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Approximate expression for the energy of a *D*-dimensional anharmonic potential

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Abstract

An approximate expression is constructed for the energy of an anharmonic potential with centrifugal barrier. In order to obtain such an analytical expression, the quasi-exact solvability is used and then a fitting of these exact solutions is done.

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1. Introduction

Unfortunately most physically relevant potentials are in the class for which the Schrödinger equation cannot be solved exactly. A happy coincidence is that the problem of the hydrogen atom is one of the exact ones, in addition to the harmonic oscillator which is a good approximation in many physical situations. Afterwards these solutions can be used in order to get some information for the cases where a more realistic potential can be taken as a perturbation over the one for which the Schrödinger equation can be solved exactly. Nevertheless the usual perturbation theory is not very reliable in some cases such as the polynomial anharmonic potentials, because it produces a nonconvergent series [1]. In past decades a certain amount of exact information for some of these anharmonic potentials was obtained, inasmuch as it was discovered that they were part of another class of potentials which have a few exact solutions, provided certain relations among their parameters hold. They were called quasi-exactly solvable (QES) potentials [2–5] because these particular analytical solutions do not cover the entire spectrum of the problem even in the case of simpler examples. Notwithstanding, in general real situations do not have potential parameters obeying the relations cited above and one is obliged to resort to numerical methods to find the complete spectra. This creates a doubt about the usefulness of these analytical solutions, which can be partially eliminated by realizing that they can be used in an interpolation to obtain an analytical approximation of the energy spectrum as a function of the potential parameters [6]. In this last work some of us discussed this approach in the case of the potential $V(r) = Ar^6 + Br^2$. In this

work we will start with the partial analytical solutions already known for the sextic anharmonic potential with centrifugal barrier including its energy spectrum but only in a recurrence relation form [2–5] and then obtain its numerical counterpart. From these numerical data we establish relations among the energy eigenvalues and the potential parameters culminating in a compact algebraic expression for the energy eigenvalues. At this point it is important to remark that some very important systems, namely interacting anyons [7, 8], Rydberg atoms in the presence of electromagnetic fields, can be mapped through point canonical transformations to the double well potential as given above, but necessarily including a centrifugal barrier [9–11]. Other important systems such as molecules of ammonia and hydrogen-bonded solids [12–14] can also be mapped into the potential $V(r) = Ar^6 + Br^4 + Cr^2 + F/r^2$. In fact one can also think of the anharmonic oscillator as an example of quantum field theory (QFT) in one dimension. It can be studied, for instance, in order to test nonperturbative methods for QFT [1, 15]. In this line of research, some work has been done discussing renormalization group properties [16, 17]. Therefore, the importance of the sextic anharmonic potential with centrifugal barrier largely justifies the search for analytical solutions even though approximately. The purpose of the present paper is to extend the approach adopted in [6] for this more general kind of potential. Finally, it is important to stress that the expression appearing in this work presents great accuracy in the range of parameters where other approaches would fail. Therefore, this leads to a second goal for this work. We intend to present energy expressions which could be used as a test ground for any new numerical method avoiding the need of additional numerical evaluations in order to perform the necessary comparisons to establish the power of a given method.

2. Analytical approach

In this section we consider the analytical properties of the time-independent Schrödinger equation ($\hbar = 1$)

$$-\frac{1}{2}\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2} + V(r)u(r) = Eu(r) \tag{1}$$

where $V(r)$ is an anharmonic sextic potential with centrifugal barrier

$$V(r) = Ar^6 + Br^4 + Cr^2 + \frac{F}{r^2} \qquad (A > 0). \tag{2}$$

We recall that equation (1) is the one-dimensional Schrödinger equation if r is defined on the whole line ($-\infty < r < +\infty$) with wavefunction normalized as $\int_{-\infty}^{+\infty} \mathrm{d}r|u|^2 = 1$ and if the centrifugal barrier is considered as an external potential. On the other hand, equation (1) is the D-dimensional radial Schrödinger equation for a central potential if r is defined on the half line ($0 \leqslant r < +\infty$) with wavefunction normalized as $\int_0^{+\infty} \mathrm{d}r\, r^{D-1}|R|^2 = \int_0^{+\infty} \mathrm{d}r|u|^2 = 1$, with $u(0) = 0$ in the event that $F \neq 0$, and if one part of the centrifugal barrier is considered as the momentum angular-dependent term of the effective potential ($l(l + D - 2)/2r^2$) and the remaining part of the centrifugal barrier is considered as an external potential.

