OBSERVABLES OF COMPLEX PT-SYMMETRIC "SHIFTED" POTENTIALS

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Received February 10, 2020

Abstract. We study complex PT-symmetric potentials, with real eigenvalues, corresponding to a complex coordinate shift $(x+i\frac{c}{2})$ of a real even potential. In this case, the rules to achieve a coherent quantum mechanics are known. They allow the calculation of observables, which are found to be independent on c. This result is illustrated by few analytical or semi analytical examples. On the other hand, trying to test this property numerically faces problems linked to the difficulty of finding the proper solutions of the Schrödinger equation. In particular, the large distance behaviour of the wave functions generates instabilities. As an example, we have studied the $(x+i\frac{c}{2})^4$ potential.

Key words: Solutions of wave equations: bound states, Quantum mechanics, Algebraic methods.

1. INTRODUCTION

Since the discovery of complex potentials with real eigenvalues, a large number of works has been devoted to this subject. Overviews and relevance for physics applications can be found in the review articles by Bender [1] and Mihalache [2], for instance, as well as in more recent papers [3, 4]. Let us also quote a few relevant works on unique properties of complex-valued external potentials and their applications in many physical settings [5–8]. At the same times, it has raised the question of building a coherent quantum mechanics for the corresponding non-Hermitian Hamiltonians. The situation has been well described by Bender [1]. One case is particularly interesting, namely the complex potentials generated from an even real potential by applying a complex coordinate shift :

$$x \ \rightarrow \ x+i\frac{c}{2}.$$

This case was first proposed by Znojil for the harmonic oscillator [9]. Its impact at the quantum mechanical level was studied by Ahmed [10]. Indeed, it is generating cases for which a coherent quantum mechanics can be easily formulated.

The purpose of the present work is to discuss observables of these shifted potentials. In fact, we shall first show, on basic principles, that the complex shift is not affecting the observables, which are actually independent of c. For illustrative

purpose, few examples shall be treated explicitly. The number of analytic cases is scarce. Numerical treatments are welcome. Unfortunately, they require a high accuracy, and face instabilities. This situation shall be illustrated by considering the $(x+i\frac{c}{2})^4$ potential.

We came across this question while studying the inverse problem in the case of complex potentials with real eigenvalues [11]. The reality of the spectrum implies the possibility of finding at least one real potential partner with the same eigenvalues. Thus, to distinguish between a real or complex potential requires to find a decisive observable. Few preliminary results have been reported at the VIth-PCMTMP conference (Tulkarem, Palestine, August 2018), and published in the Palestine Technical University Research Journal [12].

2. GENERALITIES

In the D = 1 dimensional space (with $\hbar$ = 2m = 1), we consider the Schrödinger equation on the entire x axis

$$\left[-\frac{d^2}{dx^2}+U(x)\right]\psi_n(x)=E_n\psi_n(x), \tag{1}$$

where $U(x)$is an even function. The shift $(x+i\frac{c}{2})$ generates

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

Here, $V(x)$ and $W(x)$ are even and odd functions, respectively. The obvious change of variables $(x+i\frac{c}{2})\rightarrow z$, together with $\frac{d}{dx}=\frac{d}{dz}$, proves the equivalence of the two equations. Thus, the eigenvalues are identical, up to a possible global shift of the spectrum, and the wave functions admit the same analytical forms.

In the case of quantum mechanics in the complex plane, as recalled in the review article by Bender [1], for an operator to be an observable, it has to fulfill the condition

$$A^t=CPTACPT=A, \tag{3}$$

where P and T are the parity and time reversal operators. For the shifted potentials, the operator C has been derived by Ahmed [10]. It is given by

$$C=e^{-\gamma p}P \ \text{ with } \ p=-\frac{d}{dx}, \tag{4}$$

where γ is a constant. The average value of A is thus given by

$$<n\mid A\mid m>=\int_{-\infty}^{\infty}[CPT\psi_n(x)]A\psi_m(x)dx\ . \tag{5}$$

Consider

$$x^\nu \ \rightarrow \ (x+i\frac{c}{2})^\nu \ . \tag{6}$$

The right hand side fulfils the condition (3), and thus it constitutes the equivalent operator to x^ν. Similarly, for shifted potentials, we have

$$CPT\psi_n(x+i\frac{c}{2}) = \psi_n(x+i\frac{c}{2}) \ . \tag{7}$$

Thus, the equivalent average value of x^ν is given by

$$\bar{A}_n(c,\nu) =< n \mid (x+i\frac{c}{2})^\nu \mid n >= \int_{-\infty}^{\infty} \psi_n^2(x+i\frac{c}{2})(x+i\frac{c}{2})^\nu dx \ . \tag{8}$$

