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Approximate analytic expression for the eigenenergies of the anharmonic oscillator $V(x) = Ax^6 + Bx^2$

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An approximate analytic expression for the eigenenergies of the anharmonic oscillator $V(x) = Ax^6 + Bx^2$ is introduced, starting from particular analytic solutions which are valid when certain relations between the parameters A and B are held.

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I. INTRODUCTION

A problem that has been challenging physicists and mathematicians for years is the search for analytic solutions for anharmonic oscillators. As it is well known, the general solution for this problem has not yet been found; however, particular analytic solutions have been discovered when the potential parameters obey certain relations. It is important to note that these particular analytic solutions do not cover the entire spectrum of the problem even in the case of simpler examples. Potentials with these characteristics are then called partially algebrized or quasi-exactly-solvable [1–21].

Since the complete spectra of anharmonic oscillators are not analytically known it is usual to implement numerical methods to find the energy eigenvalues. This is quite satisfactory for a particular potential with all its parameters fixed to certain numerical values. The price paid in this approach is that one cannot in general write a closed expression for the relevant functions related to the solutions of the problem as the eigenenergies or wave functions even for a more restricted class of potentials.

Clearly there is a gap between these two approaches and in this paper we want to make some effort in the direction of connecting them. To do this we will start with the partial analytic solutions known for the double-well potential $V(x) = Ax^6 + Bx^2$ $(A > 0, B < 0)$ including their energy spectrum but only in a recurrence relation form and then obtain its numerical counterpart. From these numerical data we establish relations between the energy E and the parameters A and B.

Apart from its intrinsic interest, the double-well potential also plays an important role in the quantum study of the tunneling time problem [22], in spectra of molecules such as ammonia and hydrogen-bonded solids [23], and in field theory [24]. In fact, the double-well potential that will be focused on in this work might be used as a potential model for quark confinement in quantum chromodynamics [25]. On the other hand, by performing suitable point-canonical transformations, it is possible to show that there is a mapping from the potential of Rydberg atoms in uniform magnetic fields into that of some double-well potentials [26]. Both these problems are generally studied in terms of standard perturbative approaches. It should be very profitable to obtain some analytical information, even though approximately, like that proposed here.

This paper is organized as follows. In Sec. II we review the algebraic approach for the potential $V(x) = Ax^6 + Bx^2$ and determine the energy relations for the first analytic eigenfunctions. In Sec. III we take these energy relations, which are valid when A and B satisfy a constraint relation, and interpolate them numerically. Then we obtain an expression for the energy as a function of A, B and n, the principal quantum number, for $n \leq 3$. In Sec. IV we show that these results can be extended to higher excited states and in Sec. V we present our final considerations.

II. ALGEBRAIC APPROACH

In this section we review the analytic properties of the Schrödinger equation

$$-\frac{1}{2}\,\psi'' + V\psi = E\psi \qquad (1)$$

for the sextic anharmonic potential [7,21]

$$V(x) = Ax^6 + Bx^2, \quad A > 0\,, \qquad (2)$$

obtaining explicitly the expressions for the energy corresponding to the ground and lowest excited states. As is

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well known, the Schrödinger equation for this potential can be solved by writting the wave function as

$$\Psi(x) \;=\; \tilde{\Psi}(x)\, e^{-\sqrt{2A}\, x^4/4}, \tag{3}$$

where the remaining function $\tilde{\Psi}(x)$ must be a polynomial of definite parity:

$$\tilde{\Psi}_{\rm even}(x) \;=\; \sum_{j=0,2,\ldots}^{N} a_j x^j \tag{4}$$

or

$$\tilde{\Psi}_{\rm odd}(x) \;=\; \sum_{j=1,3,\ldots}^{N} a_j x^j \;. \tag{5}$$

The exact solutions are only possible when certain relations among the coeffients a_j's are satisfied, which can be written as recurrence relations

$$a_{j+2} \;=\; -2\, \frac{E\, a_j + (N+2-j)\sqrt{2A}\, a_{j-2}}{(j+2)\,(j+1)}\;, \tag{6}$$

where E is the energy eigenvalue. Note that for $j' > N$ all $a_{j'} = 0$. This equation can be used to obtain the energy equation

$$a_N\, E \;-\; 2\sqrt{2A}\, a_{N-2} \;=\; 0\;. \tag{7}$$

These restrictions imply that the potential parameters A and B must be related by

