Finite energy ground states of the −|x|^n potentials

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Finite energy ground states of the $-|x|^n$ potentials.

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Abstract

Infinitely negative potentials have finite ground state energy if use is made of complex wave function. We study a few analytical examples and give numerical solutions for some $-|x|^n$ potentials.

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1 Introduction

The present work has been suggested by the results obtained more than 20 years ago by Bender and Boettcher [1]. In the context of PT-symmetric Non-Hermitian Hamiltonians they solved the Schrödinger equation for the $-(ix)^n$ potentials ($n > 0$). Our attention has been retained by the case n = 4. In ordinary quantum mechanics, $V(x) = -x^4$ has no bound state of finite energy. Integrating the Schrödinger equation along complex paths, Bender and Boettcher found regions of finite energy spectra. These result have incited us to study potentials infinitely attractive at large distances, among which

$$V(x) = -|x|^n \quad , \; n \; > \; 0 \tag{1}$$

is a typical example.

Note that the case $n < 0$ has been discussed in a paper by Yekken *et al* [2], in the context of energy dependent potentials. In the D=1 dimensional space, these potentials have an infinite ground state energy. However, if the coupling constant depends on energy, the ground state energy is finite.

The present approach is, in some sense, the extension of quantum mechanics to the complex plane, which could be useful for pathological potentials. It follows numerous works developed for complex potentials having real eigenvalues (see review articles on this topics, [3, 4, 5]).

To build a coherent quantum mechanics requires to define properly the scalar product and observables [6, 7, ?]. In the present paper we concentrate on the ground state energy and the normalisation of the ground state wave function. Note that it involves the extension of the probability in the complex plane [6, 8].

In a first step, we shall present a few analytical or semi analytical examples. The case $-|x|^n$ shall be treated numerically.

2 Coupled equations in the complex plane

Considering the D = 1 dimensional space with $\hbar = 2m = 1$, we start with the Schrödinger equation

$$[-\frac{d^2}{dx^2} + V(x)]\Psi_j(x) = E_j\Psi_j(x) \; ; \; V(x) \quad \leq \; 0 \tag{2}$$

Note that we restrict our study to symmetric potentials with respect to parity. Let us consider solutions of the form

$$\Psi_j(x) = R_j(x)exp[i\Phi_j(x)] \; , \quad R_j(x) \geq \; 0 \tag{3}$$

It leads to

$$-R_j''(x) - i\Phi_j''(x)R_j(x) - 2iR_j'(x)\Phi_j'(x) + (\Phi_j'(x))^2R_j(x) + V(x)R_j(x) = E_jR_j(x) \tag{4}$$

This is a complex differential equation leading in general to complex eigenvalues. However, real eigenvalues can been obtained by requiring

$$2\Phi_j'(x)R_j'(x) + \Phi_j''(x)R_j(x) = 0 \tag{5}$$

Obviously, the $(\Phi_j'(x))^2$ contribution in Eq. (4) is repulsive, and may compensate the long distance attraction of $V(x)$. A point to be proved, or at least shown by illustrative examples. Eq. (5) is a linear differential equation for the derivative of the phase. Let us write

$$g_j(x) = \Phi_j'(x) \tag{6}$$

The above condition yields

$$g_j(x) = \frac{c_j}{R_j^2(x)} \tag{7}$$

At this stage, the integration constant c_j is undetermined, but setting $c_j = 1$ seems a natural choice. We are left with a highly non linear differential equation for the modulus :

$$-R_j''(x) + V(x)R_j(x) + \frac{c_j^2}{R_j^4(x)}R_j(x) = ER_j(x) \tag{8}$$

The modulus function $R_j(x)$ has to be a real positive function not necessarily of finite norm. In this matter, following Bender and Boettcher [1], the scalar product and the norm are defined by

$$\int_{-\infty}^{\infty} \Psi_j^2(x)dx \;=\; \int_{-\infty}^{\infty} R_j^2(x)exp[2i\Phi_j(x)]dx \tag{9}$$

Note that in this case a finite norm can be ensured by rapid oscillations of the phase function at large distances. Consequently, polynomial $R_j(x)$ are acceptable, for instance.

