PT - symmetry rules applied to a class of real potentials.

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Abstract

Extending the functional space to complex eigenfunctions [1], we have shown that infinitely negative potentials at large distances admit finite energy states. The used techniques are similar to the ones applied in the case of PT symmetric complex potentials with real eigenvalues. We present the lowest part of the spectra for $-|x|^n$ potentials with $4 \leq n \leq 8$. We also discuss the norm and orthogonality of the wave functions.

Keywords : Quantum mechanics, complex wave functions, asymptotically negative potentials.

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1 Introduction

The starting point of the present work takes its roots in a paper by Bender and Boettcher [2]. These authors have obtained spectra of real eigenvalues for the $-(ix)^n$ potentials. This case belongs to the class of complex potentials having real eigenvalues, in particular potentials symmetric under parity and time reversal transformations (see, for instance, [3, 4, 5, 6, 7, 8, 9, 10]).

For $n = 4$, the potential reads $- x^4$. The ordinary quantum mechanics rejects such potentials, being infinitely negative at large distances. Intuitively it does not correspond to any simple physical situation, like the Coulomb or harmonic oscillator potentials. A possible state would acquire an infinite energy and its wave function would primarily be located at an infinitely large distance. Obviously, the finite energy spectrum obtained by Bender and Boettcher comes from the extension of the Schrödinger equation to the complex plane.

On the ground of this result, it was very tempting to check how it could be generalised to the $-|x|^n$ potentials, and more generally to potentials negative at large distances. The challenge is only possible by considering complex wave functions. As we shall see, a variable phase function generates a real confining potential, which can compensate the negative potential at large distances.

Although the problem looks as a mathematical curiosity at first glance, without physical implication, we know 2 cases in which it may have an impact. The first one concerns the calculation of the heavy quark systems. Considering the scalar confining potential γr coming from the one gluon exchange [11], the Klein-Gordon equation reads

$$p_0^2 \Psi(r) = [2p_0 r - r^2 + p^2 + m^2]\Psi(r) \ ,$$

where p_0 and p^2 are the relativistic and kinetic energies, respectively, and m the quark mass. The $-r^2$ term is neglected or ignored if use is made of the Bethe-Salpeter equation. Our method may induce a new handling of this problem.

The second example is the Glauber quantum oscillator, which contains a $-x^2$ potential [12]. A physical realisation has been obtained recently in non linear optics by Gentilini *et al* [13].

Our approach is very similar to the one applied to complex potentials having real eigenvalues, and being symmetric under parity and time reversal operations. The wave functions are complex and the Schrödinger equation gives rise to 2 coupled differential equations. Solutions are numerous and the trick is to select the ones satisfying the rules of quantum mechanics.

Our first results have been published in 2 papers [1, 14]. The present work completes our studies with a special attention to the $-|x|^n$ potentials with $4 \leq n \leq 8$, for which we give their 4 lower states.

The paper is organised as follows. The basic elements of our method are sketched in section 2. A semi-analytic example is presented in section 3 . The $-|x|^n$ potentials are discussed in section 4, followed by conclusions.

2 Sketching the method.

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

$$[-\frac{d^2}{dx^2} + U(x)]\Psi_k(x) = E_k\Psi_k(x). \tag{1}$$

For the potentials studied here, the wave functions have to be complex, and take the general form

$$\Psi_k(x) = R_k(x)exp[i\Phi_k(x)] \ , \quad R_k(x) \geq \ 0. \tag{2}$$

It leads to

$$-R_k''(x) - i\Phi_k''(x)R_k(x) - 2iR_k'(x)\Phi_k'(x) + (\Phi_k'(x))^2R_k(x) + U(x)R_k(x) = E_kR_k(x) \ . \tag{3}$$

Requiring real eigenvalues implies the complex terms to vanish :

$$2\Phi_k'(x)R_k'(x) + \Phi_k''(x)R_k(x) = 0 \ . \tag{4}$$

By setting

$$g_k(x) = \Phi_k'(x) \ , \tag{5}$$

we are left with a linear differential equation for the derivative of the phase function.

It yields

$$g_k(x) = \frac{c_k}{R_k^2(x)} \ , \tag{6}$$

The factor c_k may contain an integration constant. Here, we fix c_k to unity. As a result, $R_k(x)$ must satisfy the highly non-linear differential equation :

$$-R_k''(x) + U(x)R_k(x) + \frac{1}{R_k^4(x)}R_k(x) = E_k R_k(x) \ . \tag{7}$$

This equation is solved numerically via a Runge-Kutta routine. Its algorithm requires the extrapolation of $R_k(x)$ to define the repulsive part of the potential arising from the phase function. Excellent results are obtained by choosing a sufficiently small mesh and a Taylor expansion of $R_k(x)$ up to second order.

Equation (7) yields an approximate asymptotic behaviour for $R_k(x)$. For instance, at large distances it decays like $1/|x|^{n/4}$ for $U(x) = -|x|^n$, and $e^{-\gamma/4}$ for $U(x) = -e^{\gamma x}$.

