Accurate eigenvalues of bounded oscillators

Francisco M Fernández

INIFTA (UNLP,CCT La Plata-CONICET), División Química Teórica, Diag 113 S/N, Sucursal 4,
Casilla de Correo 16, 1900 La Plata, Argentina

E-mail: fernande@quimica.unlp.edu.ar

Abstract
We calculate accurate eigenvalues of a bounded oscillator by means of the Riccati–Padé method that is based on a rational approximation to a regularized logarithmic derivative of the wavefunction. Sequences of roots of Hankel determinants approach the model eigenvalues from below with a remarkable convergence rate.

PACS number: 03.65.Ge

1. Introduction

Some time ago, Fernández *et al* [1–11] developed a method for the accurate calculation of eigenfunctions and eigenvalues for bound states and resonances of separable quantum-mechanical models. This approach is based on Padé approximants built from the Taylor expansion of a regularized logarithmic derivative of the eigenfunction. If such rational approximations are forced to yield an additional coefficient of the Taylor expansion, then the physical eigenvalue is given by a convergent sequence of roots of Hankel determinants constructed from the coefficients of that series. One merit of this approach, called the Riccati–Padé method (RPM), is the great convergence rate of such sequences in most cases, and that the same equation applies to bound states and resonances [1–11]. Besides, in some cases the sequences yield upper and lower bounds to the eigenvalues [2].

The approach just mentioned was mainly applied to quantum-mechanical models with asymptotic boundary conditions at infinity [1–11], but it was suggested that it may be suitable for bounded problems as well [8]. In this paper, we try the RPM on the bounded anharmonic oscillator recently discussed by Ciftci and Ateser [12] that may be suitable for the study of quarkonium physics.

In secion 2, we outline the main features of the RPM. In section 3, we apply the RPM to the bounded oscillator proposed by Ciftci and Ateser [12]. In section 4, we briefly address the problem of spurious roots. In section 5, we show that the RPM applies to the central-field version of the bounded oscillator. Finally, in section 6, we draw some conclusions.

2. Method

In this section, we outline the main features of the RPM. For concreteness, we consider the dimensionless Schrödinger equation with an even-parity potential $V(x)$

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

with as yet unspecified boundary conditions. We assume that the Taylor expansion

$$V(x) = \sum_{j=0}^{\infty} V_j x^{2j} \tag{2}$$

converges in a neighbourhood of $x = 0$.

The modified logarithmic derivative $f(x) = s/x - \psi'(x)/\psi(x)$ satisfies the Riccati equation

$$f'(x) + \frac{2s}{x} f(x) - f(x)^2 - \frac{s(s-1)}{x^2} + V(x) - E = 0, \tag{3}$$

where the fourth term disappears when $s = 0$ or 1 that correspond to even or odd states $\psi(x)$, respectively. The Taylor expansion

$$f(x) = x \sum_{j=0}^{\infty} f_j x^{2j} \tag{4}$$

also converges in a neighbourhood of $x = 0$ and the coefficients f_j depend on the eigenvalue E.

The Padé approximant

$$[N + d/N] = x \frac{\sum_{j=0}^{N+d} a_j x^{2j}}{\sum_{j=0}^{N} b_j x^{2j}} \tag{5}$$

yields exactly the first $2N + d + 1$ coefficients of the series (4). We look for the values of E that allow the Padé approximant to produce the next coefficient f_{2N+d+1} exactly. Such energy values are given by the roots of the Hankel determinant $H_D^d = 0$ with matrix elements $f_{d+i+j-1}$, $i, j = 1, 2, \ldots, D$, where $D = N + 1$ is the matrix dimension, and $d = 0, 1, \ldots$ is the displacement [1–11].

Each Hankel determinant exhibits many roots but one easily identifies convergent sequences $E_n^{[D]}$, $D = 2, 3, \ldots$ that approach the actual eigenvalues E_n of the Schrödinger equation (1). If one such sequence is monotonously increasing (decreasing), then each element provides a lower (upper) bound to the eigenvalue. This property of the Hankel sequences was already proved for some problems [2].