$$B \;=\; -\sqrt{2A}\,(N \;+\; \tfrac{3}{2}), \tag{8}$$

in order to ensure exact solvability. One should observe that the parameter B is always negative. Therefore, we would not expect any kind of harmonic oscillator limit, in the case of arbitrary parameters, when A goes to zero. In order to take into account the case where B is positive, we suppose that some sort of analytical continuation should be done. Indeed, a particular case of the above mentioned potential has been studied, regarding problems related to analytical continuations of their parameters by Bender and Turbirner [27]. Moreover some discontinuities in the eigenenergy spectra of some polynomial potentials have been reported by Panday and Varma [28]. Thus it is quite clear that any limit and extrapolations should be done very carefully. In fact, the potential $V(x) = Ax^6 + Bx^2$ belongs to a general family of quasi-exactly-solvable potentials [7,21] for which partial analytic solutions are known when its parameters satisfy constraint conditions. Choosing a certain value for N, we fix also the number of exact levels that can be found in this approach: $1 + N/2$ levels when N is even and $(1 + N)/2$ levels when N is odd.

The expressions for the energy eigenvalues for the first values of N, corresponding to the potential (2), may be expressed as

$$N = 0 \text{ or } 1, \qquad 0 = E, \tag{9}$$

$$N = 2, \qquad 0 = E^2 - 2\sqrt{2A}, \tag{10}$$

$$N = 3, \qquad 0 = E^2 - 6\sqrt{2A}, \tag{11}$$

$$N = 4, \qquad 0 = E\left(E^2 - 16\sqrt{2A}\right), \tag{12}$$

$$N = 5, \qquad 0 = E\left(E^2 - 32\sqrt{2A}\right), \tag{13}$$

$$N = 6, \qquad 0 = E^4 - 60E^2\sqrt{2A} + 360A, \tag{14}$$

$$N = 7, \qquad 0 = E^4 - 100E^2\sqrt{2A} + 1512A, \tag{15}$$

$$N = 8, \qquad 0 = E\left(E^4 - 160E^2\sqrt{2A} + 5888A\right), \tag{16}$$

$$N = 9, \qquad 0 = E\left(E^4 - 240E^2\sqrt{2A} + 16128A\right), \tag{17}$$

$$N = 10, \qquad 0 = E^6 - 350E^4\sqrt{2A} + 41432E^2A - 162000\sqrt{2}A^{3/2}, \tag{18}$$

$$N = 11, \qquad 0 = E^6 - 490E^4\sqrt{2A} + 91160\, E^2A - 831600\sqrt{2}A^{3/2}. \tag{19}$$

This method may be applied for an arbitrary N, but in practice this is difficult to handle. In this analysis, we first confine ourselves to $N \leq 11$ with the advantage of finding algebraic equations for E which can be reduced to the third power (for the energy squared) so that their exact roots may be easily obtained. Finally, we obtain the complete dependence of E on the parameters A, B, and n. In Sec. IV we extend this discussion to $N = 20$ and 30, when only numerical solutions are possible.

III. ANALYTIC-NUMERICAL APPROACH

In order to find an analytic expression which gives approximate values for the eigenenergies for arbitrary parameters [not only for those satisfying (8)] we use a numerical method of adjustment and interpolation starting with the analytical eigenenergies for parameters which satisfy (8). These two variables are then fitted through a polynomial of arbitrary degree which best fit resulted in one of third degree:

$$E \;=\; a \;+\; b\,B \;+\; c\,B^2 \;+\; d\,B^3\;.$$

Noting that the coefficients a, b, c, and d must depend on the parameter A and the principal quantum number n, we write

$$E_n = a_n(A) + b_n(A)\; B + c_n(A)\; B^2 + d_n(A)\; B^3\;. \tag{20}$$

The next step is to find out these dependences explicitly. The best fit in this case is obtained by single power functions for each coefficient which read

$$a_n(A) = \alpha_n\; A^{1/4}\;, \tag{21}$$

$$b_n(A) = \beta_n\; A^{-1/4}\;, \tag{22}$$

$$c_n(A) = \gamma_n\; A^{-3/4}\;, \tag{23}$$

$$d_n(A) = \delta_n\; A^{-5/4}. \tag{24}$$

Keeping Eqs. (20) and (21)–(24) in mind, it is possible to state that the energy can be written as a function of parameters A and B and the quantum number n:

$$E_n = A^{1/4}\left[\alpha_n + \beta_n \frac{B}{\sqrt{A}} + \gamma_n\left(\frac{B}{\sqrt{A}}\right)^2 + \delta_n\left(\frac{B}{\sqrt{A}}\right)^3\right]. \tag{25}$$