As far as the boundary conditions are concerned, the value $R_k(0)$ is not given a priori and must be chosen, while $R_k'(0) = 0$ is imposed. According to the above paragraph, we search for $R_k(x)$ decaying to zero with a zero derivative.

These conditions are not sufficient to define the desired solution. Actually, because of the non-linearity of the differential equation, most of the solutions undergo oscillations. The expected modulus function and its derivative have to be continuous. In practice, we retain the modulus function closest to zero at the largest distance, and corresponding to the minimum of fluctuations.

On the other hand, if $R_k(x)$ is the "correct" solution, it can be used in a Schrödinger equation with $U_{ef}(x) = U(x) + 1/R_k^4(x)$ as effective potential. The energy obtained in this way must be equal to the one coming from the Runge-Kutta routine. Equating the 2 energies provides a particularly useful criterion.

Finally, the last point concerns the definition of the spectrum. In the usual Schrödinger case, the criterion is based on the parity and the number of nodes of the wave function. This is not possible here, because of the positive character of the modulus function. Consequently, a first way of ordering the levels is to consider their rank in the energy scale of the solutions.

Furthermore, because the derivative of the modulus function is an odd function with zeros, the number of these zeros can be used to define the order of the levels. In fact, it turns out that the modulus function has a reminiscence of the behaviour of the usual wave function, the zeros being replaced by fluctuations of $R_k(x)$, namely minima and maxima.

Nota Bene : because of the symmetry properties of the problem, we essentially work on the positive x half plane.

The modulus function $R_k(x)$ is a real, even positive function.On the other hand, the phase function, obtained by integrating $g_k(x)$, is obviously odd. Consequently, the wave function $\Psi_k(x)$ is invariant under successive time reversal and parity operations. This is very similar to the case of PT-symmetric complex potentials. It ensures the continuity equation to be fulfilled (see [5, 6, 7, 10] for details. The scalar product is defined by

$$\int_{-\infty}^{\infty} R_k^2(x) exp[2i\Phi_k(x)]dx \;=\; 2\int_0^{\infty} R_k^2(x)\cos[2\phi_k(x)]dx. \tag{8}$$

This definition ensures finite norms of the wave functions. It corresponds to an extension of the concept of probability in the complex plane [15]. Note that the cos term oscillates rapidly as the phase function becomes large. Beyond a given point, the contributions to the norm average to zero. Consequently even slowly decreasing $R_k(x)$ are normalisable.

While applying this definition of the norm, we found that for odd k state, the result comes with a negative sign. To remedy this situation, we impose a $\pi/2$ shift of the phase function for odd k, namely

$$\Psi_k(x) \to e^{i\pi/2}\Psi_k(x) \text{ for } k \text{ odd } . \tag{9}$$

This is justified by the following argument. The continuity with the usual case of real wave function is obtained by letting

$$\phi_k(x) \to 0 \ . \tag{10}$$

In this limit, the parity of the wave functions is ensured by the real parts :

$$\cos[\phi_k(x)] \text{ for } k \text{ even} \quad \text{and} \quad \sin[\phi_k(x)] \text{ for } k \text{ odd} \ , \tag{11}$$

as implied by the shift.

3 Semi-analytic examples.

As in ordinary quantum mechanics, it is possible to generate analytical or semi analytical cases. They are very efficient in illustrating the method and the situation. The procedure is relatively simple for ground states. The case of excited states is complicated by the absence of zeros of the modulus function, and will not be considered in the present work.

Postulating a form for $R_0(x)$, the phase function and the corresponding potential can be constructed. Similarly, one can start from the phase function, though this way may be less convenient. In our first paper on the subject [1], a couple of cases have been given. Here, we restrict our choice to potentials approaching $U(x) = -|x|^n$ at large distances. It generalises a similar example given previously [1].

Let us consider

$$R_0(x) = (1 + ax^2)^{-p} \ . \tag{12}$$

This is the solution for

$$U(x) = 2pa^2x^2\ \frac{3 + 2p + ax^2}{(1 + ax^2)^2} - (1 + ax^2)^{4p} \ . \tag{13}$$

The eigenvalue is given by

$$E_0 = 2ap \ . \tag{14}$$

The simple form of the ground state energies offers an opportunity to check our Runge-Kutta code. Actually they are reproduced to better than a 0.1 % accuracy.

The phase function in terms of the hyper-geometric function by

$$\phi_0(x) = x_2F_1(1/2, -2p; 3/2; -ax^2) \ . \tag{15}$$

For the sake of illustration, we look at 2 cases $p = 1/2$ and $p = 1$. In both cases, the phase function is a polynomial :

$$p = 1/2 \quad : \ \phi_0(x) = x + \frac{x^3}{3} \ , \tag{16}$$

$$p = 1 \quad : \ \phi_0(x) = x + \frac{2}{3}x^3 + \frac{1}{5}x^5 \ . \tag{17}$$

The numerical calculation of the norms is straightforward, the modulus and the phase functions being analytic. The results are displayed in fig. 1. As expected the norm becomes stabilised at large distances. The threshold of the 0.1 % stability is reached around $x = 5$ for 1/2 and $x = 2.5$ for 1.

