The Riccati - Padé method for coupled-channel equations

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Abstract.   We present a method for calculating the energies of bound and quasibound states of quantum-mechanical problems expressed in terms of coupled-channel equations. The approach is based on a rational approximation to the logarithmic derivative of the eigenfunction and leads to a simple quantization condition.

1. Introduction

The Riccati–Padé method is an efficient approach for calculating eigenvalues and eigenfunctions of the Schrödinger equation [1–3]. The procedure consists of an appropriate representation of the logarithmic derivative of the eigenfunction by means of a rational function or Padé approximant. The main advantages of the method are its simplicity, its formidable rate of convergence, and the appealing fact that the boundary conditions do not appear explicitly in its formulation. This latter feature makes the method equally suitable for the treatment of bound states and resonances (quasibound states), both given by the same quantization condition as roots of Hankel determinants [4–6]. Although the precise conditions under which the method applies have not been rigorously determined, extensive applications suggest that the method is of quite general validity [1–6].

Up until now, the Riccati–Padé method has been applied to separable problems, i.e. to a single differential equation. In this work we show how to apply this approach to coupled-channel equations which commonly arise from the treatment of nonseparable physical systems. Because the problem of convergence of the coupled-channel expansion is alien to the Riccati–Padé method, we concentrate on simple models with only two equations. The extension to systems with more channels is straightforward in principle.

2. An overview of the Riccati–Padé method

We first present the method in its simplest form by means of its application to the second-order differential equation

$$- Y''(x) + Q(x)Y(x) = 0 \tag{1}$$

where the primes stand for differentiation with respect to x, and $Q(x)$ may depend on an unknown parameter (for example, the quantum-mechanical energy).

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5825

If $Y(x) \sim x^s$ at the origin, then

$$f(x) = \frac{s}{x} - \frac{Y'(x)}{Y(x)} \tag{2}$$

is analytic at that point and can be expanded in a Taylor series:

$$f(x) = \sum_{j=0}^{\infty} f_j x^j. \tag{3}$$

In addition to this, the function $f(x)$ satisfies the Riccati equation

$$f'(x) + \frac{2s}{x} f(x) - f(x)^2 + Q(x) - \frac{s(s-1)}{x^2} = 0. \tag{4}$$

On account of the very definition of $f(x)$ one expects that a rational approximation would be a better representation of this function than the Taylor series, equation (3). Moreover, we choose the unknown parameter in such a way that the rational approximation yields one more coefficient than an ordinary Padé approximant:

$$[N + d/N](x) = \frac{\sum_{j=0}^{N+d} a_j x^j}{\sum_{j=0}^{N} b_j x^j} = \underbrace{\sum_{j=0}^{2N+d} f_j x^j}_{\text{Padé}} + \underbrace{f_{2N+d+1} x^{2N+d+1}}_{\text{present approach}} + \mathcal{O}(x^{2N+d+2}) \tag{5}$$

where $[N/M]$ represents a Padé approximant of degrees N and M in numerator and denominator, respectively. The additional requirement is not satisfied unless

$$H_D^d = \begin{vmatrix} f_{d+1} & f_{d+2} & \cdots & f_{D+d} \\ f_{d+2} & f_{d+3} & \cdots & f_{D+d+1} \\ \cdots & \cdots & \cdots & \cdots \\ f_{D+d} & f_{D+d+1} & \cdots & f_{2D+d-1} \end{vmatrix} = 0 \tag{6}$$

where $D = N + 1$ is the dimension of the Hankel determinant H_D^d. In the case of a quantum-mechanical problem the coefficients f_j are polynomial functions of the energy, and equation (6) plays the role of a quantization condition from which one obtains the energies of bound and quasibound states for sufficiently large values of D. In other words, the problem reduces to obtaining the real (bound states) and complex (quasibound states) roots of sequences of polynomials, generating convergent sequences for increasing values of the polynomial degree. Details of the calculation are given elsewhere [1–6].

It is worth mentioning that there are other systematic ways of obtaining solutions to the Riccati equation (4) that may also prove to be useful in obtaining eigenvalues. For example, continued fractions have been widely studied [7]. Here we choose the remarkably simple rational approximation outlined above.

In the case where $Y(x)$ has a definite parity (i.e. it is even or odd) one proceeds exactly in the way just indicated, except that

$$f(x) = x \sum_{j=0}^{\infty} f_j x^{2j}. \tag{7}$$

As the appropriate variable is x^2 instead of x itself, the rational approximation turns out to be $x[N + d/N](x^2)$. Afterwards the calculation proceeds exactly as indicated above.

