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Study of the singular anharmonic potentials by means of the analytic continuation method

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Abstract. Here we study the singular anharmonic potentials by applying the analytic continuation method of Holubec and Stauffer. In order to do that we have developed several approximations to the problem, because this method cannot be applied when the solution has essential singularities at any point of its domain. All the options here shown have the same precision, giving us the eigenvalues correct to all the decimal places provided by the computer.

1. Introduction

There are a number of cases where the use of singular potentials is of interest physically and mathematically [1–4]. It is known the difficulty in obtaining accurate solutions and eigenvalues to the Schrödinger equation when the potential has singularities stronger than r^{-2}. Some of these potentials appear in quantum physics and are the so called anharmonic singular potentials [2–7] which, in general can be written as

$$V(r) = r^2 + \sum_{n=1}^{N} \frac{b_n}{r^{\alpha_n}} \tag{1}$$

where $r \in [0, \infty)$, the parameters α_n are positive real numbers and, at least one of them is greater than 2. Also, much attention has been paid to the perturbative solution of the spiked harmonic potential [8, 9] defined as

$$V(x) = x^2 + \lambda |x|^{-\alpha} \tag{2}$$

where α is a positive real number. If $\alpha \geqslant 2$ the eigenfunctions must take the value zero at the origin and then we can look this problem as a particular case of (1) in the s-wave.

Different methods have been used in order to solve the anharmonic singular potential, such as numerical integration of the differential equation [6, 9], perturbative schemes specially developed for this type of potential [1, 2, 4, 10], and variational methods [7, 9, 11]. The perturbative approximation has been studied particularly extensively because of the difficulty in applying it. The reason lies in that no one terms in the potential dominates over the others: the r^2 term is more important for large values of r and the $r^{-\alpha_n}$ terms are much larger near the origin. So, only when the parameters b_n are quite small is the convergence of the series expansion acceptable. Also, perturbative expansions have been performed which give good results for large values of the coupling parameter [9]. In any case, none of the methods used to obtain the eigenvalues allows us to obtain a precision greater than six or seven decimal places.

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Neither do classical numerical integration methods work with the precision that they provide where the potential is less singular. This is because, as Killinbeck stated [6], the exact wavefunction has an essential singularity at the origin when the potential is of the type given by (1), and the energy of the bound states has an anomalous behaviour in terms of the integration step, such as occurs with the Numerov method. One can use the more elementary method of discretization for the second derivative, thus avoiding all these problems, because in this way we do not have to evaluate the potential at the origin [12]. In any case, it is known that to obtain the energy to six decimal places one must use a mesh with 80.000 points [9]. In any case, it is the essential singularity of the eigenfunction at the origin that prevents all these methods from working adequately.

There is another method [13], based on the analytic continuation of the solution of a differential equation, which has been shown to be very efficient in obtaining eigenvalues of Schrödinger operators for different potentials when these do not generate essential singularities on the eigenfunction [13–15]. In fact this is an analytic method and allows one to obtain the eigenenergies correct to all the significant digits provided by the computer. However, when the potential is such that the corresponding eigenfunctions have essential singularities, one is not able to apply this method because it is not possible to use the analyticity of the eigenfunction in the neighbourhood of $z = 0$. The aim of this work is to show how the method of analytic continuation can be applied in these above-mentioned cases. As we shall see below, the results obtained will have a precision similar to those where no essential singularities are present, i.e. we shall obtain a precision equal to all the decimal places that the computer provides.

2. Analytic continuation and essential singularities

We shall describe in this section the more important characteristic of the analytic continuation method when applied to the eigenvalues determination. A more detailed description can be seen in [13, 14]. Our problem is to find the eigenvalues of the Schrödinger radial operator which we write as

$$z^2u''(E,z) - [l(l+1) + z^2V(z) - Ez^2]u(E,z) = 0 \tag{3}$$

where we have used z instead r to extend the differential equation to the complex plane, although we are only interested in the solution on the positive real line. We use units $\hbar^2/2m = 1$.

The eigenfunction $u(E,z)$ must satisfy the conditions $u(E,0) = 0$ and $u(E,\infty) = 0$. When the potential is regular or it has, at most, a pole of second order at, for example, the origin, the solution can be expressed as

$$u(E,z) = z^{l+1}f(z) \tag{4}$$

where $f(z)$ is an analytical function, which can be expanded in a Maclaurin series, obtaining

$$u(E,z) = z^{l+1}\sum_{k=0}^{\infty} a_k(E)z^k. \tag{5}$$

The analytic continuation method uses the analyticity property of $f(z)$ which allows us to expand it around different mesh points $z_1, \ldots, z_m, \ldots$ that lie on the positive real line as

$$f(z) = \sum_{k=0}^{\infty} a_k(E)(z - z_m)^k. \tag{6}$$

It is also necessary to have an expansion for $V(z)$ in the neighbourhood of each mesh point:

$$V(z) = \sum_{k=0}^{\infty} \frac{\partial_z^k V(z)|_{z=z_m}}{k!}(z - z_m)^k \tag{7}$$

and, in order to work numerically, we must truncate this series at a term N_v in such a way that the value of the truncated series coincides with $V(z)$ within the precision of the computer. Likewise the expansion for $f(z)$ around any mesh point must be also truncated at a term N_s. We shall take this parameter in such a way that the function will be correctly described between the points z_m and z_{m+1} and therefore the final results will not be affected for this choice of N_s. It is clear that the value of this parameter is a function of the distance between two consecutive mesh points, δ_s.