To check the behaviour of $\bar{A}_n(c,\nu)$ against c let us take its derivative with respect to c. It is given by

$$\frac{d}{dc}\bar{A}_n(c,\nu) = \frac{i\nu}{2}\int_{-\infty}^{\infty} \psi_n^2(x+i\frac{c}{2})(x+i\frac{c}{2})^{\nu-1}dx + i\int_{-\infty}^{\infty} \psi_n(x+i\frac{c}{2})[\frac{d}{dc}\psi_n(x+i\frac{c}{2})](x+i\frac{c}{2})^\nu dx. \tag{9}$$

Setting

$$z = x+i\frac{c}{2} \ \ \text{together with} \ \ \frac{d}{dc} = \frac{i}{2}\frac{d}{dz} \ , \tag{10}$$

the second term can be integrated by part, and we are left with

$$\frac{d}{dc}\bar{A}_n(c,\nu) = \frac{i}{2}(\psi_n^2(x+i\frac{c}{2})(x+i\frac{c}{2})^{\nu-1}\Big|_{-\infty}^{\infty} \ . \tag{11}$$

To be normalisable, the wave functions have to decrease to zero at both limits faster than any power of x. Consequently, for such wave functions the derivative of $\bar{A}_n(c,\nu)$ with respect to c is zero. And thus it does not depend on c.

3. ILLUSTRATIVE EXAMPLES

The above statement is conclusive enough to make explicit calculations redundant. Nevertheless, for the pleasure of the "amateurs", it could be instructive to discuss few cases. Analytically, it does not bring any new aspect. However, tackling numerical examples sheds a light on the difficulties encountered in solving the Schrödinger equation for complex potentials.

3.1. THE HARMONIC OSCILLATOR

As stated in the introduction, the first example of shifted potential has been proposed by Znojil [9]. It concerns the harmonic oscillator :

$$V(x)+iW(x) = x^2+icx \ . \tag{12}$$

It is a simple matter to show that the spectrum is independent on c up to the constant shift of $\frac{c^2}{4}$. The wave functions are the usual ones of the harmonic oscillator in terms of z. Looking for an observable capable to distinguish a shifted harmonic oscillator from the real one, we have shown all the ground state moments to be independent on c. This conclusion is easily extended to other state. Moreover, we found the dipole sum rule to be also insensitive to c [12].

Here, we give the answer for the Fourier transform of the ground state density. Let

$$\psi_0^2(x) = \sqrt{\frac{\alpha}{\pi}}\, e^{-(\alpha x^2 - i\alpha c x)} \tag{13}$$

be the ground state density. Considering

$$e^{iqx} \;\rightarrow\; e^{iq(x+i\frac{c}{2})}\,, \tag{14}$$

the Fourier transform is given by

$$F(q) = \sqrt{\frac{\alpha}{\pi}}\, e^{(\frac{\alpha c^2}{4} - \frac{qc}{2})} 2\int_0^\infty e^{(-\alpha x^2)} \cos{(q-\alpha c)x} dx = e^{-\frac{q^2}{4\alpha}}. \tag{15}$$

The result is identical to the case $c = 0$.

3.2. THE SHIFTED PÖSCHL-TELLER POTENTIAL

A second analytical example is provided us by the shifted Pöschl-Teller potential [13, 14], which reads

$$V(x) = -\sigma(\sigma+1)\frac{\cosh^2(x)\cos^2(c/2) - \sinh^2(x)\sin^2(c/2)}{[\cosh^2(x)\cos^2(c/2) + \sinh^2(x)\sin^2(c/2)]^2}, \tag{16}$$

$$W(x) = 2\sigma(\sigma+1)\frac{\cosh(x)\sinh(x)\cos(c/2)\sin(c/2)}{[\cosh^2(x)\cos^2(c/2) + \sinh^2(x)\sin^2(c/2)]^2}. \tag{17}$$

Because of the cyclic character of the coefficients multiplying the hyperbolic functions, the relevant domain of the shift is $0 \leq c < \pi$. Note that for $c = 0$, the potential is real and attractive, whereas for $c = \pi$ it becomes real and repulsive. For this latter, bound states do not exist, the ground state eigenfunction has a singularity at the origin, and cannot be normalised. Consequently, this value of $c = \pi$ has to be rejected.