Another interesting feature of the RPM is that one does not have to take into account the boundary conditions explicitly. The method selects the appropriate values of E according to the singularities of the potential as we shall see below.

3. The model

Ciftci and Ateser [12] studied the Schrödinger equation (1) with the potential

$$V(x) = \frac{a^2 x^2}{\left(1 - x^2/R^2\right)^2}, \qquad (6)$$

where $a, R > 0$, $-R < x < R$, and the boundary conditions $\psi(\pm R) = 0$ which are obviously determined by the poles of $V(x)$. We begin our analysis by noticing that the change of variables $x = Lq$, where L is an arbitrary positive parameter, leads to the differential equation

$$\Phi''(q) + \left[L^2 E - \frac{a^2 L^4 q^2}{\left(1 - L^2 q^2/R^2\right)^2} \right] \Phi(q) = 0, \qquad (7)$$

for $\Phi(q) = \psi(Lq)$. Therefore, setting $L = a^{-1/2}$ or R one realizes that it is possible to choose either a or R equal to unity without loss of generality as follows from the obvious equalities $E(a, R) = R^{-2} E(aR^2, 1) = a E(1, aR)$. From a purely numerical point of view it is convenient to calculate $R^2 E(1, R)$ for small R and $E(1, R)$ for large R because $\lim_{R \to 0} R^2 E_n(1, R) = (n+1)^2 \pi^2/4$ and $\lim_{R \to \infty} E_n(1, R) = 2n + 1$, where $n = 0, 1, \ldots$ (from now on it should be assumed that $a = 1$ unless otherwise stated).

We first show that the RPM yields the exact harmonic oscillator eigenvalues when $R \to \infty$. For example, the determinant of smallest dimension for $s = 0$ and $d = 0$ is

$$H_2^0 = \frac{\begin{bmatrix} E^6 R^4 - 27 E^4 R^4 + 324 E^3 R^2 + 51 E^2 R^4 \\ -675 E^2 - 324 E R^2 - 25 R^4 - 81 \end{bmatrix}}{4725 R^4}, \qquad (8)$$

so that

$$\lim_{R \to \infty} H_2^0 = \frac{(E^2 - 25)(E^2 - 1)^2}{4725}, \qquad (9)$$

which clearly shows that two roots of the Hankel determinant give exactly the eigenvalues for the first two states of even parity of the harmonic oscillator.

Table 1. Ground-state energy of the bounded oscillator times R^2 for $R = 0.1$.

D	$d = 0$	$d = 1$
3		2.3697606944397752864
4	2.4662533354307466207	2.4674298730367798888
5	2.4674514194162024875	2.4674515378204140996
6	2.4674515390300695979	2.4674515390347723203
7	2.4674515390348029376	2.4674515390348030263
8	2.4674515390348030267	2.4674515390348030267
9	2.4674515390348030267	2.4674515390348030267
10	2.4674515390348030267	2.4674515390348030267

Table 2. Ground-state energy of the bounded oscillator for some values of R.

R	E_0	D
1	2.8848849919939971927	7
10	1.0150378624976100592	3
100	1.0001500037503748711	2

On the other hand, the present implementation of the RPM is unable to yield exact eigenvalues for $R < \infty$, and the convergence rate of the sequence of roots of the Hankel determinants decreases as R decreases. However, the RPM provides remarkably accurate results for all R as shown in what follows.

Today's available computer algebra softwares (such as Maple, Mathematica, Derive, Maxima, etc) enable one to derive the Hankel determinants analytically as well as to calculate their roots with unlimited accuracy. They are certainly much slower than standard floating-point calculations, but speed is not a relevant issue here. We have set the accuracy of the root finder to (say) 400 digits and then truncated the results to 20 meaningful ones.

According to what was said above we indicate the eigenvalues as E_{2m+s}, where $s = 0$ and 1 correspond to the even and odd states, respectively, and $m = 0, 1, \ldots$.

