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Complex potentials and the inverse problem

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Abstract: The occurrence of complex potentials with real eigenvalues has implications concerning the inverse problem, i.e. the determination of a potential from its spectrum. First, any complex potential with real eigenvalues has at least one equivalent local potential. Secondly, a real spectrum does not necessarily corresponds to a local real potential. A basic ambiguity arises from the possibility the spectrum to be generated by a complex potential. The purpose of this work is to discuss several aspects of this problem.

Keywords: local equivalent potential, basic ambiguity, conjecture

INTRODUCTION

At the end of the last century, the discovery of complex potentials having real eigenvalues originates from discussions in which D. Bessis took a key role (see the references of the paper by Bender and Boettcher [1]). It has produced a large amount of works. Many complex potentials with real eigenvalues are invariant under time reversal and parity transformation (PT invariance). However, this is neither a sufficient nor a necessary condition, and many examples have been found besides PT-invariant cases.
A surview of this domain can be found in the review articles by Bender [2] and D. Mihalache [3]. In the present work, we study its implications in the inverse problem, i.e. in the determination of a potential from its spectrum.
Here, we consider the Schro¨dinger equation in the D =1 dimensional space :

$$[-\frac{d^2}{dx^2}+V(x)+iW(x)]\psi_n(x)=E_n\psi_n(x)\ . \qquad (1)$$

The inverse problem consists in determining the potential from its observables. The most common practice is to use phase shifts from scattering data. Here we shall consider the determination of the potential from its spectrum {En}. Several cases are presented.

THE LOCAL EQUIVALENT POTENTIAL.

If a complex potential has only real eigenvalues, it possesses obviously at least 1 local equivalent potential. We shall display a couple of examples. The answer is analytical for a class of potentials including the Scarff II potential, the generalized Pochl-Teller potential and the Morse potential. By using group theoretical techniques, it has been shown by Bagchi and Quesne [4] that their complexified versions generate real eigenvalues with equivalent spectra.
The Morse potential

$$V(x)+iW(x)=(a+ib)^2e^{-2x}-(2c+1)(a+ib)exp^{-x}\ . \qquad (2)$$

has been further studied by Z. Ahmed [5]. By applying the change of variable

$$z=2(a+ib)e^{-x} \qquad (3)$$

in the Schrodinger equation, the effective parameter governing the eigenvalue is c +1/2. The eigenvalues are given by

$$E_n=-[n-c]^2\ ,\ n\ \leq\ c\ . \qquad (4)$$

This spectrum can obviously be produced by a Poschl-Teller potential

$$U(x) = -\frac{\sigma(\sigma+1)}{\cosh^2(x)} \; , \tag{5}$$

with σ = √c.
An interesting case is provided us by the potential studied by Cannata et al [6] :

$$V(x) + iW(x) = e^{2ix} \; . \tag{6}$$

Among the 2 analytic solutions found by the authors, we retained

$$E_n = [n + 1/2]^2 \; . \tag{7}$$

At large n, this spectrum approaches the one of the infinite well with opaque wall. Thus it suggests to simulate the local equivalent potential by a function with a sharp hedge at some distance, very much like a Woods-Saxon function. By using a limited number of parameters, we got satisfactory qualitative results with

$$U(x) = \epsilon_0 - (1 + x^\alpha)\frac{U_0}{[1 + exp\left(\frac{(|x|-x_0)}{p(x)}\right)]^2} \tag{8}$$

for U0 → ∞. The explicit form we obtained is given by

$$U_1(x) = -(1. + 3.642\ 10^{-5}x^8)\frac{500}{[1. + exp(\frac{(|x|-2.273)}{0.01})]} \; , \tag{9}$$

And

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

With

$$p(x) = 0.1\ \Theta(1.87 - x) + 0.005\ \Theta(x - 1.87) \; . \tag{11}$$

Here, Θ(x) is the Heaviside function.