The coefficients $a_k(E)$ of (5) are determined for each E from the differential equation, together with the boundary condition $u(E, 0) = 0$. The $a_k(E)$ of (6) are also obtained from the differential equation and from the continuity of both the function $u(E, z)$ and its first derivative at the mesh point z_m. Note that the expansion about z_1 is directly connected to the expansion about z_0. This manner of connection allows us to propagate the boundary condition at the origin and one obviously requires that the point z_m be inside the circle of convergence of the expansion made about the point z_{m-1}.

Finally, to obtain the eigenenergies we impose the condition that $u(E, z)$ goes to zero in the limit $z \to \infty$. This will be done in the following manner: for any value of E the asymptotic solution of the differential equation can be expressed in terms of two linearly independent asymptotic solutions $u_{\pm}^{\infty}(E, z)$:

$$u(E, z) = A_-(E)u_-^{\infty}(E, z) + A_+(E)u_+^{\infty}(E, z) \tag{8}$$

where $u_-^{\infty}(E, z)$ decreases to zero and $u_+^{\infty}(E, z)$ increases to infinity when z increases, and, in addition, these functions are known. The coefficients $A_{\pm}(E)$ are determined by imposing continuity on both the function and its first derivative at a point R_a far away the origin. The solution for $r \geqslant R_a$ is given by (8) and for $r \leqslant R_a$ the solution is that obtained by means of analytic continuation. The bound states correspond to the cases for which the coefficient $A_+(E)$ is zero.

Let us comment here that it is possible to obtain the eigenvalues by imposing the condition $u(E, R_a) = 0$. The precision obtained for the eigenvalues by using this condition, and for potentials of different type, is the same as that obtained by imposing the more correct condition that the coefficient $A_+(E)$ must equal zero [15]. This same has been checked in this work, when the potentials are highly singular. However, the wavefunction obtained in this way does not have a correct asymptotic behaviour.

When the potential in the radial Schrödinger equation has singularities stronger than r^{-2} the method of analytic continuation cannot be applied directly, because the solution $u(E, z)$ has an essential singularity at the origin. So, the first thing to do is to avoid it altogether or to minimize in an adequate manner the effects that this singularity has on the solutions. Several options are presented in this work, all leading to results with the same precision as those obtained where the potential is less singular [13–15].

The first option, upon which we will focus our attention, consists of approximating the required potential by

$$V_0(r, R_c) = \begin{cases} V(R_c) & \text{if } r < R_c \\ V(r) & \text{if } r \geqslant R_c\,. \end{cases} \tag{9}$$

Here R_c is a new parameter that we shall take in such a way that we obtain stability in the eigenvalues. For small values of R_c we have $V(r) \geqslant V_0(r, R_c)$, and this potential does

not have singularities. Thus we can apply the analytic continuation method directly and the eigenvalues obtained by solving the radial Schrödinger equation with this new potential $V_0(r, R_c)$ will be lower bounds on the exact eigenvalues associated with the potential $V(r)$. In addition, the new potential satisfies $V_0(r, R_c) \leqslant V_0(r, R_c')$ if $R_c \geqslant R_c'$. So by decreasing the parameter R_c we increase the corresponding eigenvalues, thus approaching the exact ones. This is the easier way of avoiding the essential singularity of the exact wavefunction. It is clear that we need to use quite small values of R_c and work near the point where the eigenfunction has the singularity. This is the more delicate point because it is necessary to do analytic continuations when $r < R_c$ with a very small step, say $\delta_c = R_c/10$. Once we reach the point R_c, we can progressively increase the step δ_c by multiplying it by a factor Δ until we reach the maximum value of the step, δ_s. We must be careful at the point R_c, where the potential $V_0(r, R_c)$ has discontinuous derivatives. Therefore the point R_c must be a mesh point, keeping in mind that we are performing the analytic continuation from the origin to larger values of r.