Similarly to the above case, it is a simple matter to verify explicitly that the shift does not affect the analytical form of the wave functions. The spectrum is identical to the real one :

$$E_n = -[n-\sigma]^2\,,\;\; n \;\leq\; \sigma. \tag{18}$$

Calculating observables is more complicated, except in few particular cases. Let us consider the case $\sigma = \frac{1}{2}$, which has a single bound state. Its squared wave

function reads

$$\psi_0^2(x+i\frac{c}{2}) = \frac{\cos(c/2)\cosh(x) - i\sin(c/2)\cosh(x)}{\cosh^2(x) - \sin^2(c/2)}. \tag{19}$$

Its norm is given by

$$N_0^{-2} = \cos(c/2)\int_{-\infty}^{\infty} \frac{\cosh(x)dx}{\cosh^2(x) - \sin^2(c/2)} = \cos(c/2)\frac{\pi}{\sqrt{1-\sin^2 c/2)}} = \pi. \tag{20}$$

The Fourier transform of the density takes the form

$$\begin{aligned} F(q) &= \frac{1}{\pi}\int_{-\infty}^{\infty} e^{[q(x+i\frac{c}{2})]} \frac{\cosh(x)\cos(c/2) - i\sinh(x)\sin(c/2)dx}{\cosh^2(x) - \sin^2(c/2)} dx \qquad (21)\\ &= \frac{4}{\pi} e^{-qc/2}\int_0^{\infty} \frac{\cos(qx)\cos(c/2)\cosh(x) + \sin(qx)\sin(c/2)\sinh(x)}{\cosh(2x) + \cos(c)}\, dx. \end{aligned}$$

With the help of integral tables [15], we get

$$F(q) = \frac{1}{\cosh(\frac{q\pi}{2})}. \tag{22}$$

Few other observables have been tested numerically, namely the average values of $(x+i\frac{c}{2})^\nu$, $\nu = 1, 2$ and 4, for $0 \leq c < \pi$. Because of the singularity of the wave function at $c = \pi$, deviations from the expected $c = 0$ value appear as c is approaching this limit. The precision depends sensitively from the integration mesh. Results displayed in Table 1 correspond to $\Delta x = 10^{-5}$. Noticeable differences arise beyond $c = 3.1$. For $\Delta x = 10^{-3}$, they appear already at $c = 3.0$ at the 1% level.

It is interesting to note the special role of $< n \mid (x+i\frac{c}{2}) \mid n >$. It relies entirely on the imaginary part of the wave function, and thus it constitutes a convenient test of it.

4. THE $(x+i\frac{c}{2})^4$ POTENTIAL

This example is essentially designed to underline the limitations arising from approximations generated by solving the Schrödinger equation numerically for complex potentials. To our knowledge, this problem has not retain attention, the WKB method being preferred [16, 17]. Recently, the finite difference method has also been considered and compared to WKB method [18]. Thus, it deserves to underline few aspects bringing special difficulties. Thus, we complete the present study with a look at the $(x+i\frac{c}{2})^4$ potential. Here we have

$$V(x) = x^4 - \frac{3}{2}c^2x^2 \tag{23}$$

Table 1

Shifted Pöschl-Teller potential. The numerical estimates of the ground state average of x^ν for ν =1,2 and 4 are displayed for values of $0 \leq c < \pi$. The integration mesh is 10^{-5}. The results show the influence of the singularity as c approaches π.

c	$<(x+ic/2)>$	$<(x+ic/2)^2>$	$<(x+ic/2)^4>$
0.0	0.	2.4674	30.440
1.0	2. 10^{-6}	2.4674	30.4397
2.0	6. 10^{-6}	2.4674	30.4398
3.0	6.8 10^{-5}	2.4672	30.4390
3.10	2.4 10^{-4}	2.4666	30.4364
3.14	6.3 10^{-3}	2.4478	30.3432
3.1415	0.10	2.1498	28.873
3.14154	0.17	1.9347	27.811
3.14159	1.27	-1.5099	10.813

and

$$W(x) = 2cx^3 - \frac{1}{2}c^3 x. \tag{24}$$

Use is made here of the Runge-Kutta method to solve coupled differential equations. Writing

$$\psi_n(x) = u_n(x) + iv_n(x)\ , \tag{25}$$

Assuming real eigenvalues, they reads

$$\begin{aligned} -u_n''(x) + V(x)u_n(x) - W(x)v_n(x) &= E_n u_n(x) \\ -v_n''(x) + V(x)v_n(x) + W(x)u_n(x) &= 0. \end{aligned} \tag{26}$$

