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Tight bounds to the Schrödinger equation eigenvalues

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Abstract. Increasingly tight upper and lower bounds to the Schrödinger equation eigenvalues are obtained from the Riccati equation for the logarithmic derivative of the wavefunction. The solution of this non-linear equation is written as a Padé approximant and the bounds are given by the roots of a sequence of determinants. Numerical results are shown for the anharmonic and quartic oscillators.

1. Introduction

Fernández and Castro [1] have recently shown that approximations to the eigenvalues of the Schrödinger equation can be obtained from the roots of the coefficients of the Taylor expansion for the logarithmic derivative of the wavefunction. The method proves to be useful in treating one-dimensional and central-field models and leads to upper and lower bounds to the energy provided rather strict conditions are satisfied. An approach to more difficult problems has also been suggested [1] which has led to analytical expressions for the energies of the Zeeman effect in hydrogen [2]. However, high-order numerical investigation of easily tractable models shows that the procedure is divergent and for this reason the accuracy of the results is limited. [1].

The purpose of the present paper is to develop an improved version of the above-mentioned method that leads to increasingly tight upper and lower bounds to the lowest eigenvalues. To this end the logarithmic derivative of the wavefunction is approximated by a sequence of Padé approximants as discussed in § 2. Results for the anharmonic and quartic oscillators are presented in § 3 and conclusions are drawn in § 4.

2. Method

The procedure discussed below applied to the ground and first excited states of one-dimensional models with parity-invariant potentials and to the s states of central-field problems. More general quantum mechanical systems will be studied elsewhere. For the sake of concreteness we consider the one-dimensional time-independent Schrödinger equation

$$\psi''(x)+(E-V(x))\psi(x)=0 \tag{1}$$

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where

$$V(x)=\sum_{j=1}^{k} v_j x^{2j} \qquad v_k>0. \tag{2}$$

Extension to rational potentials $V(x)$ is straightforward.

The function

$$f(x)=-\psi'(x)/\psi(x)+p/x \tag{3}$$

where $p=0$ for the ground state and $p=1$ for the first excited state, satisfies the Riccati equation

$$f^2-f'-2pf/x=V-E. \tag{4}$$

The function $f(x)$ is regular and can be expanded in a Taylor series around the origin

$$f(x)=\sum_{j=0}^{\infty} f_j x^{2j+1} \tag{5}$$

where the coefficients f_j are found [1] to obey

$$f_j=(2j+2p+1)^{-1}\left(\sum_{i=0}^{j-1} f_i f_{j-i}+E\delta_{j0}-\sum_{i=1}^{k} v_i\delta_{ji}\right) \qquad j=1,2,\ldots \tag{6}$$

where $f_0=E/(2p+1)$. Clearly, f_j is a polynomial function of f_0 of degree $j+1$.

A rational approximation

$$\tilde{f}(x)=\frac{A(x)}{B(x)} \qquad A(x)=\sum_{j=0}^{M} a_j x^{2j+1} \qquad B(x)=\sum_{j=0}^{N} b_j x^{2j} \tag{7}$$

can be found so that

$$\tilde{f}(x)=\sum_{j=0}^{M+N+1} f_j x^{2j+1}+O(x^{2M+2N+5}). \tag{8}$$

To this end the coefficients a_j and b_j have to satisfy

$$a_m=\sum_{j=0}^{m} b_j f_{m-j} \qquad m=0,1,\ldots,M \tag{9}$$

$$\sum_{j=0}^{m} f_{m-j} b_j=0 \qquad m=M+1,M+2,\ldots,M+N+1 \tag{10}$$

where $b_j=0$ if $j>N$. In order to have a non-trivial solution to the homogeneous linear equations (10) it is necessary that

$$\det \mathscr{F}=0 \tag{11}$$

where $\mathscr{F}$ is the matrix of the system (10). The roots of (11) determine a set of f_0 values. Some of them prove to be bounds to $E/(2p+1)$ for the ground and first excited states of (1).