As an exercise, we found interesting to determine the first excited state. The results are summarised in table 1. We note the large gap between the ground and first excited states. It is related to the low value of $R_1(0)$, simulating a large confining potential already at short distances. Somehow it reflects the situation of the ordinary potential, for which the odd wave functions are zero at $x = 0$.

The figures 2 and 3 show the modulus functions and their derivatives. We note the large difference in scale between $p = 1/2$ and $p = 1$. An effect of the confining potential needed to balance the negative part of the potential. As stated above, we remark that the ground state derivative is zero at the origin and at infinity, while for the first excited state a zero exists at an intermediate value of x.

Finally, we checked the orthogonality between the ground and excited state wave functions. It is fulfilled to the level of 1 %.

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

The question of the $-|x|^n$ potentials has already been touched in our previous publications [1, 14]. Here we present results for the 4 lower states of potentials with $4 \leq n \leq 8$. This choice is motivated by the fact that for low n, the modulus function extends over very large distances. At the other limit, if n is too large, the confining effect of the phase function confines the modulus function to a very small space. In both cases it generates numerical difficulties unnecessary to overview the problem.

The results for the spectra of the 5 potentials are displayed in table 2. The $R_k(0)$ values and the energies are listed. The n dependences are non-monotonic for both quantities, with a minimum appearing between $n = 7$ and $n = 5$ according to k. Note that for $n = 4$, the present result is in good agreement with the value given by Bender and Boettcher [2].

In view of the confining aspect of the spectra, it is tempting to search for approximate potentials reproducing the energies. In principle, with a large enough ensemble of levels, it could be possible to construct local equivalent potentials [16, 17]. In the present case, among various possible hypothesis, we got inspired by the $-(ix)^3$ potential previously treated by the inverse problem techniques. In this case we found the local equivalent potential to be dominated by x^3 [17]. Consequently, we have tried the simple form

$$U(x) = \lambda |x|^n \ , \tag{18}$$

adjusting the coefficient λ to the ground state energy. Denoting the approximate energies by ϵ_k, we display in table 3 the ratio ϵ_k / E_k for the 3 excited states. The agreement reaches almost 90 % for n = 4, and is regularly improved as n increases.

Because the ground state energies are the simplest to calculate, this approximation offers perhaps a useful lower bound estimate of the excited state energies. However, this conclusion is obtained from a small number of cases, and should be tested over a larger sample.

Concerning the modulus functions and their derivatives, results are displayed in figs 4-7 for n = 4 and n= 8. They are well representative of the general behaviour of these 2 functions.

The interesting point concerns the derivatives. They all start with 0 at the origin, and tend to 0 with a 0 tangent at large distances, ideally at infinity, by negative values. In the intermediate range, the number of zeros is linked to the index k of the state. It corresponds to the fluctuations of the modulus function, which reflects the zeros of the wave function in the ordinary real potential case. This is illustrated by figs. 8 and 9 showing the modulus function derivatives at short distances for k = 2 and 3, n = 4 - 8. Consequently, this characteristic gives a way to order the excited levels.

Concerning the orthogonality of the wave functions, they have been checked, and results are displayed in tables 4 and 5 for n= 4 and 8. Generally speaking, the integrals are of the order of 10^{-5}, while the norm reach about 10^{-2}. Thus the orthogonality is satisfied at the 0.1 % level, which underlines the difficulty to get numerically accurate wave functions, in particular modulus functions.

5 Conclusions.

In recent works, we have shown that real potentials, infinitely negative at large distances, possess finite energy states. This is obtained by using complex wave functions. The applied

techniques are very similar to the one used in the case of PT symmetric complex potentials with real eigenvalues.

The wave function is expressed as the product of a modulus and a phase functions. The differential equation for the modulus part is highly non-linear but can be solved by a Runge-Kutta algorithm. The number of solutions is infinite, and criterions are needed to select the solution corresponding to a quantum mechanical case.

In the present work, the method has been applied to a semi analytic case, which means analytic for the ground state, and for $-|x|^n$ potentials with $4 \leq n \leq 8$. The results underline a confining aspect of the spectra. The behaviours of the modulus functions and their derivatives exhibit analogies with wave functions of ordinary real potentials. The number of zeros of the derivatives gives a way to fix the state ordering.

The next step in this framework is the calculation of observables. Because a real spectrum can be reproduced by a local equivalent potential [16], this point is essential to check the relevance of dealing with potentials negative at large distances. It requires the proper definition of observables. A point to be discussed in future works.

As far as physical implications are concerned. Two examples have been quoted in the introduction. We note also that, in some sense it remains us the case of curved waveguides, which exhibit bound states in an unusual situation [18, 19, 20, 21].