The results are displayed in the fig 1.
A more sophisticated, and more general method, relies on the connection between the excitation energies and the moments of the ground state density. For obvious reasons, the method can be applied if and only if the number of bound states is sufficiently large. A unique answer is obtained in the case of an infinite number of bound states, namely for confining potentials. More details concerning the procedure and its constraints can be found in the work by Yekken et al [7].
Here, use is made of

$$< x^{2n} >= f(n)\frac{n(2n-1)}{E_n - E_0} < x^{2n-2} > \; , \tag{12}$$

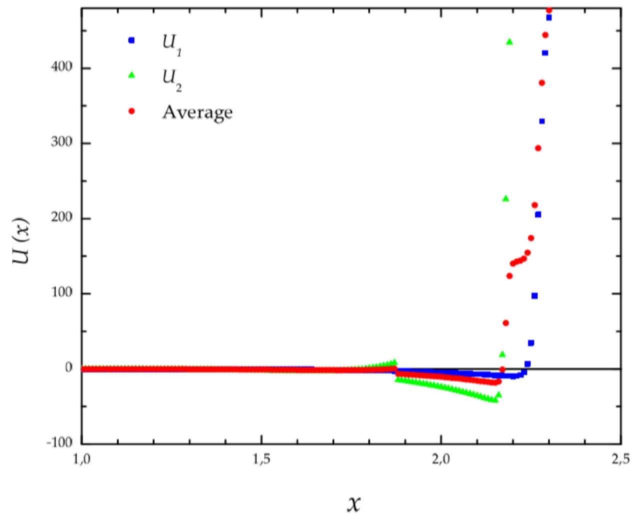

Figure 1: Example of U(x) fitting the lowest 14 levels to better than 1 %.

where f(n) has to be determined iteratively. Note that f(n) = 1 ∀ n in the case of the harmonic oscillator.
The next difficulty consists in the reconstruction of | ψ0(x) |2 from its moments. It can be achieved by means of the Fourier transform of | ψ0(x) |2 and its approximate expansion via Pad´e approximants.
Uniqueness of the answer : the ground state density being a positive definite function, the answer is unique if the number of known moments tends to infinity. In practice, a finite number of known moments results with uncertainties for the density requiring a statistical analysis. Knowing the lowest 12 - 15 levels yields already a reasonable answer.

The ground state density provides us with the ground state wave function. The potential is obtained by reversing the Schrodinger equation.

$$V(x) = \frac{\psi_0''(x)}{\psi_0(x)} + E_0 \; . \tag{13}$$

The method has been applied to

$$V(x) + iW(x) = -(i\ x)^3\ . \tag{14}$$

Its spectrum has been given by Bender and Boettcher [1]. Up to n = 4, the values have been obtained with the Runge-Kutta method. For larger n, the spectrum is well approximated by

$$E_n = [2.1558(n + 1/2)]^{1.2} \quad , \quad n \geq 5\ . \tag{15}$$

We found the local equivalent potential to be given by

$$U(x) = \left[-0.1009 - 0.604x + 2.28x^2\right]\Theta(0.8 - x) + 1.538x^3\Theta(x - 0.8)\ . \tag{16}$$

It approximates the exact spectrum to better than 0.1 %, as illustrated in table 1.

Table 1: Eigenvalues of U(x), Eq. (16), compared to the exact values of Bender and Boettcher [1].

n	exact values	approximated values
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

A BASIC AMBIGUITY.

Because of the existence of complex potential with real eigenvalues, the determination of the potential from its spectrum suffers from a basic ambiguity. From the above considerations, a real spectrum arises first from a local real potential. But the latter may admit complex partners with the same spectrum. Consequently, observables beyond the eigenvalues are needed to determine the potential and its nature, real or complex. We illustrate this situation in the following way. Consider an even potential given by

$$U(x) = \sum_n a_n x^{2n}\ . \tag{17}$$

The shift

$$x\ \rightarrow\ x + i\frac{c}{2} \tag{18}$$

produces

$$V(x) + iW(x) = \sum_n \alpha_n x^{2n} + i\sum_n \beta_n x^{2n-1}\ . \tag{19}$$

Such a potential is manifestly P T symmetric. Moreover : the Schrodinger equation is invariant under

$$z\ =\ x + i\tfrac{c}{2}.$$

Thus formally, to the ensemble ψn(x) of solutions to U(x) corresponds the ensemble ψn(z) of solutions to V (x)+iW(x) with the same spectrum En up to a constant. The parameter c is not determined by the spectrum, so that the transformation (18) generates an infinity of complex partners with identical spectrum.
We shall illustrate this situation by 2 examples. First, let us look at the shifted harmonic oscillator introduced years ago by Znojil [8].