We first notice that $\tilde{f}$ defines a potential $V(x)+R(x)$ given by

$$\tilde{f}^2-\tilde{f}'-2p\tilde{f}/x=V+R-W \qquad W=(2p+1)f_0 \tag{12}$$

and an approximate wavefunction $\tilde{\psi}$, $\tilde{\psi}'=-\tilde{f}\tilde{\psi}$, which behaves asymptotically as

$$\tilde{\psi}\sim\exp[-a_M x^{2(M-N+1)}/2(M-N+1)b_N] \tag{13}$$

when $x \to \infty$. It cannot yield the exact asymptotic behaviour

$$\psi \sim \exp[-v_k^{1/2} x^{k+1}/(k+1)] \tag{14}$$

unless $2(M-N) = k-1$.

If $M+N+2 = J$, where $J = \max\{2M+1, 2N+k\}$, then it follows from (6)-(10) that R reduces to only one term. When $2M+1 > 2N+k$ we have

$$R = a_M^2 x^{4M+2}/B^2 \tag{15}$$

and it can be easily proved that $W > E$ provided

$$\int_{-\infty}^{\infty} \psi\tilde{\psi}\, dx < \infty. \tag{16}$$

Since $\tilde{\psi} \sim \exp(-a_M x^4/4b_M)$, this last equation always holds for $k > 3$.

On the other hand, when $2M+1 < 2N+k$ it is found that

$$R = -v_k x^{4N+2k}/B^2. \tag{17}$$

Since $-\tilde{\psi}''/\tilde{\psi} + V = W - R \geqslant W$, it follows from theorem 3 of [3] that $W \leqslant E$. Our algorithm can therefore yield both upper and lower bounds to the first two eigenvalues of (1).

In the case of the anharmonic oscillator ($k = 2$) one can choose $M = N+s$, $s = 0, 1$ and the bounds are found to be given by the roots of the Hankel-Hadamard determinants (cf (10) and (11))

$$H_N^s = \det \mathscr{F} \qquad \mathscr{F}_{ij} = f_{i+j+s-1} \qquad i, j = 1, 2, \ldots, N+1. \tag{18}$$

It is worth noticing that the Riccati equation (4) applies to central-field models provided that $0 < x \equiv r < \infty$ and $p = l+1$, where $l = 0, 1, \ldots$ is the angular momentum quantum number.

3. The anharmonic oscillator

In order to check the conclusions drawn in § 2 we consider here the anharmonic oscillator potential

$$V(x) = x^2 + \lambda x^4 \tag{19}$$

because the Schrödinger equation eigenvalues have been accurately calculated [4-6]. A tedious but straightforward calculation using (6) and (18) shows that

$$H_1^0 = [(W^2-1)^2(W^2-25)/63 + 6\lambda W(W^2-1)/7 - \lambda^2]/25 \tag{20}$$

$$H_1^1 = [(W^2-1)^2(W^2-25)(W^2+3)/3 - 6\lambda W(W^2-1)(31W^2-47) + \lambda^2(222W^2-294)]/99\,225 \tag{21}$$

for the ground state and

$$H_1^0 = [(W^2-9)^2(W^2-49)/91\,125 + 8\lambda W(W^2-9)/3645 - \lambda^2]/49 \tag{22}$$

$$H_1^1 = [(W^2-9)^2(W^2-49)(W^2+11)/1125 - 2\lambda W(W^2-9)(17W^2-233)/15 + \lambda^2(122W^2-1458)]/1964\,655 \tag{23}$$

for the first excited state. When $\lambda = 0$ the roots of H_1^0 and H_1^1 agree with the actual harmonic oscillator eigenvalues $E_0 = 1$, $E_1 = 3$, $E_2 = 5$, and $E_3 = 7$. As shown in table 1 the implicit analytical expressions $H_1^s(W, \lambda) = 0$, $s = 0, 1$, yield acceptable estimates of E_0 and E_1 for all values of λ, and $W_n(H_1^0) < E_n < W_n(H_1^1)$ as was mentioned above. The second and third excited states can also be obtained from the roots of H_1^1 but the accuracy is poor for $\lambda > 0.1$. The problem posed by such excited states will be studied in a forthcoming paper.