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p	1/2	1
$R_(0)$	1.0	1.0
E_0	1.0	2.0
$R_1(0)$	0.3270	0.293
E_1	86.45	134.660

Table 1: Modulus wave functions at the origin and energies of the ground and first excited states for the potential (13) for $p = 1/2, a = 1$ and $p = 1, a = 1$.

	k= 0	k = 1	k = 2	k = 3
n = 4				
$R_k(0)$	1.051	0.6325	0.5396	0.4823
E_k	1.4768	6.006	11.8028	18.4757
n = 5				
$R_k(0)$	1.139	0.6356	0.5462	0.48605
E_k	1.385	5.396	11.3718	17.8922
n = 6				
$R_k(0)$	1.2146	0.62251	0.551825	0.4814
E_k	1.3547	5.2628	11.2351	18.4974
n = 7				
$R_k(0)$	1.28194	0.604304	0.55662	0.4763065
E_k	1.3510	5.2645	11.3491	19.0633
n = 8				
$R_k(0)$	1.34355	.5845938	0.562008	0.4702378
E_k	1.3599	5.32048	11.55998	19.65285

Table 2: Values of $R_{n,k}(0)$ and $E_{n,k}$ for $-|x|^n$ potentials with $4 \leq n \leq 8$.

		ϵ_k/E_k		
n	λ	k = 1	k = 2	k = 3
4	2.6955	0.867	0.880	0.878
5	2.218	0.952	0.920	0.943
6	1.9952	0.974	0.955	0.943
7	1.790	0.986	0.973	0.969
8	1.674	0.992	0.983	0.979

Table 3: Ratio between the approximated energies obtained from the multiplicative potentials $\lambda|x|^n$ and the exact values E_k. λ is adjusted to the ground states energies.

$n = 4$			
	k = 1	k = 2	k = 3
k = 0	-i 9.33 10^{-5}	2.35 10^{-5}	-i 1.25 10^{-5}
k = 1		i 4.08 10^{-5}	4.81 10^{-5}
k = 2			0.91 10^{-5}

Table 4: Test of the orthogonality. The modulus functions are not normalised.

$n = 8$			
	k = 1	k = 2	k = 3
k = 0	-i 3.3910^{-4}	7.8810^{-5}	i 5.06 10^{-5}
k = 1		i 0.36 10^{-5}	- 0.65 10^{-5}
k = 2			-i 0.14 10^{-5}

Table 5: Test of the orthogonality. The modulus functions are not normalised.

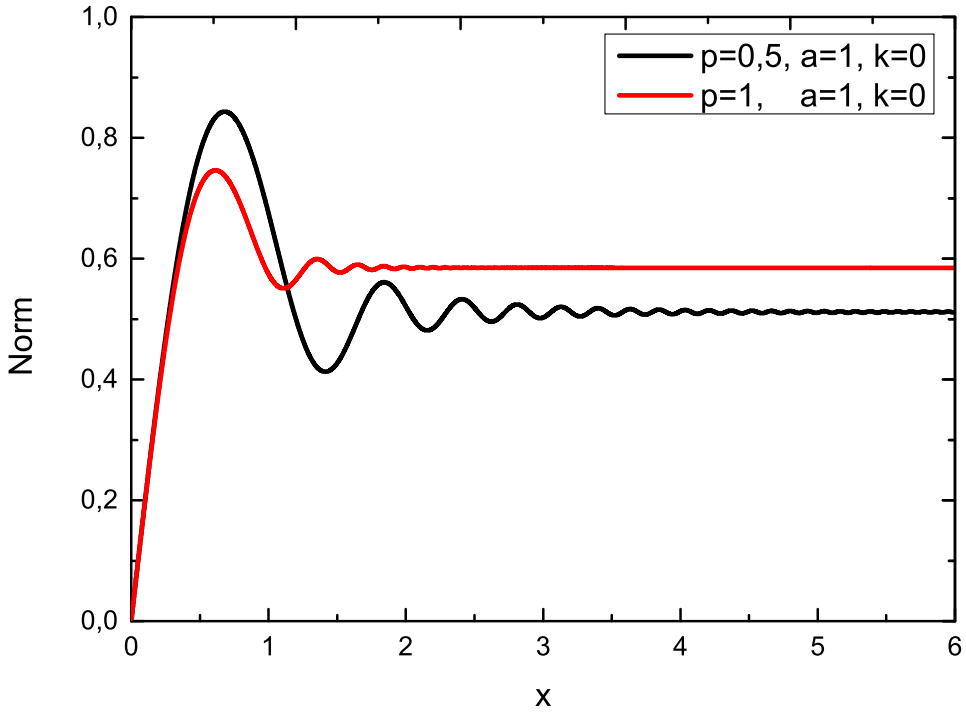

Figure 1: Norm of the wave function as function of the upper integral limit for the case p = 1/2 and 1, respectively.