$$U(x) = \alpha^2x^2 \rightarrow V(x) + iW(x) = \alpha^2x^2 + i\ \alpha^2cx = \alpha^2z^2 + \frac{\alpha^2c^2}{4}\ . \tag{20}$$

It is a simple matter to verify that its spectrum corresponds to the ordinary harmonic oscillator spectrum shifted by $\alpha^2c^2/4$, and its wave functions are those of the usual H.O. in terms of z.
Looking for a simple observable able to fix the value of c, we have checked the dipole transition between the ground and first excited state. Before presenting the results, it is important to recall that in the case of non-Hermitian systems, the necessary conditions to generate a coherent quantum mechanics imply the definition of the scalar product and the observables.
In brief, we have to ensure the positivity of the norms and to get rid of incoherent statements. For instance, the average value of a positive definite operator must be positive definite.
This problem does not admit a simple general form, but has to be solved for each potential. In general, the proper definition is given by

$$\int_{-\infty}^{\infty} [CPT\psi_n(x)]\, A\psi_m(x)dx\ , \tag{21}$$

where P and T, are the parity and time reversal operators. To be an observable A must satisfy

$$A^t = CPTACPT = A \ . \tag{22}$$

For the shifted potential, the operator C has been derived by Ahmed [9] :

$$C = e^{-cp}P \quad with \quad p = -i\frac{d}{dx} \ . \tag{23}$$

In particular, it yields

$$x^n \ \rightarrow \ (x + i\frac{c}{2})^n \ . \tag{24}$$

Back to the harmonic oscillator case Eq. (20), the ground and first excited state wave functions are given by

$$\Psi_0(x) = \left[\frac{\alpha}{\pi}\right]^{1/4} e^{-\alpha(x+i\frac{c}{2})^2} \tag{25}$$

and

$$\Psi_1(x) = \sqrt{2}\left[\frac{\alpha^3}{\pi}\right]^{1/4} (x + i\frac{c}{2}) \ e^{-\alpha(x+i\frac{c}{2})^2} \ , \tag{26}$$

respectively. Furthermore, the spectrum is given by

$$E_n = \alpha(2n+1) + \alpha^2\frac{c^2}{4} \ . \tag{27}$$

With these elements, two kind of results can be established.
First, the equivalent of the x2 average on the ground state

$$\left[\frac{\alpha}{\pi}\right]^{1/2} \int_{-\infty}^{\infty} e^{-\alpha(x+i\frac{c}{2})^2}(x + i\frac{c}{2})^2 dx \ = \ \frac{1}{2\alpha} \ . \tag{28}$$

Thus the result is independent on c. For the higher ground state moments, use can be made of the recurrent relationship

$$< 0 \mid (x + i\frac{c}{2})^{2k+2} \mid 0 >= -\left[\frac{\alpha}{\pi}\right]^{1/2} \ \frac{d}{d\alpha}\int_{-\infty}^{\infty} e^{-\alpha(x+i\frac{c}{2})^2}(x + i\frac{c}{2})^{2k} dx \ . \tag{29}$$

As a consequence, all the ground state even moments are independent on c.
A similar result can be obtained for the odd moments. Indeed we have

$$< 0 \mid (x + i\frac{c}{2})^{2k+1} \mid 0 >= -\left[\frac{\alpha}{\pi}\right]^{1/2} \ \frac{d}{d\alpha}\int_{-\infty}^{\infty} e^{-\alpha(x+i\frac{c}{2})^2}(x + i\frac{c}{2})^{2k-1} dx \ , \tag{30}$$

here with k ≥ 1. Moreover, because for k = 1 the ground state average is zero, all the odd ground state moments are zero.
Consider the dipole transition operator $x+i\frac{c}{2}$

the contribution of the lowest excited state is given by

$$< 1 \mid (x + i\frac{c}{2}) \mid 0 >= \ \alpha\left[\frac{2}{\pi}\right]^{1/2} \int_{-\infty}^{\infty} e^{-\alpha(x+i\frac{c}{2})^2}(x + i\frac{c}{2})^2 dx \ = \ \frac{1}{\sqrt{2\alpha}}. \tag{31}$$

It is easy to check that the lowest excited state is exhausting the dipole sum rule :

$$\sum_n (E_n - E_0) \mid< n \mid x + i\frac{c}{2} \mid 0 >\mid^2 = \ (E_1 - E_0) \mid< 1 \mid x + i\frac{c}{2} \mid 0 >\mid^2 = 1 \ , \tag{32}$$

which is actually a property of the harmonic oscillator. In other words, we conclude that for the harmonic oscillator the shift of the $i\frac{c}{2}$ ordinate by has little if no impact on the physics, and thus is irrelevant.