3 Analytic and semi analytic cases

Actually, though Eq. (8) is highly non-linear, it is not difficult to build analytical cases. Let us consider the almost trivial exponential case :

$$V(x) = -e^{|x|} \tag{10}$$

Dealing only with the ground state, the index j has been dropped from expressions of energy, wave function and phase function. The problme being symmetric we shall consider only the positive x axis. Setting

$$R(x) = e^{-\alpha x/4} \tag{11}$$

in Eq. (8), the resulting equation

$$-\frac{\alpha^2}{16} - e^x + e^{\alpha x} = E \tag{12}$$

is solved for $\alpha = 1$. The ground state energy is negative but finite. Furthermore, the phase function $\Phi(x)$ admits an analytical form :

$$\Phi(x) = \int_0^x g(t)dt = \int_0^x e^{t/2}dt = 2[e^{x/2} - 1] \tag{13}$$

The norm is given by

$$N = 2\int_0^\infty e^{-x/2}\cos\left[4(e^{x/2} - 1)\right]dx = 16\int_0^\infty \frac{cos(y)}{(y+4)^2}dy \tag{14}$$

where we have set

$$4(e^{x/2} - 1) = y \tag{15}$$

This integral admits a analytical expression in terms of $Si(4 + y)$ and $Ci(4 + y)$, the sine- and cosine-integrals.

Another example is provided us by

$$V(x) = -\cosh(x) - \frac{5}{16}\frac{1}{\cosh^2(x)} \tag{16}$$

In this case, the solution is given by

$$R(x) = \cosh^{-1/4}(x) \quad \text{with} \quad E = -\frac{1}{16} \tag{17}$$

3.1 A polynomial form.

To get closer to the $-|x|^n$ potentials, let us consider

$$V(x) = \frac{n}{4}x^2\left[\frac{(3 + n/4 + x^2)}{(1+x^2)^2}\right] - (1+x^2)^{n/2} \tag{18}$$

This potential tends asymptotically to $-|x|^n$. The function

$$R(x) = \frac{1}{(1+x^2)^{n/8}} \tag{19}$$

solves Eq (8) with an eigenvalue of $E = \frac{n}{4}$.

The phase function takes the form

$$\Phi(x) = \int_0^x (1+t^2)^{n/4}dt \tag{20}$$

It corresponds to a compact expression in few cases like

$$n = 2 \quad : \; \Phi(x) = \frac{x}{2}\sqrt{(1+x^2)} \tag{21}$$

$$n = 4 \quad : \ \Phi(x) = x + \frac{x^3}{3} \tag{22}$$

The general expression is an hyper-geometric function :

$$\Phi^{(n)}(x) = x \ {}_2F_1(1/2, -n/4; 3/2; -x^2) \tag{23}$$

At this point, we recall the importance of the phase function to ensure the normalisation of the wave function. As $R(x)$ is decreasing with $1/x^n$ asymptotically, its norm or higher moments are not necessarily finite a priori. However, because the phase is varying very rapidly as x increases, the integrand is averaged to zero beyond a certain value of x. Thus, the norm and the moments get stabilised.

3.2 Numerical examples.

We end up this section by presenting numerical results for two polynomial potential of the above form with n = 2 and n = 4.

The Eq. (8) with $V(x)$ given by Eq. (18) is solved by fixing the energy E and the boundary conditions $R(0) = 1$ and $R'(0) = 0$, by using the Runge-Kutta method. A priori, all solutions with $R(x)$ definite positive and with no singular behaviour are acceptable. We do not get a single energy but an area of energies. Thus, a criterion has to be found to single out the solution corresponding to the analytical energy.

In terms of self-consistency, Eq. (8) admits a unique solution for $R(x)$. Instead, the Runge-Kutta method provides us with an ensemble of $R(x, E_{RK})$, from which effective potentials can be calculated and introduced in the Schrödinger equation.

If the $R(x, E_{RK})$ calculated from Runge-Kutta is the correct one, it must solve the corresponding Schrödinger equation with the same energy, which we quote E_S. Consequently, $E_{RK} = E_S$ should be the criterion to select the correct energy. For all other E_{RK} energies, the effective $V(x)$ potential is different from the original one, resulting in $E_{RK} \neq E_S$. A sample of results are displayed in table 1 for the cases n= 2 and 4. They show the necessary precision of the numerical codes to select the solution on the energy basis.

A second criterion is provided us by the behaviour of the wave functions. It appears that the $R(x)$ corresponding to the analytic energy is the one extending over the longest distance and showing the less oscillations. The situation is even clearer with $S(x)$. Not only the analytic energy yields the wave function extending over the larger distance but for other energies the corresponding $S(x)$ diverge rapidly. These results are illustrated in figs 1 and 2.