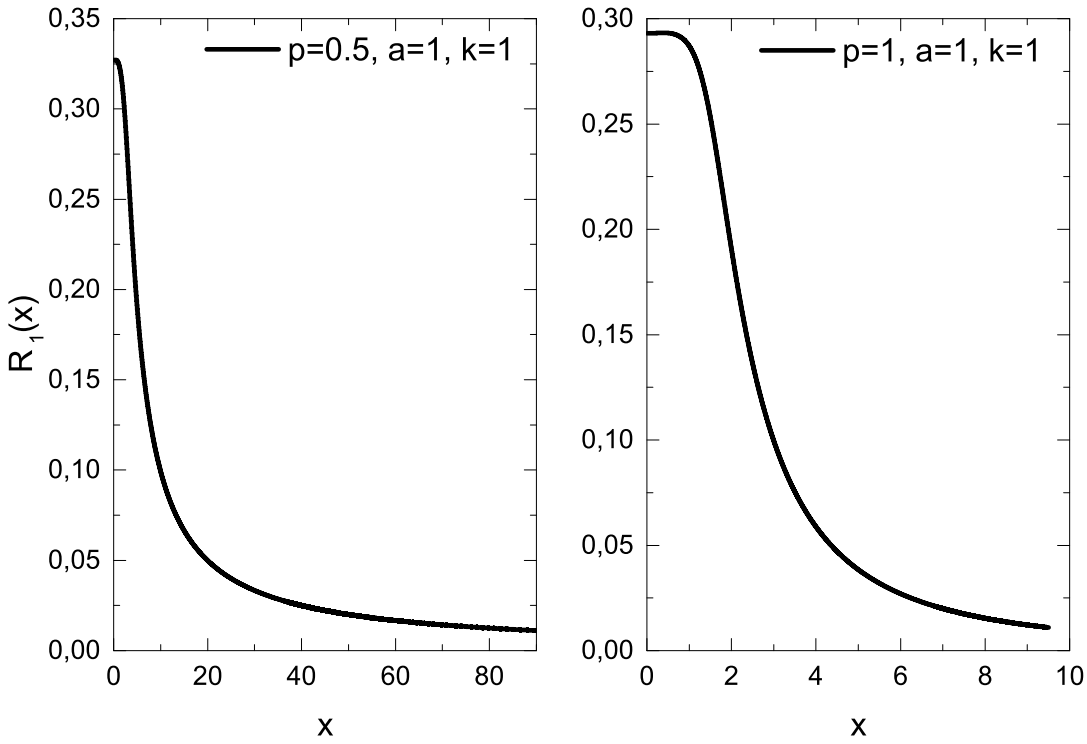

Figure 2: Modulus function of the first excited state for p = 1/2 and 1, respectively.