Table 1 shows two sequences of roots of the Hankel determinants that converge towards the ground-state eigenvalue of the bounded oscillator given as $R^2 E_0(1, R)$, for $R = 0.1$. The first ten digits of the present result agree with those reported by Ciftci and Ateser [12]. The velocity of convergence of the RPM sequences is as remarkable as in previous applications of the method to problems with asymptotic boundary conditions at infinity [1–11].

We have decided to keep 20 digits in all our results although in some cases not all of them are exact. In this way one can clearly estimate the accuracy of an entry by its agreement with the neighbours in the same column and row, making it easier to appreciate the appearance of new stable digits as D or d increases.

Table 2 shows the ground-state energy for some values of R and the smallest determinant dimension at which all the reported digits are stable ($d = 0$ in all the cases).

The convergence rate of the RPM sequence decreases as the quantum number increases. The reason is that N should increase in order to take into account the increasing oscillation of the excited states. Table 3 shows two RPM sequences converging towards the eigenvalue E_2 for $R = 1$. The first six digits of our result agree with those reported by Ciftci and Ateser [12].

Table 3. Energy of the first even excited state for $R = 1$.

D	$d = 0$	$d = 1$
4	24.086798714692429504	24.361407377724659906
5	24.424509979572052554	24.428687415859914431
6	24.429124533510868656	24.429142207076630442
7	24.429143334496913081	24.429143367079353985
8	24.429143368495260376	24.429143368526373359
9	24.429143368527356872	24.429143368527373946
10	24.429143368527374357	24.429143368527374363

Table 4. Energy of the first excited state of the bounded oscillator with $R = 1$.

D	$d = 0$	$d = 1$
3	11.134110459186094281	11.158800510018056742
4	11.161646658411540522	11.161732939936591584
5	11.161737758990207575	11.161737854670925624
6	11.161737857894423316	11.161737857940626897
7	11.161737857941670476	11.161737857941681848
8	11.161737857941682032	11.161737857941682034
9	11.161737857941682034	11.161737857941682034
10	11.161737857941682034	11.161737857941682034

4. Spurious roots

As said above, the Hankel determinants exhibit many roots and one has to select those corresponding to the chosen state and model. Equation (9) shows that there is a double root corresponding to the ground state $E_0 = 1$, and a single root corresponding to the next higher even state $E_2 = 5$. Multiple roots in an exactly solvable problem become multiple sequences converging to the eigenvalue of a nontrivial problem [1–11]. However, one easily identifies the sequence with the best convergence rate looking for the root of H_{D+1}^d closest to the previously chosen root of H_D^d. As D increases, more roots appear in the neighbourhood of the actual eigenvalue which is an additional indication of sound convergence.

The change of variables $x \to ix$ transforms the Hamiltonian operator with potential $V(x) = \frac{x^2}{(1 - x^2/R^2)^2}$ into minus the Hamiltonian operator with potential $V_2(x) = \frac{x^2}{(1 + x^2/R^2)^2}$. This transformation accounts for the spurious roots $E = -1$ and -5 in equation (9) (for $R \to \infty$) as discussed earlier in a more general way [8]. When $R < \infty$ the potential $V_2(x)$ does not support bound states (the RPM does no longer select Dirichlet boundary conditions at $\pm R$, and $-\infty < x < \infty$). In this case, one expects resonances with complex values of E, and outgoing or ingoing waves as $x \to \pm\infty$ [6]. For example, when $R = 1$ there is a sequence of Hankel roots that converge towards $E = -0.015565600439810503080$ that appears to be minus the real part of a resonance of $V_2(x)$. The complex part of this resonance seems to be quite small. We do not discuss this feature of the RPM any further because we are mainly interested in bounded oscillators.