We end up this section with the question of the norm. As stated above, the normalisation of $R(x)$ depends essentially on the phase function $\Phi(x)$. Typically, we get for n = 2

$$\int_0^\infty R^2(2,x)dx = \int_0^\infty \frac{1}{\sqrt{(1+x^2)}}dx = \log(x + \sqrt{(1+x^2)}|_0^\infty \tag{24}$$

Table 1: Results for the n = 2 and 4 cases of the potential (18). The eigenvalue range of acceptable solutions of the Runge-Kutta method is given. Selected eigenvalues around the analytical value are compared for the Runge-Kutta method and the Schrödinger equation.

n	Eigenvalue range	Runge-Kutta	Schrödinger	x_{max} for S(x)
2	E = 0.42 - 0.59	0.45	0.4506	67.1
	x_{max} = 290 for R(x)	0.50	0.5000	290
		0.55	0.5506	67.8
4	E = 0.54 - 1.59	0.60	0.6116	8.9
		0.70	0.7097	9.5
		0.80	0.8075	10.4
		0.90	0.9049	12.0
	x_{max} = 91 for R(x)	1.00	1.0000	35.5
		1.10	1.1049	12.1
		1.20	1.2076	10.6
		1.30	1.3098	9.8
		1.40	1.4118	9.3
		1.50	1.5135	8.9

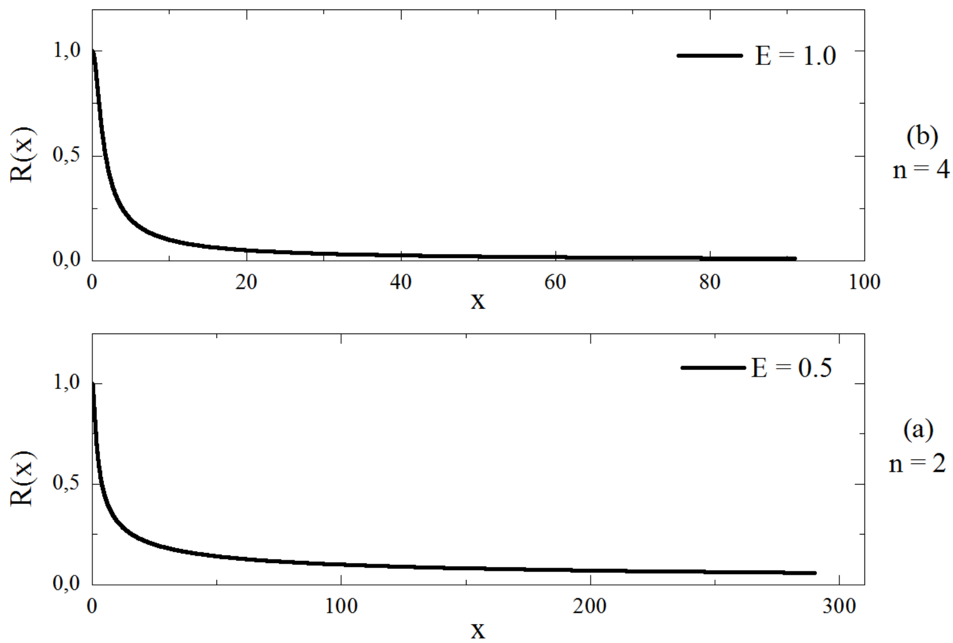

Figure 1: Runge-Kutta wave functions in the case n = 2 and 4.

which is logarithmically diverging.