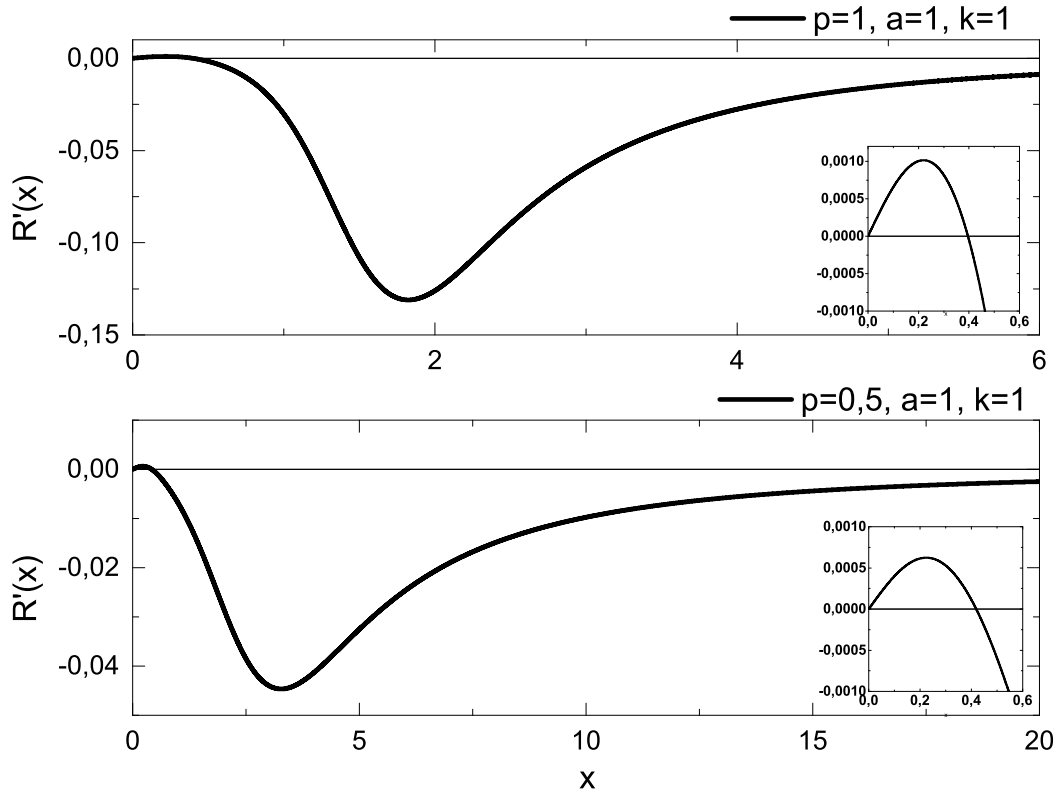

Figure 3: Derivative of the modulus function of the first excited state for p = 1/2 and 1, respectively, the behaviour near the origin is also shown.

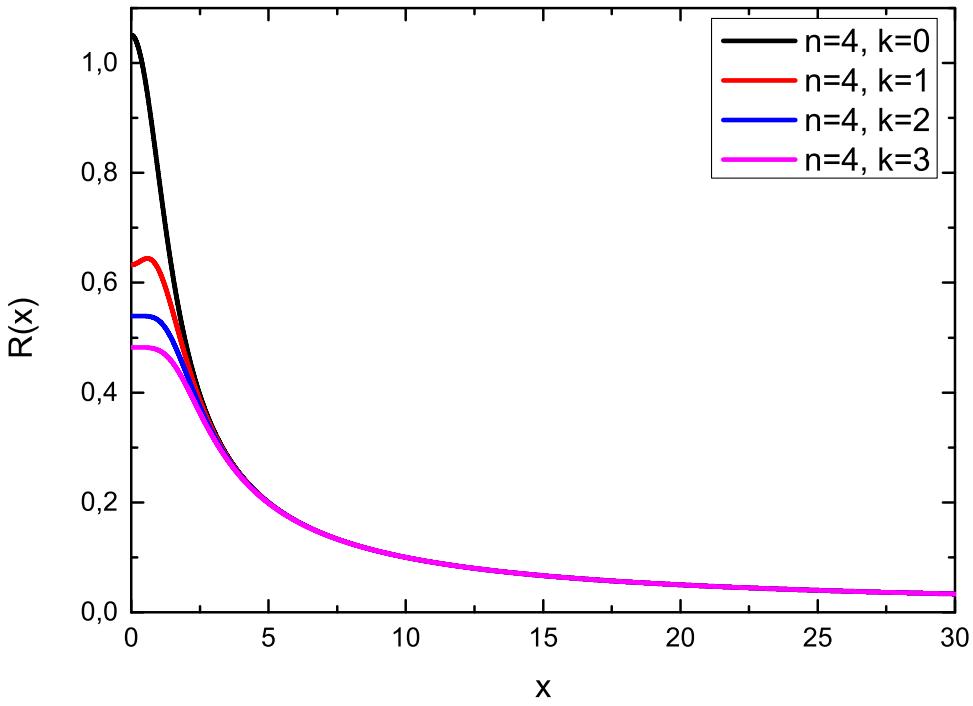

Figure 4: Modulus functions of the 4 lowest states for n = 4.

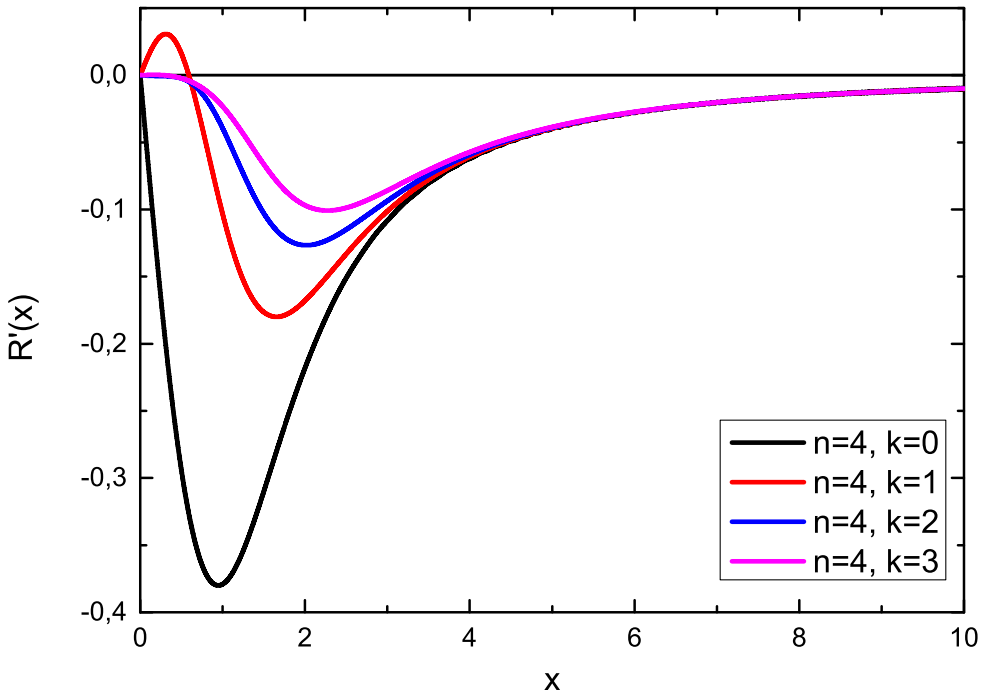

Figure 5: Modulus function derivatives of the lowest 4 states for n = 4.

