U_1(x) + 0.30 \ U_2(x) + \epsilon_0,
\]

with

\[
U_1(x) = -(1. + 3.642 \times 10^{-5} \ x^8) \frac{500}{1. + \exp\left(\frac{\left|\left|x \right|-2.273\right|}{0.01}\right)},
\]

and

\[
U_2(x) = -(1. + 1.8915 \times 10^{-4} \ x^8) \frac{500}{1. + \exp\left(\frac{\left|\left|x \right|-2.18\right|}{p(x)}\right)},
\]

with

\[
p(x) = 0.1 \ \Theta(1.87-x) + 0.005 \ \Theta(x-1.87).
\]
Here, $\Theta(x)$ is the Heaviside function. The recourse to an average mean reflects the difficulty to shape the potential around its sharp hedge with a simple form and a restricted number of parameters. Actually, the potential $U_2(x)$ has a discontinuity at the point where the slope of the exponential is changing. This is not important at the present qualitative stage. The sketch of the potential shapes is illustrated in Fig. 1, where the two components are displayed. Their corresponding eigenvalues and the weighted mean are listed in Table 1, and compared to the exact values. It shows that the distortions of the $U_1(x)$ and $U_2(x)$ spectra are somewhat complementary.

![Fig. 1 – Potentials $U_1(x)$, Eq. (12) and $U_2(x)$, Eq. (13), and their weighted average $U(x)$ Eq. (11) plotted against $x$: filled squares, triangles, and circles, respectively. The functions $U_1$, $U_2$, and $U$ being even, their negative $x$ parts are symmetric to the ones displayed here.](image)

In principle, it should be possible to reach a more accurate shape for the equivalent potential by applying the techniques we have developed. However, it would
require an effort at the level of the numerical analysis, which is not really justified.

Table 1

Eigenvalues of $U_1(x)$, Eq. (12), $U_2(x)$, Eqs. (13) and (14) and of their weighted average $U(x)$, Eq. (11), compared to $E_n = 1/2(n + 1/2)^2$.

<table>
<thead>
<tr>
<th>$n$</th>
<th>exact values</th>
<th>$U_1$</th>
<th>$U_2$</th>
<th>weighted average values</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
<td>0.125</td>
</tr>
<tr>
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<td>1.125</td>
<td>1.125</td>
<td>1.125</td>
<td>1.125</td>
</tr>
<tr>
<td>2</td>
<td>3.125</td>
<td>3.125</td>
<td>3.125</td>
<td>3.125</td>
</tr>
<tr>
<td>3</td>
<td>6.125</td>
<td>6.183</td>
<td>6.004</td>
<td>6.129</td>
</tr>
<tr>
<td>5</td>
<td>15.125</td>
<td>15.295</td>
<td>14.383</td>
<td>15.022</td>
</tr>
<tr>
<td>7</td>
<td>28.125</td>
<td>28.225</td>
<td>27.560</td>
<td>28.026</td>
</tr>
<tr>
<td>8</td>
<td>36.125</td>
<td>36.099</td>
<td>36.087</td>
<td>36.095</td>
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<tr>
<td>9</td>
<td>45.125</td>
<td>44.906</td>
<td>45.819</td>
<td>45.180</td>
</tr>
<tr>
<td>10</td>
<td>55.125</td>
<td>54.645</td>
<td>56.676</td>
<td>55.254</td>
</tr>
<tr>
<td>11</td>
<td>66.125</td>
<td>65.312</td>
<td>68.579</td>
<td>66.292</td>
</tr>
<tr>
<td>12</td>
<td>78.125</td>
<td>76.905</td>
<td>81.448</td>
<td>78.268</td>
</tr>
<tr>
<td>13</td>
<td>91.125</td>
<td>89.422</td>
<td>95.206</td>
<td>91.157</td>
</tr>
</tbody>
</table>

2.3. THE $(ix)^3$ CASE

Finally, we consider one of the potentials studied by Bender and Boettcher [11]:

$$V(x) + iW(x) = -(ix)^3.$$  \hspace{1cm} (15)

The energies are taken from the paper [11]. They are the exact numerical values up to $n = 4$. For the higher levels, use is made of their WKB approximation, which reads

$$E_n = [2.1558(n + 1/2)]^{1.2} \quad n \geq 5.$$  \hspace{1cm} (16)

According to the method developed in [10], the moments of the ground state density are approximated by the relation

$$<x^{2n}>_{a} = \frac{n(2n-1)}{E_n - E_0} <x^{2n-2}> f(n).$$  \hspace{1cm} (17)

Here, $f(n)$ is an empirical correction factor, constructed by taking advantage from the fact that for $<x^4>$ we have an absolute upper bound:

$$<x^4>_{ub} \leq \frac{4}{E_2 - E_0} <x^2> + <x^2>^2.$$  \hspace{1cm} (18)
The correction factors are then given by

\[ f(n) = f(2)^{n-1}. \]  

(19)

Note that for \( n = 1 \), \( < x^2 >_a \) is also a strict upper bound. It corresponds to an inequality first derived by Bertlmann and Martin from the dipole sum rule [23].