5. Central-field models

Ciftci and Ateser [12] mentioned a possible application of a three-dimensional bounded oscillator to quarkonium physics. The application of the RPM to central-field models is straightforward [1, 3, 5, 6]. The Riccati equation for the radial part of the Schrödinger equation becomes

$$f'(r) + \frac{2s}{r} f(r) - f(r)^2 - \frac{s(s-1)}{r^2} + V(r)$$
$$+ \frac{l(l+1)}{r^2} - E = 0 \qquad (10)$$

where $f(r) = s/r - \psi'(r)/\psi(r)$ and $\psi(0) = 0$. In this case, $l = 0, 1, \ldots$ is the angular-momentum quantum number and we choose $s = l + 1$ in order to remove the centrifugal term and make $f(r)$ regular at origin [1, 3, 5, 6]. When $l = 0$ the results are identical to those of the odd states of the

one-dimensional problem that satisfy the same boundary condition at origin. Table 4 shows two Hankel sequences converging towards E_1 (or the energy of the ground state of the central-field model), when $R = 1$ (notice that $s = 1$ in this case). The first six digits of our result agree with those reported by Ciftci and Ateser [12].

It is worth mentioning that the sequences shown in tables 1, 3 and 4 are monotonously increasing, and, therefore, they provide lower bounds to the corresponding eigenvalues of this particular model.

6. Conclusions

We have shown that the RPM gives accurate eigenvalues for some one-dimensional and central-field bounded oscillators. The approach automatically selects the physical energies according to the singularities of the potential-energy function. In addition to enlarging the field of application of the RPM, we have verified that the perturbation variant of the asymptotic iteration method (AIM) proposed by Ciftci and Ateser [12] yields reasonably accurate results for most physical purposes. However, the RPM appears to be much more accurate and straightforward. It does not require factorization of the asymptotic behaviour of the wavefunction, and its Hankel sequences converge monotonously from below, providing lower bounds to the eigenvalues of this particular model. In this respect, the RPM is a suitable complement to the variational methods that render upper bounds.

Besides, the AIM has not yet proved suitable for the calculation of complex eigenvalues that the RPM yields easily and accurately [5, 6, 8, 9, 11]. It is worth mentioning that the RPM is not restricted to the Schrödinger equation. We have recently applied a variant of the RPM, which we may call the Padé–Hankel method [13], to nonlinear two-point boundary value problems, obtaining very accurate results for the unknown parameters in several models of physical interest [14–16].

References

[1] Fernández F M, Ma Q and Tipping R H 1989 *Phys. Rev.* A **39** 1605
[2] Fernández F M, Ma Q and Tipping R H 1989 *Phys. Rev.* A **40** 6149
[3] Fernández F M 1992 *Phys. Lett.* A **166** 173
[4] Fernández F M and Guardiola R 1993 *J. Phys. A: Math. Gen.* **26** 7169
[5] Fernández F M 1995 *Phys. Lett.* A **203** 275
[6] Fernández F M 1995 *J. Phys. A: Math. Gen.* **28** 4043
[7] Fernández F M 1995 *J. Chem. Phys.* **103** 6581

[8] Fernández F M 1996 *J. Phys. A: Math. Gen.* **29** 3167
[9] Fernández F M 1996 *Phys. Rev.* A **54** 1206
[10] Fernández F M 1997 *Chem. Phys. Lett.* **281** 337
[11] Fernández F M 2008 *J. Phys. A: Math. Theor.* **41** 065202
[12] Ciftci H and Ateser E 2007 *Phys. Scr.* **76** 517
[13] Amore P and Fernández F M 2007 Rational approximation for two-point boundary value problems *Preprint* 0705.3862
[14] Boisseau B, Forgács P and Giacomini H 2007 *J. Phys. A: Math. Theor.* **40** F215
[15] Bervillier C, Boisseau B and Giacomini H 2008 *Nucl. Phys.* B **789** 525
[16] Bervillier C, Boisseau B and Giacomini H 2008 Analytical approximation schemes for solving exact renormalization group equations. II Conformal mappings *Preprint* 0802.1970v1