The behavior of the coefficients α, β, γ, and δ against n results in the polynomials

$$\alpha_n = 0.2310 + 2.995n - 1.466n^2 + 0.4490n^3\ , \tag{26}$$

$$\beta_n = (-1.224 + 9.067n - 4.919n^2 + 0.9516n^3) \times 10^{-1}, \tag{27}$$

$$\gamma_n = (-11.00 - 3.057n + 9.876n^2 - 2.562n^3) \times 10^{-2}, \tag{28}$$

$$\delta_n = (-1.778 - 1.953n + 4.176n^2 - 1.073n^3) \times 10^{-3}\ . \tag{29}$$

These results were obtained for range of values $0.01 \leq A \leq 100$ and $-12.5 \leq \frac{B}{\sqrt{2A}} \leq -1.5$ (and $0 \leq N \leq 11$). The expression (25) is in excellent agreement with the energy levels obtained analytically for $n \leq 3$. In these cases the error was always less than 1%, except for $n = 2$, which presents a maximum discrepancy that is still smaller than 4%. This can be seen from the Table I, where we show the energy eigenvalues, exact and approximate, for the case $A = 1$.

IV. EXTENSION TO HIGHER EXCITED STATES

So far we have only considered the energy for the ground state and the first three excited states. This was so because we have chosen the order N of the polynomials (4) and (5) to be no higher than 11. In that case, the solutions for the energy equation were obtained exactly. With that choice we have varied the parameters A and B through large ranges. As a matter of fact, the choice $N = 11$ leads to six exact levels, but as we take the safe limit of four values of the eigenenergies to be interpolated, we have found the expression (24) for $n \leq 3$ only.

In order to study the behavior of higher excited states we increase N for specific values of the parameters A and B, satisfying relation (8). Choosing $N = 20$ and applying Eq. (6) iteratively, similarly to what has been done for Eqs. (10)–(19), we find that the energy-squared levels $y = E^2$ obeys the equation (for $\sqrt{2A} = 10^{-4}$)

$$\sqrt{y}\,(y^5 - 0.44y^4 + 0.605299y^3 - 2.99171 \times 10^{-3}y^2 + 4.58305 \times 10^{-5}y - 1.25083 \times 10^{-7}) = 0\ , \tag{30}$$

which leads to the energy eigenvalues shown in Table II, with the corresponding principal quantum number n. The best fitting for these points leads to the equation

$$E_n^{N=20}|_{\sqrt{2A}=10^{-4}} = -0.482986 + 7.44313 \times 10^{-2}n - 3.91992 \times 10^{-3}n^2 + 1.30664 \times 10^{-4}n^3. \tag{31}$$

Analogously, for $N = 30$ we find ($\sqrt{2A} = 10^{-10}$) a polynomial equation of eigth power for the energy squared, which leads to the eigenvalues also shown in Table II. These data lead to the equation

$$E_n^{N=30}|_{\sqrt{2A}=10^{-10}} = -8.95776 \times 10^{-4} + 9.16173 \times 10^{-5}n - 3.18989 \times 10^{-6}n^2 + 7.08864 \times 10^{-8}n^3. \tag{32}$$

TABLE I. Comparison between the exact and approximate results for the eigenenergies with $A = 1$. The precision of the approximate solutions is measured by $\delta \equiv (E_{\text{exact}} - E_{\text{approx}})/E_{\text{exact}}$.

B	E_{exact}	E_{approx}	δ
		n=0	
-2.1213	0.0000	0.0037	
-4.9497	-1.6818	-1.6722	5.7×10^{-3}
-7.7782	-4.7568	-4.7557	-2.3×10^{-4}
-10.6066	-8.9651	-8.9482	-1.9×10^{-3}
-13.4350	-14.0098	-14.0272	1.2×10^{-3}
-16.2635	-19.7569	-19.7516	2.6×10^{-4}
		n=1	
-3.5355	0.0000	-0.0016	
-6.3640	-2.9130	-2.9076	-1.8×10^{-3}
-9.1924	-6.7272	-6.7324	8.2×10^{-4}
-12.0208	-11.3917	-11.3914	-3.0×10^{-5}
-14.8492	-16.8011	-16.7985	-1.5×10^{-4}
-17.6777	-22.8680	-22.8690	5.0×10^{-4}
		n=2	
-4.9497	1.6818	1.6682	-8.1×10^{-3}
-7.7782	0.0000	0.0548	
-10.6066	-2.1164	-2.1984	3.9×10^{-2}
-13.4350	-5.4771	-5.4223	-1.0×10^{-2}
-16.2635	-9.9345	-9.9482	1.4×10^{-3}
		n=3	
-6.3640	2.9130	2.9101	-9.8×10^{-4}
-9.1924	0.0000	0.0111	
-12.0208	-3.4134	-3.4302	4.9×10^{-3}
-14.8492	-7.5588	-7.5477	-1.5×10^{-3}
-17.6777	-12.4725	-12.4754	2.3×10^{-3}