In order to guarantee the asymptotic behaviour of the Schrödinger equation when $r \to \infty$ and $r \to 0$, so that

$$\frac{\mathrm{d}^2u}{\mathrm{d}r^2} \to 2(Ar^6 + Br^4 + Cr^2)u \qquad (r \to \infty) \tag{3}$$

$$\frac{\mathrm{d}^2u}{\mathrm{d}r^2} \to \frac{2F}{r^2}u \qquad (r \to 0) \tag{4}$$

$u(r)$ should look like

$$u(r) = \mathrm{e}^{-(\alpha r^4+\beta r^2)} \qquad (r \to \infty) \tag{5}$$

$$u(r) = r^{-g} \qquad (r \to 0). \tag{6}$$

Substituting the above eigenfunctions in the corresponding asymptotic equations, one gets the following relations among the arbitrary parameters introduced in the eigenfunctions and the potential parameters:

$$\alpha = \frac{\sqrt{2A}}{4} \qquad \beta = \frac{B}{2\sqrt{2A}} \qquad g(g+1) = 2F. \tag{7}$$

This asymptotic behaviour suggests a suitable ansatz for the eigenfunction $u(r)$,

$$u(r) = r^{-g}\tilde{u}(r)\,\mathrm{e}^{-(\alpha r^4+\beta r^2).} \tag{8}$$

Now, we choose the function $\tilde{u}(r)$ given by a power series expansion

$$\tilde{u}(r) = \sum_{j=0}^{\infty} a_j r^j. \tag{9}$$

So, after the substitution in the Schrödinger equation, we verify that one must have

$$a_1 g = 0 \tag{10}$$

and also have the recurrence relation

$$\frac{(j+2)(j+1-2g)}{2}a_{j+2} + \left[E - \frac{B}{\sqrt{2A}}\left(j + \frac{1}{2} - g\right)\right]a_j + \left\{\frac{\sqrt{2A}}{2}[2(g-j)+1] + \frac{B^2}{4A} - C\right\}a_{j-2} = 0. \tag{11}$$

From equation (10), it can be seen that if $g \neq 0$ then $a_1 = 0$, and from the recurrence relation, that all the odd terms will vanish. On the other hand, when $g = 0$ both parities are admissible. Furthermore, we impose that g is a nonpositive number, to avoid singularity of the eigenfunction at the origin. In order to obtain acceptable solutions for $r < 0$ in the one-dimensional case the condition that g is an integer must be additionally imposed. In this particular case, the centrifugal barrier for $g \leqslant -2$ represents an infinitely high potential barrier separating the space symmetrically. This fact implies two-fold degeneracy of the levels associated with N (even) and $N+1$ (odd).

In general, $\tilde{u}(r)$ is an infinite series. In order to keep control of the normalization of the eigenfunction and also of its convergence, though, we did truncate the series at $j = N$. As a consequence of this imposition two things happen. First, the potential parameters become constrained through the equation

$$C = -\sqrt{2A}\left(N + \frac{3}{2} - g\right) + \frac{B^2}{4A} \tag{12}$$

and moreover the energy spectrum will come from the roots of a polynomial equation for the energy given by

$$\left[E - \frac{B}{\sqrt{2A}}\left(N + \frac{1}{2} - g\right)\right]a_N + 2\sqrt{2A}a_{N-2} = 0 \tag{13}$$

where the coefficients $a_j(E)$ obey the recurrence relation

$$a_{j+2} = -2\frac{\left[E - \frac{B}{\sqrt{2A}}\left(j + \frac{1}{2} - g\right)\right]a_j + (N-j+2)\sqrt{2A}a_{j-2}}{(j+2)(j+1-2g)}. \tag{14}$$

The Schrödinger equation for this potential can be analytically solved when the potential parameters obey relation (12). In this case the polynomial in the energy will permit us to obtain $1 + N/2$ real solutions when N is even, and $(N + 1)/2$ real solutions when N is odd. In fact this parameter N is an important one, because it not only defines the number of exact solutions but also the corresponding potential parameters, through equation (12). Below we present the first four cases:

$$N = 0 \qquad E - \frac{B}{\sqrt{2A}}\left(\frac{1}{2} - g\right) = 0 \tag{15}$$

$$N = 1 \qquad E - \frac{B}{\sqrt{2A}}\left(\frac{3}{2} - g\right) = 0 \tag{16}$$

$$N = 2 \qquad E^2 + E\frac{B}{\sqrt{2A}}(2g - 3) + \frac{B^2}{2A}\left[\frac{5}{4} + g(g - 3)\right] + 2\sqrt{2A}(2g - 1) = 0 \tag{17}$$

$$N = 3 \qquad E^2 + E\frac{B}{\sqrt{2A}}(2g - 5) + \frac{B^2}{2A}\left[\frac{21}{4} + g(g - 5)\right] + 6\sqrt{2A}(g - 1) = 0. \tag{18}$$

It is easy to see that for larger values of N, the algebraic equations become more involved, generally requiring numerical solutions for $N \geqslant 6$. Nonetheless, if $B = 0$ the roots of the algebraic equations are symmetrically disposed around $E = 0$ and they can be analytically found for $N \leqslant 11$. It is important to remark that now the difficulties are quite different and less than that of solving the Schrödinger differential equation numerically.

