Upper and lower bounds to the eigenvalues of an anharmonic oscillator

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Abstract
We obtain tight upper and lower bounds to the eigenvalues of an anharmonic oscillator with a rational potential. We compare our bounds with results given by other approaches.

1 Introduction

Barakat has recently proposed a shifted large–dimension expansion (SLNT) implemented by means of the Asymptotic iteration method (AIM) [1]. According to the author, this alternative approach corrects “serious difficulties” of previous applications of that successful perturbation theory. He applies this improved SLNT to an anharmonic oscillator with a rational potential–energy function. The results are not impressive because the perturbation series are restricted to order six and contain only four terms because the odd coefficients vanish. However, the article title promises a large–order calculation [1].

The purpose of this paper is to calculate some eigenvalues of the anharmonic oscillator with the rational potential accurately by means of the Riccati–Padé method (RPM) that has proved to be successful for other problems [2–14]. In Sec. 2 we show the model and outline the application of the

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RPM. In Sec. 3 we discuss the results and compare Barakat’s approach [1] with other applications of the SLNT.

2 The Riccati–Padé method

For concreteness we consider the eigenvalue equation

\[-\chi''(x) + \left[ x^2 + \frac{bx^2}{1+cx^2} + \frac{l(l+1)}{x^2} \right] \chi(x) = E \chi(x) \quad (1)\]

that applies to one–dimensional and central–field problems. In the former case we have \( l = -1 \) and \( l = 0 \) for even and odd states, respectively, and in the latter case \( l = 0, 1, \ldots \) is the angular–momentum quantum number. One easily generalizes this equation to take into account a central–field model for any other space dimension. It is sufficiently general for our present goals. For comparison purposes we choose \( n = 0, 1, \ldots \) to be the radial quantum number [1].

The simple function

\[ \chi_e(x) = x^{l+1}(1 + cx^2)e^{-x^2} \quad (2) \]

is an exact solution to equation (1) if

\[
\begin{align*}
  b &= -2c[c(2l + 3) + 2] \\
  e &= (2l + 3)(1 - 2c) 
\end{align*} \quad (3)
\]

The modified logarithmic derivative of the solution

\[ f(x) = \frac{l + 1}{x} - \frac{\chi'(x)}{\chi(x)} \quad (4) \]

can be expanded in a Taylor series about the origin

\[ f(x) = x \sum_{j=0}^{\infty} f_j x^{2j} \quad (5) \]

where the coefficients \( f_j \) are polynomial functions of the energy \( E \).

If we require that the rational approximation

\[ [M/N](x^2) = \frac{\sum_{j=0}^{N+d} a_j x^{2j}}{\sum_{j=0}^{N} b_j x^{2j}} \quad (6) \]
satisfies
\[ [M/N](x^2) - \sum_{j=0}^{2N+d+1} f_j x^{2j} = \mathcal{O}(x^{2(2N+d+2)}) \]
then the Hankel determinant \( H_d^D \) with elements \( f_{d+i+j+1}, i, j = 0, 1, \ldots, N \) vanishes. \( D = N + 1 \) is the determinant dimension and \( d = 0, 1, \ldots \). The main assumption of the RPM is that there are sequences of roots \( E_d^D, D = 2, 3, \ldots \) of the Hankel determinant that converge towards the eigenvalues of the equation (1) for a given \( d \). Previous applications of this approach have shown that the Hankel series of roots exhibit remarkable rate of convergence and yield accurate results for a wide variety of problems [2–14]. If \( E_d^D < E_{d+1}^D \) \( (E_d^D > E_{d+1}^D) \) then the Hankel series provide lower (upper) bounds. This property has been proved for some simple models [3] but it is more practical to proceed by inspection of the series.

The RPM yields the exact result in the partially solvable cases; for example, when \( b = -0.46 \) and \( c = 0.1 \), then \( H_0^D = (5E - 12)^{D-1} P(E) \), where the roots of the polynomial \( P(E) \) give the approximations to the other eigenvalues. Notice that the RPM yields the exact result \( E = 12/5 = 2.4 \) for the ground state of the model \( (n = l = 0) \), while, on the other hand, the AIM with the large–dimension expansion gives this eigenvalue only approximately [1].