A CONJECTURE.

It is very tempting to state that for any PT symmetric shifted potential the spectrum and the observables based on the ground state moments do not depend on the complex shift. However, this conjecture is simply based on the formal change affecting the Schrodinger equation under the change of variable. The positive illustrating example may essentially reflect the very special properties of the harmonic oscillator. Consequently the confirmation or the rejection of this conjecture require more effort. Here we shall pursue the discussion by investigating a second example.
Let us consider the Poschl-Teller potential :

$$U(x) = -\frac{\sigma(\sigma+1)}{cosh^2(x)} \tag{33}$$

with its spectrum

$$E_n = -[n - \sigma]^2 \ , \quad n \ < \sigma \ . \tag{34}$$

The shifted potential reads

$$V(x) = -\sigma(\sigma+1)\frac{\cosh^2(x)\cos^2(c/2) - \sinh^2(x)\sin^2(c/2)}{[\cosh^2(x)\cos^2(c/2) + \sinh^2(x)\sin^2(c/2)]^2} \tag{35}$$

$$W(x) = 2\sigma(\sigma+1)\frac{\cosh(x)\sinh(x)\cos(c/2)\sin(c/2)}{[\cosh^2(x)\cos^2(c/2)+\sinh^2(x)\sin^2(c/2)]^2} . \quad (36)$$

This potential is obviously P T symmetric. Because of the cyclic character of the coefficients multiplying the hyperbolic function, it is sufficient to consider $0 \leq c < \pi$ The formal derivation in terms of the z variable should be valid ∀c in this domain. However, take the upper limit $c = \pi$, it reduces to

$$V(x) = \frac{\sigma(\sigma+1)}{\sinh^2(x)} , \quad (37)$$

which has no bound state !
To get more insight, consider the case $\sigma = 1$, for which a single bound state exists with $E0 = -1$. The wave function reads

$$\Psi_0(x) = \frac{1}{\cosh(x+i\frac{c}{2})} = \frac{\cosh(x)\cos(c/2) - i\sinh(x)\sin(c/2)}{\cosh^2(x)\left[\cos^2(c/2)+\sinh^2(x)\sin^2(c/2)\right]} . \quad (38)$$

It is a simple matter to verify that for $c = \pi$, this wave function reduces to

$$-i\frac{1}{\sinh(x)} . \quad (39)$$

It satisfies the Schrodinger equation with above mentioned eigenvalue. However, because of its singularity at the origin, this wave function is not square integrable and thus has to be rejected from the Hilbert space.

On the other hand, if we calculate the norm and the average $(x+i\frac{c}{2})^2$,

the results are stable, equal to their values at $c = 0$ until the vicinity of the singularity is reached. Note that these results are obtained by numerical integrations, which are very sensitive to the integration mesh size as the singularity is approached. To be specific, with a mesh of 10^{-3}, the results deviate from the $c = 0$. values at $c = 3.131$ to a 10^{-10} level, the limit $c = 3.1405$ is reached with a mesh of 10^{-4}, and $c = 3.14150$ with a mesh of 10^{-5}.

Actually, by expanding the wave function for $c = \pi-\varrho$, we obtain

$$\Psi_0(x) = \frac{(\epsilon/2)\cosh(x) - i\sinh(x)}{(\epsilon^2/4)\cosh^2(x)+\sinh^2(x)}, \text{ with } \lim_{x\to 0}\Psi_0(x) = \frac{1}{\epsilon} . \quad (40)$$

It indicates a $\frac{1}{\epsilon}$ divergence.
These results suggest the above conjecture to be true for all c values for which the wave function is normalizable.

CONCLUSIONS.

In this work, we are dealing with complex potentials having real eigenvalues. Such potential admit a real local equivalent potential, which is more or less obvious. Some examples of the determination of real local equivalent potentials have been given.
More interesting is the fact that any real even potential possesses an infinite number of complex partners, by a simple complex change of coordinate like $x \to x + ic\,2$. This change leaving the Schrodinger equation unchanged, the spectrum is the same, independently of c. The 2 studied examples indicate that actually the values of other observables are unchanged. A point to be studied more thoroughly.

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