The prime and double prime represent the first and second derivative with respect to x, respectively. For even states, the boundary conditions at the origin are $u_n(0) = 1$, $u_n'(0) = 0.$, $v_n(0) = 0$, $v_n'(0)$ has to be fixed. At infinity $u_n(x)$ and $v_n(x)$ have to vanish sufficiently fast the wave function to be normalisable.

In the case of real potentials, the number of nodes and the occurrence of a zero at large distance, simulating an asymptotic decrease of the wave function, are sufficient criteria to choose the solution to a desired approximation. This is not valid in the complex case, because of the oscillatory behaviour of both the real and imaginary part of the wave function. Thus, one has to rely on the large distance behaviour of the wave function modulus. It is a positive definite function. Thus it never crosses the x axis, but approximate solutions show a sharp minimum at large x. It should be possible to add a second test by looking at the derivative of the modulus near its large distance minimum. However, from the few examples we have worked out, this

is strongly affected by instabilities in the tail of the wave function, and thus it is not efficient.

On the other hand, the coupled equations (26) can be written for the modulus and the phase. If

$$\psi_n(x) = \rho_n(x) e^{i\phi_n(x)} \ , \tag{27}$$

we get

$$\begin{aligned} -\rho_n''(x) + V(x)\rho_n(x) + g_n^2(x)\rho_n(x) &= E_n \rho_n(x) \\ g_n'(x) + 2\frac{\rho_n'(x)}{\rho_n(x)} g &= W(x), \end{aligned} \tag{28}$$

where we have set

$$\phi_n'(x) = g_n(x). \tag{29}$$

Provided the derivative of the phase to be known, Eq. (28) is similarly to an ordinary Schrödinger equation.

A convenient strategy would be to start with Eqs. (26), which provides an estimate of $g_n(x)$:

$$g_n(x) = \frac{v_n'(x)u_n(x) - u_n'(x)v_n(x)}{u_n^2(x) + v_n^2(x)}. \tag{30}$$

Introducing this quantity in Eqs. (28) for any solution of Eqs. (26), it gives the same eigenvalue as the system (26) if and only if it corresponds to the correct solution. Though quite useful, this criterion is not absolutely safe, precisely because of the instabilities of $\phi_n(x)$ at large distances. In the tails of the wave functions and of the modulus, the approximations are not the same in Eqs. (26) and (28). The differences are expected to increase with c, requiring increased precision in the numerical codes as c gets large.

For the sake of illustration, we have worked out the case of the ground state ($n = 0$). The phase $g_0(x)$ is obtained from Eqs. (26), and fitted by a polynomial form

$$g_{0a}(x) = \sum_{k\ even} a_k x^k. \tag{31}$$

Note that from Eqs. (28), $\rho_0(x)$ being an even function and $W(x)$ being odd, $g_{0a}(x)$ has to be an even function. Use has been made of a polynomial of order $k = 18$. The phase function is introduced in Eqs. (28), and we retain the solution for which the two estimates of E_0 are in close agreement, *i.e.* usually better than $0.1\ \%$.

The results for a sample of c values, up to $c = 1.0$, are displayed in Table 2. The ground state energy E_0 is compared to the expected value

$$E_{0,c} = E_{0,0} - \frac{c^4}{16}. \tag{32}$$

Few moments, namely $(x+ic/2)^\nu$ for $\nu = 0, 2 \text{ and } 4$, are compared to their values at $c = 0$. The results agree with the expected values to better than 0.1 %, except for $< (x+ic/2)^4 >$ at $c = 1.0$.

We complete these results by displaying the modulus and the phase function for a couple of c values in Figs. 1 and 2, respectively. The variation of the modulus with c is rather small. The phase function, however undergoes quite sensitive changes with c, becoming sharper in the tail as c increases.