Once the ground state moments are calculated, the ground state density

\[ \rho_0(x) = \psi_0^*(x)\psi_0(x) \]  

(20)

is reconstructed from its moments. To this aim use is made of the formal series expansion of its Fourier transform:

\[ F(q) = 2 \int_0^\infty \cos(qx)\rho(x)dx = \sum_n (-)^n \frac{<x^{2n}>}{(2n)!} q^{2n}. \]  

(21)

This formal series expansion has a finite convergence radius. To circumvent this difficulty and recover the density from the inverse transform, the expansion is replaced by Padé approximants. We recall that a Padé approximant \( P(N,D) \) is a rational function, which has a Maclaurin expansion agreeing as far as possible with the series expansion under study. Here, \( N \) and \( D \) are the degrees of the numerator and denominator, respectively. In principle, a statistical analysis of all approximants compatible with the Fourier transform has to be performed.

At the same time, the use of Padé approximants is a good way to perform a sensible determination of the potential while considering a finite number of levels, which means a finite number of moments.

In the present case, only the lowest levels up to \( n = 8 \) have been considered, which means dealing with the ground state moments up to \( < x^{16} > \). For the sake of simplicity, the effort have been concentrated on \( P(0,16), P(2,14), \) and \( P(4,12) \). Their inverse Fourier transforms yield an average first order estimate of \( \rho_0(x) \), from which \( \psi_0(x) \) is deduced. A first approximation for the potential is then obtained by inverting the Schrödinger equation

\[ U(x) = \frac{\psi_0''(x)}{\psi_0(x)} + E_0. \]  

(22)

where \( \psi_0''(x) \) is the second derivative of \( \psi_0 \) with respect to \( x \). Solving the Schrödinger equation with this potential allows us to check how it approximates the spectrum. It provides also a way to improve the correction factors, and start an iterative procedure.

Actually, because of numerical instabilities, the potential is well determined only on the interval \( 0 \leq x \leq 2 \). This is clearly insufficient. However, it turns out that postulating a power-law potential, it is found that asymptotically

\[ U_{ass}(x) \equiv 1.538 |x|^3 \]  

(23)

is reproducing the eigenvalues \( E_n \) for \( n \geq 4 \) to better than 0.1 %. Consequently, this
is taken as the asymptotic form of the potential, to be matched to the part determined near the origin.

Without entering into details, three iterations were sufficient to get a potential reproducing the original spectrum with an agreement better than 0.1%. It reads

\[ U(x) = \left[ -0.10085 - 0.6039x + 2.28x^2 \right] \Theta(0.8 - x) + 1.538x^3 \Theta(x - 0.8), \tag{24} \]

where \( \Theta(x) \) is the Heaviside function. The resulting energies are displayed in Table 2 and compared to the actual values [11].

\begin{table}
\centering
\caption{Eigenvalues of \( U(x) \), Eq. (24), compared to the exact values of Bender and Boettcher.}
\begin{tabular}{|c|c|c|}
\hline
\( n \) & exact values & approximated values \\
\hline
1 & 1.156 & 1.156 \\
2 & 4.109 & 4.100 \\
3 & 7.562 & 7.540 \\
4 & 11.31 & 11.30 \\
5 & 15.29 & 15.28 \\
6 & 19.44 & 19.43 \\
7 & 23.76 & 23.75 \\
8 & 28.21 & 28.19 \\
9 & 32.78 & 32.77 \\
10 & 37.46 & 37.45 \\
\hline
\end{tabular}
\end{table}

To give an idea of the convergence of the method, the ground state density moments are displayed in Table 3 from their 0 to 3-order approximations.

\begin{table}
\centering
\caption{Successive estimates of the ground state density moments as a function of the order \( i \) of the iterations.}
\begin{tabular}{|c|c|c|c|}
\hline
\( n \) & \( < x^{2n} > \) \\
\hline
\hline
\( i = 0 \) & \( i = 1 \) & \( i = 2 \) & \( i = 3 \) \\
\hline
1 & 0.3386 & 0.3370 & 0.3378 & 0.3379 \\
2 & 0.3260 & 0.3256 & 0.3241 & 0.3240 \\
3 & 0.4950 & 0.4978 & 0.4952 & 0.4959 \\
4 & 1.008 & 1.031 & 1.023 & 1.024 \\
5 & 2.551 & 2.654 & 2.631 & 2.636 \\
6 & 7.660 & 8.116 & 8.052 & 8.065 \\
7 & 26.49 & 28.65 & 28.42 & 28.46 \\
8 & 103.4 & 114.15 & 113.3 & 113.5 \\
\hline
\end{tabular}
\end{table}

To go beyond the present analysis requires, as in the previous example, a nu-
merical effort we are not considering here. Nevertheless, the potential \( U(x) \) of Eq. (24) is a sufficient approximation to substantiate our present claims.