The second option consists of approximating the required potential by

$$V_1(r, R_c) = \begin{cases} \infty & \text{if } r < R_c \\ V(r) & \text{if } r \geqslant R_c\,. \end{cases} \tag{10}$$

For this potential the initial condition at the origin must be changed by the condition $u(E, z = R_c) = 0$ and we must take R_c as the first mesh point. Note that $V(r) \leqslant V_1(r, R_c)$ for any R_c and that $V_1(r, R_c) \geqslant V_1(r, R_c')$ if $R_c \geqslant R_c'$. So by applying the analytic continuation method to the potential $V_1(r, R_c)$ with the aforementioned initial condition we shall obtain a set of upper bounds on the exact eigenvalues. These upper bounds will approximate to the exact values as the parameter R_c becomes smaller.

Finally, the third option can be applied when we know the behaviour of the wavefunction near the origin analytically. This is the case of the potentials given by (1) for which the solution for small values of r is

$$u(E, z) \propto \exp\left(-\frac{b}{r^\beta}\right) \tag{11}$$

where the parameters b and β depends on the smaller exponent and the corresponding coefficient of the potential in (1). Thus we know the value of the wavefunction and of its derivatives at a point $R_c > 0$ and then from this we can start the process of analytic continuation. This requires that the analytical expression for the eigenfunction is numerically acceptable at the point R_c.

We shall see below that all these methods give us the same results for the corresponding eigenvalues when the parameter R_c is sufficiently small. These methods include a set of parameters that we shall now enumerate. They must be fixed by requiring stability in the results obtained and they are as follows:

- R_c is the value which defines the new potentials V_0 and V_1. When R_c becomes smaller we must obtain better values for the eigenvalues.
- R_a is the point where we connect the function obtained by mean of the analytic continuation and the asymptotic one.
- δ_c is the initial step, around the point R_c.
- δ_s is the final step. We go from δ_c to δ_s by multiplying by a factor Δ, that is another parameter.
- N_v and N_s give us the number of terms that we take in the expansion of $V(z)$ and $f(z)$, respectively. They must be sufficiently large in order that the results do not depend on them.

3. Results

To analyse the precision of the methods proposed here, we compare our results with some special case for which both the eigenvalue and the eigenfunction are known analytically. This is the case for the potential given by

$$V(r) = r^2 + \frac{a}{r^4} + \frac{b}{r^6} \tag{12}$$

with $a = b = 1$, which has been studied by Znojil [2] and Guardiola and Ros [7] and which has a ground-state energy $E = 5$. This exact value can be obtained with different sets of values for the free parameters. A typical set is

$$\begin{aligned} &N_v = 15 \qquad N_s = 15 \qquad \delta_c = 0.01 \qquad \delta_s = 0.2 \\ &\Delta = 1.05 \qquad R_c = 0.125 \qquad R_a = 8 \end{aligned} \tag{13}$$

and we can obtain the eigenvalue $E = 5$ working with any of the options presented here.

Table 1. Values of the ground-state energies for the singular anharmonic potential with $b_4 = b_6 = 1$ in terms of the parameter R_c. The E_i, $i = 1, 2, 3$ are the values obtained with each of the three options. Note how the values E_1 and E_2 are respectively lower and upper bounds on the exact energy ($E = 5$). Here $\delta_c = 0.01$ and $\Delta = 1.05$.

R_c	E_1	E_2	E_3
0.25	4.999 999 993 551 034	5.000 002 446 703 359	5.000 000 274 214 582
0.23	4.999 999 999 722 652	5.000 000 205 720 335	5.000 000 023 933 230
0.21	4.999 999 999 995 094	5.000 000 008 368 000	5.000 000 001 007 228
0.19	4.999 999 999 999 995	5.000 000 000 119 759	5.000 000 000 014 873
0.17	4.999 999 999 999 996	5.000 000 000 000 361	5.000 000 000 000 043
0.15	4.999 999 999 999 998	5.000 000 000 000 000	5.000 000 000 000 000
0.13	4.999 999 999 999 999	5.000 000 000 000 000	5.000 000 000 000 000

The parameter R_c defines the family of potentials that we have used. In table 1 we analyse the behaviour of the different options here proposed in terms of R_c, once the other parameters have been fixed. We denote the eigenvalues obtained with the different options by the symbols E_i, $i = 1, 2, 3$. One can notice how the lower, E_1, and upper, E_2, bounds on the exact eigenvalue approach it when the parameter R_c decreases. When this parameter is small enough the numerical results coincide with the analytical one within the precision of the computer. As can also be seen the same occurs with the third method.

Once we have established that all the options give us the results with all the digits correct, in the next tables we shall write the eigenvalues obtained with the first option. In table 2 we show the value of the energy for the ground state of the potential given by (1) and for several cases studied in the literature by using different approximation methods. The upper part of this table shows the eigenvalues corresponding to the case $b_6 = 0$ and different values of the parameter b_4. The lower part shows the eigenenergies corresponding to different values of the parameter b_6 and $b_4 = 0$. All these cases lack analytical solutions and we compare the results obtained here with those considered as exact of Fernández [11] and of Solano Torres *et al* [16].