Table 2

The $(x+i\frac{c}{2})^4$ potential. The ground state energy and observables obtained by solving Eqs. (26) are compared to expected values for few values of c. The energy $E_{0,c}$ refers to Eq. (32) ; for the moments the expected values are those of $c = 0$.

c	$E_{0,c}$	E_0	$< (x+i\frac{c}{2}) >$	$< (x+i\frac{c}{2})^2 >$	$< (x+i\frac{c}{2})^4 >$
0.0		1.060429	0.0	0.3620	0.3534
0.01	1.060429	1.060377	$2.1\ 10^{-6}$	0.3619	0.3534
0.1	1.060423	1.060472	$9.7\ 10^{-5}$	0.3619	0.3529
0.2	1.060329	1.060413	$8.5\ 10^{-5}$	0.3621	0.3536
0.5	1.056523	1.056482	$-9.0\ 10^{-7}$	0.3620	0.3534
1.0	0.997929	0.997922	$-7.8\ 10^{-3}$	0.3648	0.3679

4.1. A POSSIBLE ITERATIVE PROCEDURE

The case $c = 1.0$ deserves attention. It provides us with an example of instabilities of $g_0(x)$, specially in its tail. It suggests also the possibility of an iterative procedure.

Because we choose the phase function giving the smallest difference between the two energy estimates, it may be considered as a good first approximation to generate an iterative procedure of Eqs. (28). If the process is converging, we may reach the correct solution. The new phase function will differ from the one given by Eqs. (26). The solutions of Eqs. (26) being approximative in any case, this difference is not in contradiction with the basic postulate stating the equivalence of the two systems of equations. In principle, it would allow us to start from any approximate solution of Eqs. (26).

However, the situation does not follow this ideal scheme. The behaviour of $\rho_0(x)$ in its tail, introduces large instabilities. In turn these instabilities render the integration of the $g_0(x)$ equation quite hazardous. The few cases we have worked out were unsatisfactory, leading to diverging results. It may be due to the finite accuracy of our codes, but it may also underline that expressing $g_0(x)$ in term of a finite polynomial is not sufficient to reach the exact solution.

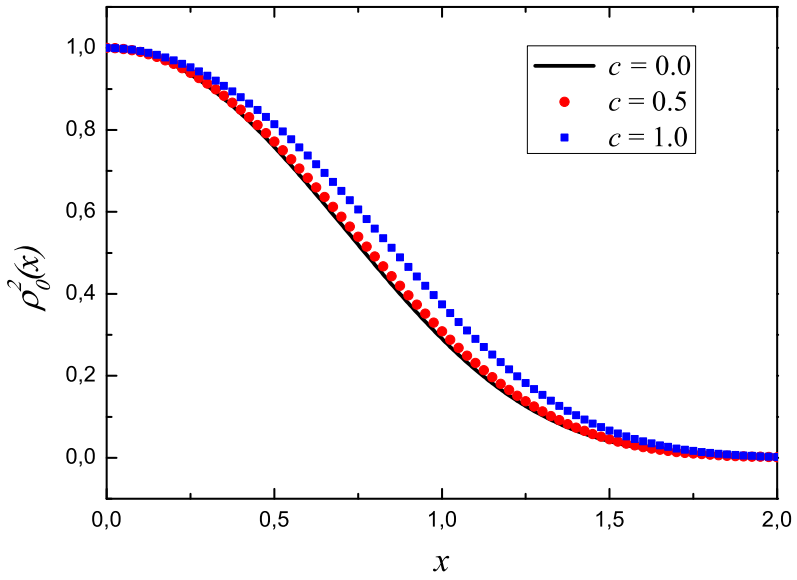

Fig. 1 – The $(x+i\frac{c}{2})^4$ potential. Squared modulus of the ground state wave function as function of x for $c=0$ (full line), $c=0.5$ (filled circles) and $c=1.0$ (filled squares).