To test the convergence of the method we consider the most unfavourable case of the quartic oscillator

$$V(x) = x^4. \tag{24}$$

The relative deviations $\delta_N^s = [W_n(H_N^s) - E_n]/E_n$ for the two first eigenvalues E_0 and E_1 [5, 6] are shown in table 2 for $s = 0, 1$ and increasing N values. In both cases the proper root of H_N^0 increases providing tight lower bounds. On the other hand, H_N^1 exhibits two zeros $W_n(H_N^1)^L$ and $W_n(H_N^1)^U$ when $N > 1$ so that the former increases and the latter decreases as N increases. It is found that $W_n(H_N^1)^L < W_n(H_N^0) < E_n < W_n(H_N^1)^U$ for $n = 0$, 1 and $N > 1$. Besides, the convergence rate of the algorithm is formidable with $(\delta_N^1)^L$, δ_N^0 and $(\delta_N^1)^U$ being roughly of order 10^{-2N+2}, 10^{-2N} and 10^{-2N-1}, respectively. We are at present unable to account for the lower bound $W_n(H_N^1)^L$.

Table 1. Upper and lower bounds on the first two eigenvalues of the anharmonic oscillator (19) obtained from the roots of $H_1^s(W, \lambda)$, compared with the exact values E_0 and E_1 taken from [4, 5].

λ	$W_0(H_1^0)$	$W_0(H_1^1)$	E_0	$W_1(H_1^0)$	$W_1(H_1^1)$	E_1
10^{-1}	1.065 166	1.065 292	1.065 286	3.2775	3.306 915	3.306 872
10^{0}	1.389	1.392 67	1.392 352	4.5407	4.650 2	4.648 813
10^{1}	2.432	2.451	2.449 174	8.33	8.606	8.599 003
10^{2}	4.955	5.005	4.999 418	17.22	17.846	17.830 193
10^{3}	10.54	10.651	10.639 789	36.76	38.122	38.086 833
10^{4}	22.64	22.889	22.861 609	79.03	81.979	81.903 317

Table 2. Relative deviations $\delta_N^s = [W_n(H_N^s) - E_n]/E_n$ from the first two exact eigenvalues $E_0 = 1.060\,362\,090\,484\,182\,89$ [5, 6] and $E_1 = 3.799\,673\,029\,801\,394\,16$ of the quartic oscillator (24).

	$n = 0$			$n = 1$		
N	δ_N^0	$(\delta_N^1)^L$	$(\delta_N^1)^U$	δ_N^0	$(\delta_N^1)^L$	$(\delta_N^1)^U$
1	-9.6×10^{-3}		1.0×10^{-3}	-8.4×10^{-3}		9.3×10^{-4}
2	-1.2×10^{-4}	-1.3×10^{-2}	1.3×10^{-5}	-1.0×10^{-4}	-1.3×10^{-2}	1.1×10^{-5}
3	-1.4×10^{-6}	-2.0×10^{-4}	1.5×10^{-7}	-1.2×10^{-6}	-1.9×10^{-4}	1.3×10^{-7}
4	-1.9×10^{-8}	-2.9×10^{-6}	4.9×10^{-10}	-1.3×10^{-8}	-2.6×10^{-6}	1.4×10^{-9}
5	-1.9×10^{-10}	-3.9×10^{-8}	1.5×10^{-11}	-1.5×10^{-10}	-3.4×10^{-8}	1.5×10^{-11}
6	-1.9×10^{-12}	-1.4×10^{-9}	1.1×10^{-13}	-1.6×10^{-12}	-4.5×10^{-10}	1.5×10^{-13}
7	-8.0×10^{-14}	-6.9×10^{-12}	1.0×10^{-14}	-3.9×10^{-14}	-5.1×10^{-12}	1.0×10^{-14}

4. Further comments and conclusions

The method just developed yields rapidly convergent upper and lower bounds to the Schrödinger equation eigenvalues. For this reason we believe that it is worth further investigation. A difficult problem to be dealt with in most cases is the occurrence of undetermined coefficients f_j. This happens, for instance, when $V(x)$ has no definite parity because $f(x)=f_0+f_1x+\ldots$, where $f_1=E+f_0^2$. Therefore, both E and f_0 are to be determined. Such a difficulty is reminiscent of the missing moment problem discussed by Handy and Bessis [7]. However, although they found one missing moment for both the anharmonic and quartic oscillators, there are no undetermined coefficients f_j when using our procedure. In addition to this, our bounds converge faster than theirs as can be easily verified by comparing table 2 of the present paper with table 4 of [7].

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