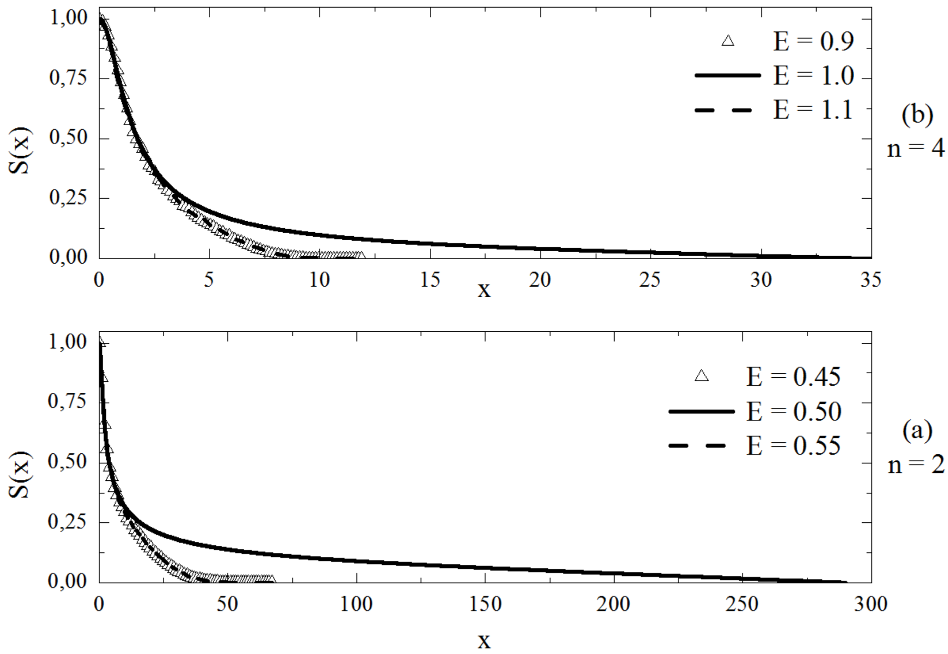

Figure 2: Schrödinger wave functions in the cse n = 2 and 4.

For n = 2 and 4, we have integrated Eq. (9) between 0 and a variable limiting x_L. The results are displayed in fig 3. They show the asymptotic result of the norm to be rather rapidly obtained.

4 The $-|x|^n$ potentials.

The same strategy is applied to the $-|x|^n$ potentials. Solving Eq. (8), the solutions yielding positive definite $R(x)$ are retained. This procedure determines areas of acceptable energies. Inserting $1/R(x)^4$ as an effective potential in the Schrödinger equation, we select the energy in closest agreement with the one obtained with the Runge-Kutta method. It also corresponds to the largest extension of the wave function.

The results are displayed in table 2 for $2 \leq n \leq 5$. As a function of n, the energies are well fitted by

$$0.928 + 0.247n - 0.018n^2 \tag{25}$$

It suggests the arising of a maximum at or beyond n = 7. This conjecture is supported by the fact that for $V(x) = -e^x$, considered as the limit of $-x^\infty$, the energy is slightly negative.

As far as the wave functions are concerned, examples of $R(x)$ and $S(x)$ are showed in fig 4 and

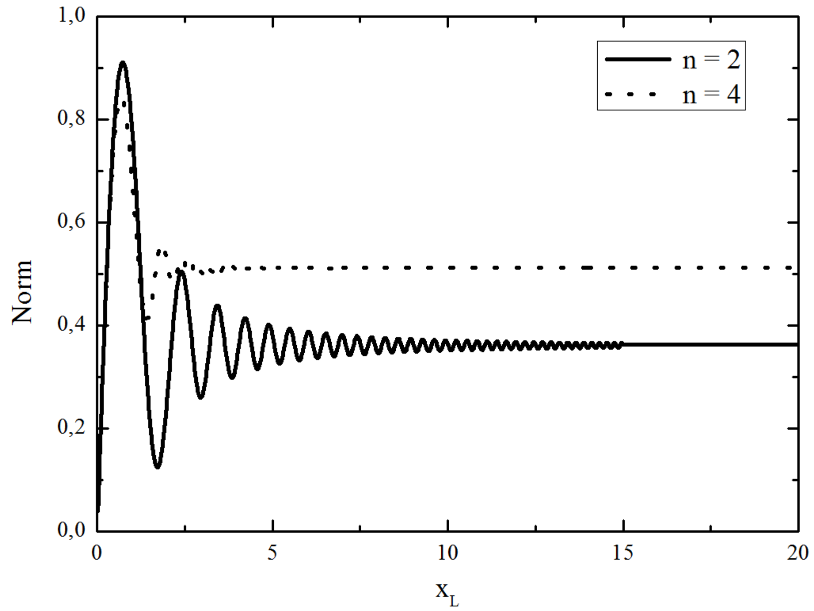

Figure 3: Norm of the ground state wave function in the case n = 2 and 4 as function of x_L, the upper limit of the integral.

5.