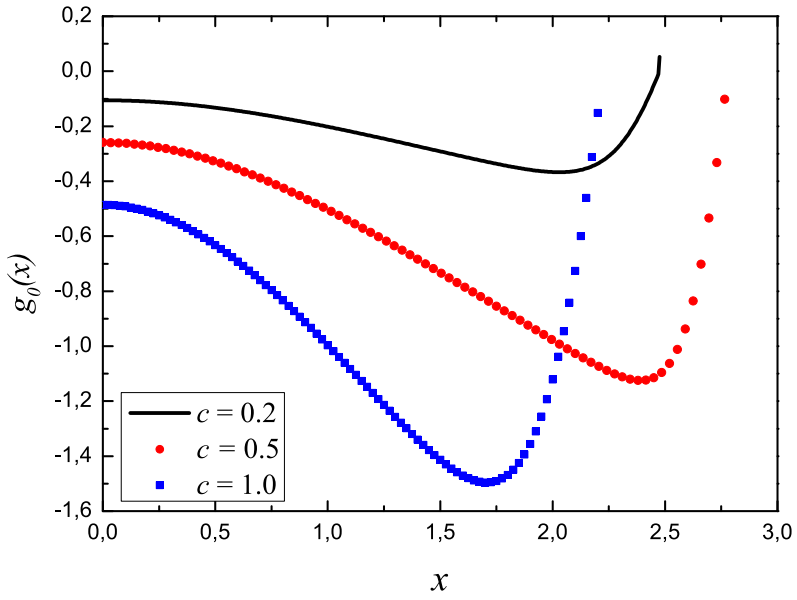

Fig. 2 – The $(x+i\frac{c}{2})^4$ potential. Derivative of the phase of the ground state wave function $g_0(x)$. The full line corresponds to $c=0.2$, filled circles and squares to $c=0.5$ and $c=1.0$, respectively.

We end this study with the following exercise. For $c = 1.0$, starting with $g_{0a}(x)$, we solve Eqs. (28) to get a new phase $g_{01}(x)$. In a kind of first iteration, we search for

$$g_{02}(x) = g_{0a}(x) + \alpha g_{01}(x) \ , \tag{33}$$

such that g_{02} brings the eigenvalue in close agreement with the one given by Eqs. (26). This is achieved with $\alpha = 0.0045$. The smallness of α indicate how close g_{0a} is from the exact solution. As we have checked, the differences appear essentially in the tail of the phase function.

The results are displayed in Table 3 for few solutions of Eqs. (26) very close to the exact one. This naive trick improves all the observables, except $(x + i\frac{c}{2})$, which indicates uncertainties in the imaginary part of the wave function.

Table 3

The $(x + i\frac{c}{2})^4$ potential. Ground state observables obtained from Eqs. (28) by adjusting the phase $g_{02}(x) = g_{0a}(x) + \alpha g_{01}(x)$ as explained in the text are compared to values given by Eqs. (26).

$v_0'(0)$	EQS	E_0	$< (x + i\frac{c}{2}) >$	$< (x + i\frac{c}{2})^2 >$	$< (x + i\frac{c}{2})^4 >$
-0.48566	(26)	0.997864	$-8.0\ 10^{-3}$	0.3649	0.3683
	(28)	0.992594	$-1.1\ 10^{-2}$	0.3622	0.3558
		0.997926	$-1.4\ 10^{-2}$	0.3619	0.3552
-0.48561	(26)	0.997928	$-7.8\ 10^{-3}$	0.3648	0.3679
	(28)	0.992764	$-1.1\ 10^{-2}$	0.3621	0.3554
		0.997920	$-1.4\ 10^{-2}$	0.3618	0.3550
-0.48541	(26)	0.998163	$-7.2\ 10^{-3}$	0.3643	0.3661
	(28)	0.993452	$-1.0\ 10^{-2}$	0.3618	0.3543
		0.997929	$-1.2\ 10^{-2}$	0.3616	0.3540

5. CONCLUSIONS

Complex potentials generated by a complex shift $(x + ic/2)$ of a real even potential are very attractive. In particular, the way to calculate observables is known [1, 10], and thus it gives rise to a coherent quantum mechanics. However, it turns out that the observables are independent on the imaginary shift. For confining potentials, the vacuum energy is affected by the value of c, but the energy differences between the levels are the one obtained for $c = 0$.

The independence of the observables with respect to c has been obtained from basic principles. It has been illustrated by two examples: the harmonic oscillator

and the Pöschl-Teller potential. The case of the $(x+i\frac{c}{2})^4$ potential has been chosen to underline the difficulties encountered when solving the Schrödinger equation for complex potentials.

Concerning the observables, whether a similar situation occurs for other complex potentials with real eigenvalues remains an open question. At first glance it sounds to be different. However, no statement can be made without establishing in each case the way to calculate observables.

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