A similar study has been performed in table 3 for the eigenvalues of the spiked potential given by (2) when $\alpha = \frac{5}{2}$ and for several values of the parameter λ. We compare these results with those labelled as exact in [9].

Table 2. Values of the ground-state energies for the singular anharmonic potential compared with others obtained by numerical integration of the Schrödinger equation. The upper part corresponds to the case $b_6 = 0$ and different values of b_4 and the lower to the case $b_4 = 0$ and different values of b_6.

b_4	E^a	$E^{b \text{ or } c}$
0.001	3.068 763 170 918 247	NA
0.01	3.205 067 495 068 930	3.205 067 49[b]
0.1	3.575 551 991 226 094	3.575 55
1	4.494 177 983 369 188	4.494 18
10	6.606 622 512 024 944	6.606 62
100	11.265 080 431 752 83	11.265 08
1000	21.369 462 532 163 43	NA
b_6	E^a	$E^{b \text{ or } c}$
0.001	3.279 855 825 921 856	NA
0.0025	3.353 919 317 108 725	3.353 919 30
0.01	3.505 452 275 995 097	3.505 452 39
1	4.659 939 969 573 538	4.659 940
10	6.003 209 028 895 745	6.003 209

[a] Present work.
[b] [11].
[c] [16].
NA denotes not available.

Table 3. Values of the ground-state energies for the spiked potential for $\alpha = \frac{5}{2}$ and for various values of λ compared with those of Aguilera-Navarro *et al* [9].

λ	E^a	E^b
0.001	3.004 011 251 013 044	3.004 022
0.005	3.019 140 107 276 879	3.019 142
0.1	3.266 873 026 113 018	3.266 873
1	4.317 311 689 247 366	4.317 311
10	7.735 111 103 489 141	7.735 111
1000	44.955 484 788 095 62	44.955 485

[a] Present work.
[b] [9].

In all cases the analytical continuation method works to maximum precision, independently of the values of the potential parameters. This clearly shows that we may use this method for any kind of singularity in the potential and/or wavefunction. Note that we have improved significantly the best previous results for all the potentials.

Finally in table 4 we illustrate the applicability of the method to the problem of obtaining the energies of different excited states. In particular the energies of the four first excited states in l-wave of (i) the anharmonic singular potential with $b_4 = 1$ and $b_6 = 0.8$ (upper part of the table), and of (ii) the spiked potential with $\alpha = \frac{7}{2}$ and $\lambda = 0.01$ (lower part) are shown. The precision obtained is the same that for the ground states, working with the same set of free parameters.

Table 4. Eigenenergies of different excited states. In particular the energies of the four first excited states in l-wave of the anharmonic singular potential (upper part of the table), and of the spiked potential (lower part). See the text for details.

l	$E^{(1)}$	$E^{(2)}$	$E^{(3)}$	$E^{(4)}$
0	4.934 719 654 208 102	9.449 469 323 017 711	13.820 014 025 153 72	18.118 296 927 675 69
1	5.826 516 364 862 367	10.189 739 413 922 72	14.477 689 594 185 10	18.721 286 131 021 72
2	7.337 966 318 320 429	11.528 662 793 952 46	15.703 099 694 993 76	19.863 901 016 045 18
3	9.152 115 604 044 834	13.237 870 853 570 27	17.325 653 157 929 63	21.413 724 618 088 92
0	3.134 824 476 759 598	7.186 617 411 387 038	11.222 786 115 502 59	15.251 451 037 676 74
1	5.009 008 428 229 980	9.013 577 267 716 157	13.017 629 772 211 79	17.021 341 728 433 79
2	7.002 761 202 108 935	11.003 793 296 129 79	15.004 745 148 821 64	19.005 639 422 514 53
3	9.001 382 138 376 020	13.001 784 880 371 65	17.002 162 317 727 45	21.002 520 522 262 53

4. Conclusions

We have shown how the analytic continuation method, which can only be applied where the solution does not have essential singularities, can also be applied in this case by introducing a family of non-singular potentials which depend on a parameter R_c and which tend to the exact potential as R_c tends to zero. The application of the standard method to this family of potentials allows us to obtain eigenvalues, which approach the exact ones as the potential does.

Although we have also introduced a third analytical option (only applicable in some cases), the best way of studying the eigenvalue problem for any potential is by using one of the two first methods, because we approach to the exact result from below or from above, and their results can be considered as lower or upper bounds on the exact eigenvalue.

This method is very simple to apply as a standard numerical method, its speed also being similar. Note that it is not necessary to work with equally spaced mesh points, although this is easier. In fact we needed to work with a very small step near the singularity, increasing it as we move away.

Finally let us comment here that the method can be applied to potentials with more than one singularity, working in a similar way as we have done when the potential is singular at the origin.

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