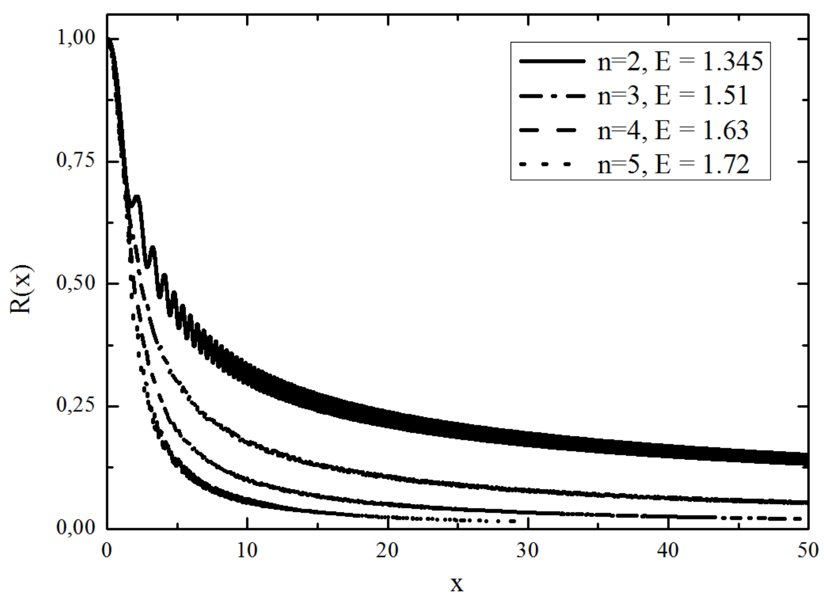

Figure 4: Runge-Kutta wave functions of $-|x|^n$, for n = 2,3,4 and 5.

Table 2: The eigenvalue ranges and selected eigenvalues solutions of the Runge-Kutta and Schrödinger equations for the $-|x|^n$ potentials with $2 \leq n \leq 5$

n	Energy range	Runge-Kutta	Schrödinger	x_{max}
2	1.27 - 1.43	1.345	1.3471	39.7
2.5	1.32 - 1.57	1.44	1.4426	27.1
3	1.27 - 1.80	1.51	1.5124	21.8
3.5	1.24 - 1.99	1.57	1.5705	30.5
4	1.23 - 2.14	1.63	1.6341	12.3
4.5	1.25 - 2.24	1.67	1.6777	8.8
5	1.28 - 2.29	1.72	1.7314	7.0

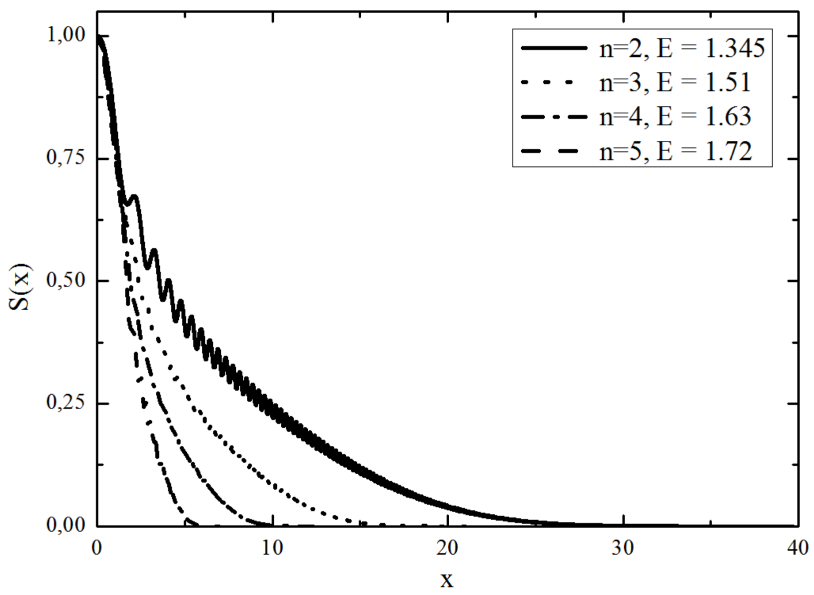

Figure 5: Schrödinger wave functions of $-|x|^n$, for n = 2,3,4 and 5.

5 Conclusions.

This paper is dealing with aspects of the quantum mechanics in the complex plane, i.e. when the wave function is a complex function. This extension has no impact in the case of ordinary potentials. Here, it allows to find finite energy solutions for potentials infinitely negative at large distances.

The problem is well defined mathematically. Physically it still requires further studies. The first question concerns the definition of observables, which will be the subject of future work.

Secondly we may search for the domain of application of the present method. A point we also keep for further investigations.

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