3. THE QUESTION OF UNIQUENESS

In quantum mechanics, it is commonly accepted that knowing the eigenvalues of a couple of discrete states is not sufficient to determine the corresponding potential, and the physics lying behind. Limited to the domain of real potentials, our study of the inverse problem shows that a large number of measured eigenvalues is constraining the shape of the potential. The determination converges towards a unique solution as the number of known energies tends to infinity.

However, the present work underlines the ambiguity arising from the possibility of a real spectrum to be generated by a complex potential. Considering \( D = 1 \), we can prove, indeed, that such an ambiguity occurs for any even real potential.

**Proposition:** Consider \( U(x) \) an even potential on \(-\infty \leq x \leq \infty\), and its spectrum \( E_n \) generated from the Schrödinger equation. This potential has at least two complex conjugate partners with the same real eigenvalues.

The potential \( U(x) \) being an even function, it can be expanded on the even powers of \( x \). Considering the change of variable

\[
x \rightarrow x \pm ic = z ,
\]

each term of the series expansion is obtained from

\[
x^n \rightarrow (\pm ic)^n [\frac{x}{ic} \pm 1]^n n \text{ even} .
\]

It is a simple matter to verify that the real part of the transformed potential contains only the even powers of \( x \), while the odd powers are building the complex part. Consequently the transformed potential is \( PT \)-symmetric. Moreover, the above variable change leaves the Schrödinger equation unchanged. Thus \( U(z) \) has the same spectrum as \( U(x) \).

Suppose \( U(x) \) contains terms like \(| x |\). The expansion in even powers of \( x \) may be lengthy. However, use can be made of

\[
|x| = \sqrt{x^2} \rightarrow \sqrt{(x \pm ic)^2} = (x^4 + 2c^2x^2 + c^4)^{1/4} \exp[i\phi(x)] ,
\]

with

\[
\phi(x) = \frac{1}{2} \arctan \frac{-2cx}{x^2 - c^2} .
\]

Clearly, the same conclusions as above apply to this case.

At this point, it is interesting to underline that the linear potential

\[
V(x) + iW(x) = \lambda | x | + icx ,
\]
which differs only slightly from $U(x \pm ic) = |x \pm ic|$, is also a $\mathcal{PT}$-symmetric potential, but its spectrum contains complex eigenvalues unless $c = 0$ [24].

4. CONCLUSIONS

The present work is dealing with the search of real potentials equivalent to complex potentials having a real spectrum. Beyond simple analytical cases, two examples have been studied:

$$V(x) = e^{2ix} \quad \text{and} \quad V(x) = (ix)^3.$$  \hspace{1cm} (30)

Approximate solutions have been reached. More precise answers are possible in principle but require sophisticated numerical techniques.

The present results are nevertheless sufficient to underline clearly the ambiguity arising from the existence of complex potentials with real eigenvalues. It stresses the fact that the knowledge of a spectrum is not sufficient to determine the potential, even if a large number of eigenvalues are measured. Other observables are needed to understand the physical situation.

The present work has been done in the one-dimensional space. We are confident that similar conclusions hold in higher dimensions.

Appendix: A remark about the inverse problem.

In our previous papers on the inverse problem from discrete states, it was implicitly assumed that the excitation energies

$$\Delta(n) = E_n - E_0$$  \hspace{1cm} (31)

have to be discrete values of a continuous function. This condition is important to ensure the existence of a connection between $\Delta(n)$ and the moments of the ground state density. These last quantities are defined by

$$M(n) = 2\int_0^\infty |\psi_0(x)|^n \, dx,$$  \hspace{1cm} (32)

which is a continuous function of $n$, unless $\psi_0(x)$ has a peculiar behavior. It then becomes obvious that a relationship of the form

$$M(n) = F[\Phi(n), \Delta(n)]$$  \hspace{1cm} (33)

must exist. The functional can take various forms and the connecting function $\Phi(n)$ is not known a priori. Both cannot be derived from general principles. The relationships we are using is derived from lower bounds of the moments obtained from sum rules, extending a technique proposed by Bertlmann and Martin [23]. In this case, $\Phi(n)$ can be established analytically for the harmonic oscillator in any dimensions, and in $D \geq 2$ for the Coulomb potential [25]. In the general case, $\Phi(n)$ is approached by iterations.
While writing the present article, we became aware of works achieved by mathematicians on the subject. Out of an abundant literature, we quote the book by Pöschel and Trubowitz [26], the papers by McLaughlin [27], and Chung-Tsun Shieh and Yurko [28]. The main difference with our approach lies in the choice of the data used to get the potential. To the best of our knowledge the connection between the spectrum and the moments of the ground state density has not been investigated by mathematicians.

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