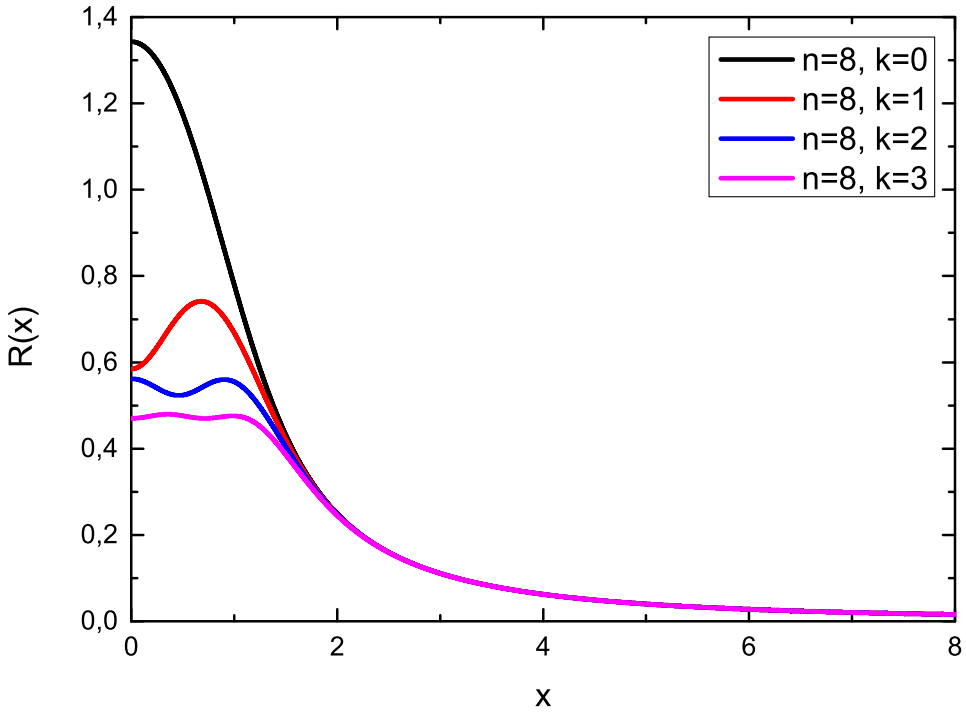

Figure 6: Idem Fig 4 for n = 8.

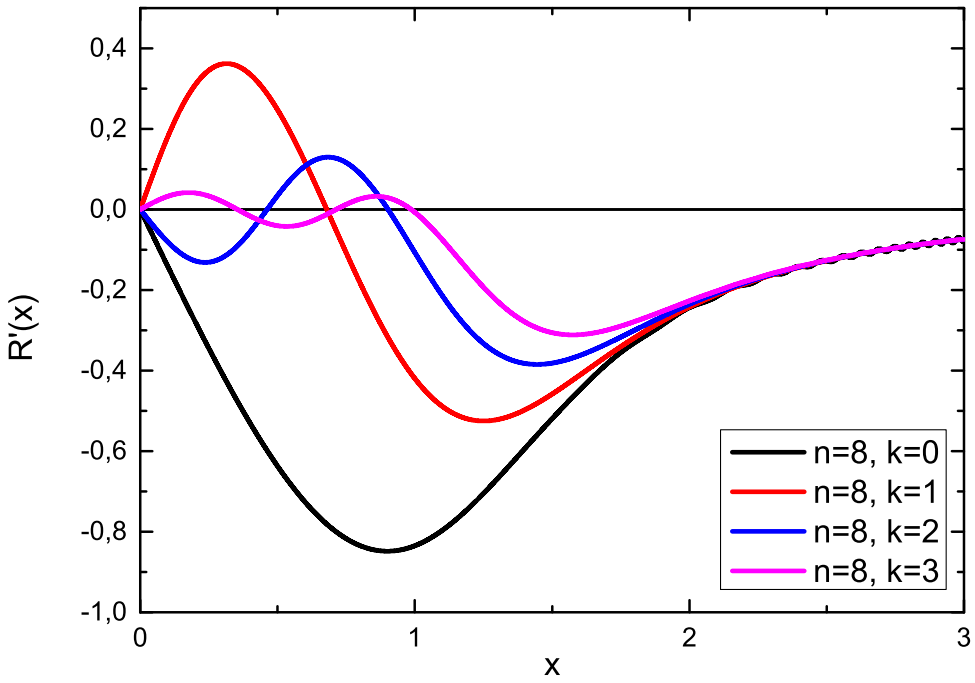

Figure 7: Idem Fig 5 for n = 8.