3. Scale covariance

As the potential under study here has many parameters, it is very interesting to use a scale covariance present in this kind of potential. It is easy to show that under the scale transformation $r = \lambda y$ [18], the Schrödinger equation keeps its form if its new parameters are rewritten in terms of the former, and the scaling parameter as

$$\mathcal{A} = \lambda^8 A \qquad \mathcal{B} = \lambda^6 B \qquad \mathcal{C} = \lambda^4 C \qquad \mathcal{F} = F \qquad \mathcal{E} = \lambda^2 E. \tag{19}$$

It is interesting to note that, in the same way as the Schrödinger equation, the constraint relation appearing in (12) is covariant. This implies that the scaled potential is still a quasi-exactly solvable one. The previous equations say that, once one has solved the Schrödinger equation in the original parameters, that corresponding to the new parameters is automatically solved, and vice versa, for a fixed N. In fact a whole class of potentials is related through a convenient choice of the scaling parameter. Because we only have even powers of λ in the above relations, we can identify seven sets of potential parameters (if λ is restricted to a real number) which can be related to one another inside each set by the scale transformation. The parameter A is always positive, but B and C can be positive, negative or zero, and F can be determined through the constraint equation, depending on the possibilities of choice of B and C. Nonetheless, (12) implies that C is always a negative number in the event of $B = 0$. This way one ends with seven sets. Below we will choose λ in order to factorize the dependence

on the parameter A in the energy. For this we use $\lambda = A^{-\frac{1}{8}}$. Note, though, that this implies a singular expression in the limit $A \to 0$.

4. Analytical-numerical approach

From the above discussion of the scale covariance, it is not hard to see that one can define a new kind of energy, related to the former through

$$\mathcal{E} = \frac{E}{A^{\frac{1}{4}}} \tag{20}$$

and similarly another variable

$$z \equiv \left(\frac{B^2}{4A\sqrt{2A}} - \frac{C}{\sqrt{2A}} + g \right)^{\frac{1}{2}} \tag{21}$$

both of them invariant under scaling. Note that these variables are suggested by the quasi-exact solvability condition (12). In order to find an analytical expression which gives approximate values for the eigenenergies expressed by (20) for arbitrary parameters (not only for those satisfying (12)), we use a numerical method of adjustment and interpolation starting with the analytical eigenenergies for parameters which satisfy (12). These two variables are then fitted through a polynomial of arbitrary degree whose best fitting resulted in a polynomial of degree 7:

$$\mathcal{E} = \sum_{i=0}^{7} \alpha_i z^i \tag{22}$$

where the coefficients α_i depend on the principal quantum number n. We also find a best fit for a polynomial of degree 7:

$$\alpha_i = \sum_{j=0}^{7} b_{ij} n^j. \tag{23}$$

It is quite remarkable that (22) implies a symmetry among some sets of potentials which have different parameters and the same energy spectra.

Along with this process, we take into account N up to 55 and the principal quantum number n up to 15, obtaining $(N-n)/2+1$ states for $n \leqslant N$. Higher values of N would permit us to analyse states with higher values of n. Nonetheless, as N increases the power of the polynomial equation from which we find the eigenenergies also increases, leading to technical difficulties in calculating the roots. Each step of the process of obtaining the coefficients b_{ij} was checked against the exact data. From the above discussion it is easy to conclude that our approximated analytical expression for the energy is given by

$$E = A^{\frac{1}{4}} \sum_{i=0}^{7} \sum_{j=0}^{7} b_{ij} n^j z^i. \tag{24}$$

The process of obtaining the coefficients b_{ij} establishes the kind of source required for obtaining precise energies which can be useful for comparisons. The comparison among the exact energies resulting from the roots of the algebraic equations given by (13) and those coming from the above approximate analytical expressions, gives us errors between 10^{-6} and $10^{-1}\%$. This was obtained in a region where the potential parameters were $A = 0.1, -1 \leqslant B \leqslant 1, -1 \leqslant C \leqslant 1$, and for up to $n = 14$. The parameter F was determined by the constraint relations. In table 1 we present the coefficients b_{ij} for a particular

Table 1. Coefficients b_{ij} ($\times 10^{+2}$) of (24) for the set of parameters such that $B < 0$ and $C > 0$.