In those cases that the eigenvalue equation (1) is not exactly solvable the RPM provides upper and lower bounds. For concreteness we choose a model with intermediate values of the parameters: \( b = c = 1 \). Fig. 1 shows \( \log |E_0^D - E_1^D| \), which is is a clear indication of the convergence of the upper \( E_0^D \) and lower \( E_1^D \) bounds towards each other, for the states with \( n = l - 1 = 0, \) and \( n = l = 1 \). It is well known that the convergence rate of the Hankel sequences decreases as the number of radial zeros (given by \( n \)) increases because we need larger values of \( N \) to take into account the increasing number of poles of \( f(x) \) [2–14]. We clearly appreciate this fact in Fig. 1 where the lower curve corresponds to the state with \( n = 0 \). For this state we obtain the bounds \( E_{20}^0 = 5.6513933067559477094 > E(n = 0, l = 1) > E_{20}^1 = 5.6513933067559476997 \). Notice that both the variational \( E_{var} = 5.65139331725017 \) [15] and AIM–SNLT \( E_{AIM} = 5.654047914 \) [1] results lie outside the bounds and display a misleading number of wrong digits. For the state \( n = l = 1 \) we conclude that the sixth–order AIM–SNLT estimate \( E_{AIM} = 9.708 \) lies outside our bounds \( E_{20}^0 = 9.7137541388484906057 > E > E_{20}^1 = 9.7137541388484891570 \). We realize that the RPM enables one to
estimate the accuracy of other approaches.

We can also monitor the convergence rate of a sequence $s_n$, $n = 1, 2, \ldots$ by means of a sort of logarithmic error $\log |s_{n+1} - s_n|$. Fig. 2 shows this logarithmic error for the sequences $E_D^0$ and $E_D^1$. We can improve our results by means of an interpolation of the upper and lower bounds: $i_D(p) = (E_D^0 + pE_D^1)/(1 + p)$. If $D = K$ is our largest determinant dimension we obtain the optimal value of $p$ from the condition $i_K(p) = i_{K-1}(p)$. Fig. 2 shows also the logarithmic error for the sequence $i_D(p)$ and we appreciate what appears to be a considerably gain of accuracy. From the interpolated sequence we estimate $E(n = 0, l = 1) = 5.6513933067559477064$ that is clearly between the bounds given above.

3 Conclusions

We have shown that the RPM yields much more accurate results than the perturbation version of the AIM. The partial sums of the perturbative AIM appear to converge towards the RPM results but they may by asymptotic divergent. It is impossible to state that a series converges by simple inspection of the first four terms. In the particular case of the anharmonic oscillator the RPM provides tightly accurate upper and lower bounds to the eigenvalues that are most useful to estimate the accuracy of the results.

Finally, we want to discuss one of Barakat’s comments regarding an early application of the HPM [16]. He states “However, the previous authors in their work did not give explicit expressions of their algorithm, each order getting progressively much more complicated than the previous one, and the derivations were tediously long. Thus, the need arises here to have a relatively simple, fast and effective method that will provide large-order shifted $1/N$ expansions.” This sentence is surprising (to say the least) because Maluendes et al [16] gave a recurrence relation from which one obtains perturbation corrections of any order, either numerically (in those days) or analytically by the aid of today computer algebra systems. Despite the fact that each order “gets progressively more complicated than the previous one” Maluendes et al [16] carried out perturbation calculations of order twenty five, while Barakat [1] has not managed to obtain more that six. Besides, that very same hypervirial perturbation method has enabled us to derive analytical expressions of the perturbation coefficients for any order and arbitrary potential–energy functions [17]. On the other hand, Barakat presents nu-
merical perturbation coefficients for some particular states and particular values of the potential parameters [1]. I doubt that the AIM may be able to provide analytical expressions like those just mentioned [17]. Of course, the general analytical expressions [17] are bound to look more cumbersome than the numbers in Table 1 in Barakat’s paper [1] that apply to particular cases. It is also important to remember that the AIM does not give results in terms of arbitrary quantum numbers. Any such result has been obtained by induction from results for \(n = 0, 1, \ldots\) [18–22]. This is possible for extremely simple problems but it is much more difficult in general. Besides, in those cases the authors simply verified that their particular results agreed with the analytical expression derived by other more efficient strategies. Notice that Barakat presents only the correction of order zero in terms of \(n\) [1]. On the other hand, the unperturbed energy \(\varepsilon_{nl}^{(0)}\) appears explicitly in the main equations of the hypervirial perturbative method and, consequently, all the corrections are straightforwardly given in terms of it [16,17].

Finally, we mention that a variant of the RPM [23] has been successfully applied to several nonlinear problems of physical interest [24–26]. It is not clear that the AIM can be suitable for the treatment of such problems.

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Figure 1: Logarithm of the difference between the upper bound and lower bound for the states with $n = l - 1 = 0$ (squares) and $n = l = 1$ (circles)

Figure 2: Logarithmic error $\log|s_{D+1} - s_D|$ for the sequences $E_D^0$ (squares), $E_D^1$ (filled squares), and interpolation (circles)