Note that Eqs. (31) and (32) have the same form as Eq. (25), since all of these expressions are given by polynomials of third degree in n. One should also note that these equations have a scaling symmetry, since if we choose, for example, $\sqrt{2A} = 1$, we find that the energy eigenvalues of Table II are only shifted by the factors 10^2 and 10^5 for $N = 20$ and 30, respectively. This scaling symmetry is a consequence of the fact that the energy eigenvalues are proportional to $A^{1/4}$, as could be observed in Eqs. (10)–(19) or (25) as well. This exact dependence was also observed by Bender and Turbirner [27] by applying a variational method. Note that the reflection symmetry between the negative and positive energy eigenvalues appearing in Table II are due in part to the method employed here and also to the quasiexact symmetry of potential (2).

TABLE II. Eigenenergies for $N = 20$ and $N = 30$.

E_n	n
N=20	
-4.783810×10^{-1}	0
-3.564750×10^{-1}	2
-2.446070×10^{-1}	4
-1.442440×10^{-1}	6
-5.878460×10^{-2}	8
0.000000	10
5.878460×10^{-2}	12
1.442440×10^{-1}	14
2.446070×10^{-1}	16
3.564750×10^{-1}	18
4.783810×10^{-1}	20
N=30	
-8.84041×10^{-4}	0
-7.32793×10^{-4}	2
-5.89470×10^{-4}	4
-4.54646×10^{-4}	6
-3.29087×10^{-4}	8
-2.13924×10^{-4}	10
-1.11289×10^{-4}	12
-2.93390×10^{-5}	14
2.933904×10^{-5}	16
1.112891×10^{-4}	18
2.139249×10^{-4}	20
3.290873×10^{-4}	22
4.546464×10^{-4}	24
5.894709×10^{-4}	26
7.327931×10^{-4}	28
8.840412×10^{-4}	30

Analyzing the behavior of the higher excited states discussed above for $N = 20$ and 30, we expect that their properties will also be accompanied by situations with arbitrary N. In practice, however, as N increases, the power of the polynomial equation from which we find the energy eigenvalues also increases, leading to technical difficulties in calculating its roots. In fact, the levels are not equally spaced and as the number of roots increases, one can find that these differences may be of many orders of magnitude, for which a numerical approach requires rapidly increasing precision. It is important to remark that the behavior of E_n, as always being a polynomial of third degree in n, appears to be a kind of "exact behavior" in the case studied, because it persists when the number of analytically obtained excited states increases.

V. CONCLUSIONS

Some final considerations are now in order. First, we observe that the above developed method, apart from the obvious advantage of producing an approximate energy spectrum for arbitrary values (restricted to a given region of validity) of the potentials parameters, permits at least in principle an approximate analytical expression also for the wave function. This can be achieved by truncating the series appearing in the wave function, defined through the expressions (2)–(4), in a term such that

$$j = \mathrm{R}\left(- \left(\frac{B}{\sqrt{2A}} + \frac{3}{2} \right) \right), \tag{33}$$

where $\mathrm{R}(x)$ rounds x to the nearest integer. In the case where the parameters A and B are such that $j = N$, we get the exact solutions. In the remaining cases we have an approximation for the wave function, which in turn permits us to have some information about the probabilities of a given process, not only about its eigenenergies. There is another approach that gives an analytical approximation for the wave function introduced by Chhajlany and Malnev [18] and improved by Fernández. [29] It is based on an approach where exact solutions of a potential of a higher order are obtained and then, taking convenient limits, one can restrict the power of this potential to the desired one of interest, for which no exact solution could be found. It would be very interesting to compare these two approaches.

We intend to extend the approach developed here in order to include other polynomial potentials. Furthermore, we are also improving the statistics with more points, for obtaining the full analytical energy expression for greater values of the principal quantum number n. These and other questions are under study and we expect to report on them in the near future.

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