$j\backslash i$	0	1	2	3
0	−5.110 116 3083	−56.864 496 2138	68.141 705 1894	−30.237 697 2789
1	−0.040 362 3346	−53.235 552 878	63.452 323 0593	−28.083 768 325
2	0.000 549 0447	−3.819 425 1189	4.544 010 9565	−2.006 139 9261
3	0.000 002 9422	−0.031 826 6762	0.037 797 0874	−0.016 647 5518
4	−0.000 565 8753	84.512 627 0636	−100.828 543 709	44.683 777 5396
5	−0.000 342 5886	18.483 078 7293	−22.009 802 1861	9.729 150 8222
6	−0.000 022 6538	0.469 699 5852	−0.558 301 6301	0.246 188 6136
7	−0.000 000 1334	0.000 916 6636	−0.001 087 6931	0.000 478 529

$j\backslash i$	4	5	6	7
0	6.524 289 8597	−0.732 804 7081	0.041 073 7165	−0.000 905 2399
1	6.040 899 463	−0.676 214 2221	0.037 768 0854	−0.000 829 4387
2	0.430 259 3967	−0.048 009 1791	0.002 672 5856	−0.000 058 5013
3	0.003 560 5927	−0.000 396 1208	0.000 021 9845	−0.000 000 4798
4	−9.626 293 3327	1.079 366 4033	−0.060 390 078	0.001 328 5617
5	−2.089 650 2471	0.233 534 0457	−0.013 021 4825	0.000 285 4905
6	−0.052 726 3482	0.005 874 4082	−0.000 326 5108	0.000 007 1362
7	−0.000 102 2151	0.000 011 3558	−0.000 000 6293	0.000 000 0137

(Continued.)

Table 2. Exact and approximate eigenenergies for the set of parameters such that $B < 0$ and $C > 0$. Furthermore, n is the quantum number and z is the variable defined in (21).

n	z	E_{exact}	E_{approx}	Per cent deviation
0	1.5	−517.079 996	−517.079 994	0.000 000
0	3.5	−524.836 412	−524.836 430	0.000 003
0	5.5	−532.241 653	−532.241 622	−0.000 006
0	7.5	−539.293 903	−539.293 899	−0.000 001
0	15.5	−563.938 470	−563.938 461	−0.000 002
2	3.5	−486.084 099	−486.084 117	0.000 004
2	5.5	−493.661 383	−493.661 286	−0.000 020
2	7.5	−500.879 218	−500.879 323	0.000 021
2	9.5	−507.735 583	−507.735 641	0.000 011
2	15.5	−526.116 485	−526.116 375	−0.000 021
4	5.5	−455.618 510	−455.618 198	−0.000 068
4	7.5	−463.012 192	−463.012 154	−0.000 008
4	9.5	−470.037 490	−470.035 675	−0.000 386
4	11.5	−476.692 145	−476.689 327	−0.000 591
4	15.5	−488.880 807	−488.874 579	−0.001 274

set of parameters ($B < 0, C > 0$) and in table 2 we present a few results coming from expression (24) and their comparison with those coming from QES solutions.

At this point it is very important to remark that the energy expression obtained here has some advantages compared with those obtained by other approaches. First, as far as we know this is the first time that it is considered for higher excited states. The majority of the papers in the literature deal with the ground state or the lowest excited states [19]. Furthermore, these results are in general obtained for one-dimensional potentials, without centrifugal barriers,

which in turn are quite essential to describe more realistic systems. On the other hand, the energy expressions obtained through the Rayleigh–Schrödinger perturbation theory are nonconvergent [1], so leading to very poor results. In such a state of affairs, the approach presented in this paper generates a complete energy spectrum, with the correct physical limits and including the centrifugal barrier term.

5. Conclusions

In this work we presented an approximate analytical expression for the eigenvalues of an anharmonic oscillator with centrifugal barrier for arbitrary values (restricted to a given region of validity) of the potential parameters. This was done by using the quasi-exact solutions for this potential and then interpolating them, and also using the scaling covariance of the system in order to diminish the number of independent variables. The presentation of the coefficients b_{ij} of the expression for eigenenergies (24) was done because the approximate results may be useful for exploratory purposes. The comparison with exact results was done, giving very good accuracy (errors between 10^{-6} and $10^{-1}\%$) in the region of validity of the expression presented. The exact results used for this comparison were those coming from the input themselves, i.e. the solutions of the algebraic equations for the energy eigenvalues for the QES potentials (13). It is worthwhile mentioning that these exact results correspond to $\sqrt{N+3/2}$ in (21).

The approximate solution presented in this paper can be used to study the behaviour of physically interesting systems, such as interacting anyons, Rydberg atoms in strong magnetic fields, molecules of ammonia, hydrogen-bonded solids, etc. This approach can be extended to other situations where quasi-exact solutions do exist or even by using numerically calculated eigenvalues [20].

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