It is worth mentioning that the quantization condition equation (6) also follows from an appropriate truncation of either the numerator or denominator of the Padé determinant. For example, $b_N = 0$ leads to $H_N^{d+1} = 0$, and $a_{2N+d+1} = 0$ leads to $H_{N+1}^d = 0$.

3. The Ricatti–Padé method for two coupled-channel equations

Throughout this paper we consider two coupled-channel equations of the form

$$\begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \begin{pmatrix} A(x) \\ B(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \tag{8}$$

where

$$\begin{aligned}
L_{11} &= -\frac{d^2}{dx^2} + Q_{11}(x) \\
L_{22} &= -\frac{d^2}{dx^2} + Q_{22}(x) \\
L_{12} &= L_{21} = Q_{12}(x).
\end{aligned} \tag{9}$$

The functions $Q_{jj}(x)$ in the diagonal elements of the matrix operator depend on the energy E. The treatment of more than two equations should be a straightforward extension of the algorithm for the present simple case.

For the kind of problems considered here, the regular solutions of equation (8) behave near the origin as $A(x) \sim A_0 x^s$ and $B(x) \sim B_0 x^{s'}$, where the values of $s, s' \geqslant 0$ are determined by the indicial equations. We assume that A_0, B_0 and E are the only unknowns when we expand $A(x)$ and $B(x)$ in a Taylor series about $x = 0$. In other words, by virtue of equation (8), all the coefficients of such series depend only on the three parameters indicated. We are allowed to arbitrarily choose either $A_0 = 1$ or $B_0 = 1$ so that just two undetermined parameters remain.

Before proceeding with the description of the method it is worth mentioning possible transformations of equation (8) by means of 2×2 unitary matrices $\mathbf{U}$ independent of the coordinate x:

$$\mathbf{U} \begin{pmatrix} L_{11} & L_{12} \\ L_{21} & L_{22} \end{pmatrix} \mathbf{U}^{-1} = \begin{pmatrix} \tilde{L}_{11} & \tilde{L}_{12} \\ \tilde{L}_{21} & \tilde{L}_{22} \end{pmatrix}. \tag{10}$$

A straightforward application of the rational representation outlined above to each of the logarithmic derivatives

$$\begin{aligned}
f(x) &= \frac{s}{x} - \frac{A'(x)}{A(x)} \\
g(x) &= \frac{s'}{x} - \frac{B'(x)}{B(x)}
\end{aligned} \tag{11}$$

leads to two equations like equation (6) that completely determine the energy E and either A_0 or B_0 (whichever is assumed to be unknown). Finally, one has to solve two nonlinear coupled equations with two unknowns.

The required coefficients f_j and g_j of the Taylor expansions of $f(x)$ and $g(x)$, respectively, are related to the coefficients A_j and B_j of the corresponding expansions of $A(x)$ and $B(x)$ through equation (11).

4. Applications

4.1. Coupled harmonic oscillators

First, we consider two displaced harmonic oscillators coupled by a linear interaction

$$
\begin{aligned}
Q_{11}(x) &= x^2 + \epsilon_1 - E \\
Q_{22}(x) &= x^2 + \epsilon_2 - E \\
Q_{12}(x) &= \lambda x
\end{aligned}
\tag{12}
$$

where ϵ_1 and ϵ_2 are energy shifts, and λ determines the strength of the coupling. This simple problem is a schematic representation of the nuclear-electronic coupling of diatomic molecules, which is used to explain fluorescence phenomena in diatomic molecules (see, e.g. [8])

Written in a different way, this model proved itself useful to be suitable for testing the applicability of the generator coordinate approximation for the description of the nuclear-electronic coupling in diatomic molecules [9]. In fact, through the orthogonal transformation given by

$$
\mathbf{U} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}
\tag{13}
$$

we obtain

$$
\begin{aligned}
\tilde{L}_{11} &= -\frac{d^2}{dx^2} + x^2 + \lambda x + \frac{\epsilon_1 + \epsilon_2}{2} - E \\
\tilde{L}_{12} &= \frac{\epsilon_1 - \epsilon_2}{2} \\
\tilde{L}_{22} &= -\frac{d^2}{dx^2} + x^2 - \lambda x + \frac{\epsilon_1 + \epsilon_2}{2} - E
\end{aligned}
\tag{14}
$$

which is essentially the model considered in [9].