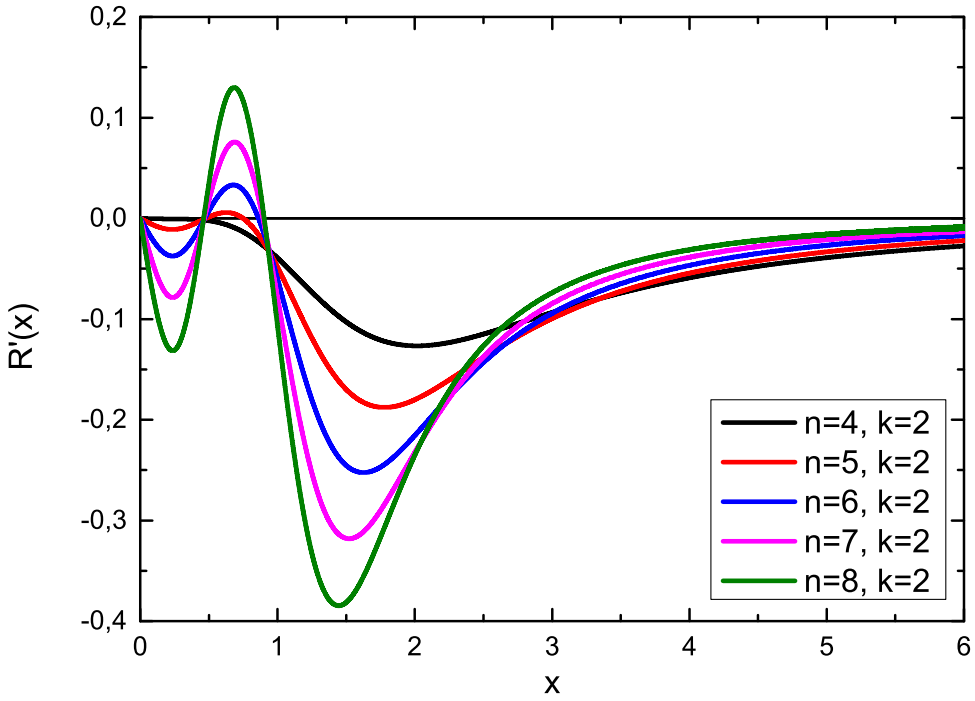

Figure 8: Modulus function derivatives at short distances of the second excited states as function of n.

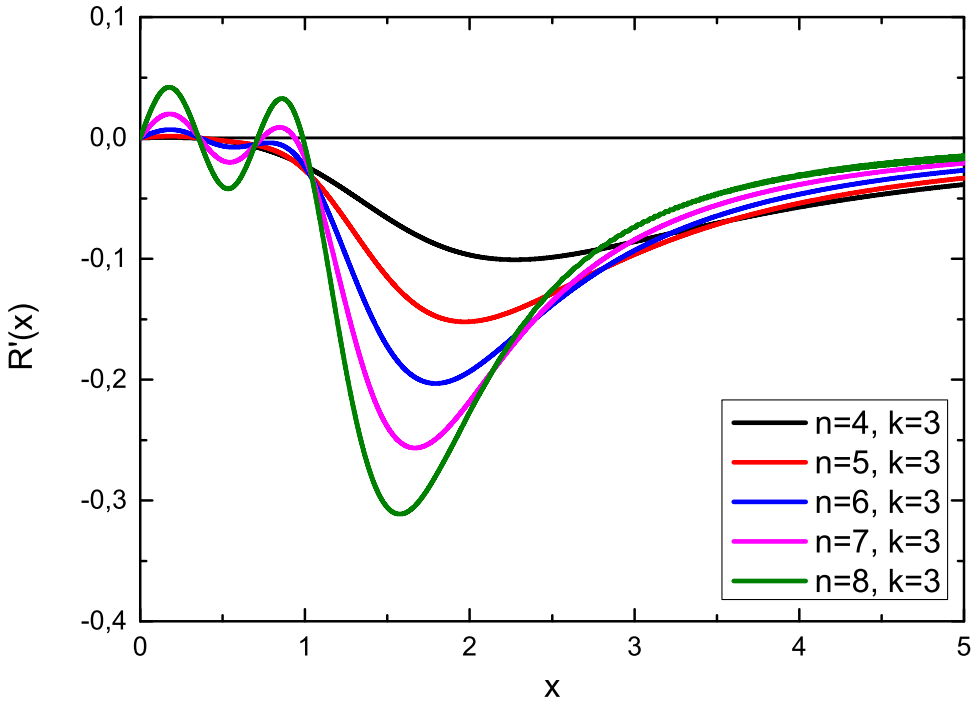

Figure 9: Idem Fig 8 for the third excited state.