The solutions $A(x)$ and $B(x)$ of the untransformed equations have definite but opposite parity: if $A(x)$ is even (odd) then $B(x)$ is odd (even). The unperturbed problem ($\lambda = 0$) exhibits degenerate states when the difference of energy shifts is an even integer, $\epsilon_2 - \epsilon_1 = 0, 2, 4, \ldots$. In particular when $\epsilon_1 = \epsilon_2$, and the equations given by the transformed operator equation (14) are uncoupled.

We have considered the nondegenerate case, with $\epsilon_1 = 1$ and $\epsilon_2 = 2$. Determinants of dimension $D \leqslant 5$ are sufficient to obtain the first four allowed values of the energy with 10 exact digits for all $0 < \lambda < 1$. Such results, shown in figure 1, have been confirmed by accurate numerical integration of the coupled equations.

4.2. A Coulomb-like problem

The model just discussed only supports bound states. A more interesting and richer example is provided by a Coulomb potential in either a channel or linear coupling:

$$
\begin{aligned}
Q_{11}(x) &= 2(\epsilon_1 - E - 1/x) \\
Q_{12}(x) &= 2\lambda x \\
Q_{22}(x) &= 2(\epsilon_2 - E - 1/x) \qquad x \in [0, \infty]
\end{aligned}
\tag{15}
$$

which approximately reproduces some of the relevant features of the Stark effect in hydrogen.
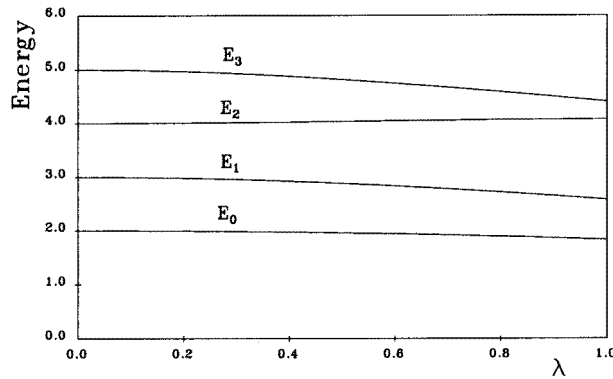
Figure 1. Eigenvalues of the harmonic oscillator with linear coupling.

In the particular case $\epsilon_1 = \epsilon_2$ the system equation (8) is separable into two independent one-dimensional equations by means of transformation (10) with the orthogonal matrix equation (13). One of the equations supports only bound states, whereas the other exhibits no bound state but resonances embedded in the continuum:

$$\tilde{L}_{11} = -\frac{d^2}{dx^2} + 2\left(\lambda x - \frac{1}{x} - E\right)$$

$$\tilde{L}_{12} = 0 \tag{16}$$

$$\tilde{L}_{22} = -\frac{d^2}{dx^2} - 2\left(\frac{1}{x} + \lambda x + E\right).$$

We apply the Riccati–Padé method to the separate and nonseparate forms of this model when $\epsilon_1 = \epsilon_2 = 0$. We already know that the approach gives accurate results in the former case [5], and by comparison we test the present generalized version for coupled-channel equations.

Figure 2 shows the rate of convergence of the sequences of roots for the first real (bound state) and complex (quasibound state) eigenvalues obtained from determinants with shift $d = 0$ (setting $d = 1$ leads to a slight improvement). These results for the *nonseparate* form of the model suggest that the Riccati–Padé method may be of practical utility for the calculation of bound states and resonances in coupled-channel equations. The expression *significant figures* in figure 2 means that the error is of at most two units in the last digit.

4.3. Zeeman effect in hydrogen

The next example is a hydrogen atom in a strong magnetic field along the Z-axis. The diamagnetic part of the Hamiltonian operator in atomic units reads

$$H = -\frac{1}{2}\nabla^2 - \frac{1}{r} + \lambda(x^2 + y^2) \qquad r^2 = x^2 + y^2 + z^2 \tag{17}$$

where λ is proportional to the square of the magnetic-field strength. The eigenstates of the Hamiltonian equation (17) may be characterized by the magnetic quantum number m, because H commutes with the third component L_z of the angular momentum operator. On the other hand, H does not commute with $\boldsymbol{L}^2$, and l is not a good quantum number. This problem has been the subject of intensive research since the first detection of quadratic effects in the measurements of Jenkins and Segrè [10] and their interpretation by Schiff and
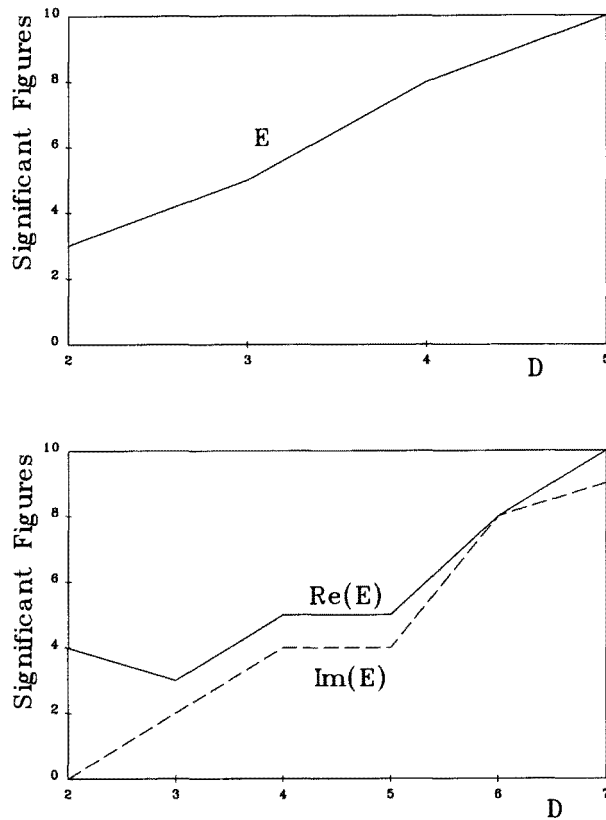
Figure 2. Rate of convergence of two eigenvalues supported by the Coulomb-like potential with linear coupling.

Snyder [11] by means of second-order perturbation theory. Moreover, large-field effects are of astrophysical interest [12]. A review on the Zeeman effect in hydrogen may be found in [13].

To obtain the solution of equation (17) we expand the eigenfunction Ψ in terms of the spherical harmonics $Y_l^m(\theta, \phi)$ (m fixed)

$$\Psi(r, \theta, \phi) = \frac{1}{r} \sum_{l=|m|}^{\infty} \Phi_l(r) Y_l^m(\theta, \phi) \tag{18}$$

giving rise to the coupled equations

$$\left[-\frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{2r^2} - \frac{1}{r} + \lambda C(l, l, m) r^2 - E \right] \Phi_l + \lambda C(l, l-2, m) r^2 \Phi_{l-2}$$
$$+ \lambda C(l, l+2, m) r^2 \Phi_{l+2} = 0 \tag{19}$$

where the matrix elements $C(l, l', m) = \langle Y_l^m | \sin(\theta)^2 | Y_{l'}^m \rangle$ are easily obtained in terms of Clebsch–Gordan coefficients. Here we restrict ourselves to states with $m = 0$.

In order to test the performance of the Riccati–Padé method on this problem we have compared the eigenvalues produced by this method with numerical integration of the same set of coupled equations.
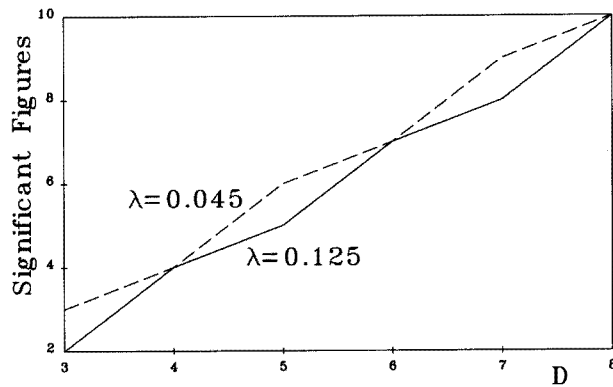
Figure 3. Rate of convergence for the ground state of the diagonal equation with $l = 0$ of the Zeeman effect in hydrogen.

The Riccati–Padé method converges rapidly for the diagonal equations (obtained by entirely neglecting the couplings), as shown in figure 3 for $l = 0$ and two values of λ. These results suggest that the present approach correctly takes into account the singularity of the potential-energy function at infinity (due to the term $r^2 \geqslant x^2 + y^2$).

As a test example for the case of coupled equations we consider only the first two equations for $m = 0$:

$$
\begin{aligned}
&\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r} + \lambda C(0,0,0)r^2 - E \right] \Phi_0 + \lambda C(0,2,0)r^2\Phi_2 = 0 \\
&\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{3}{r^2} - \frac{1}{r} + \lambda C(2,2,0)r^2 - E \right] \Phi_2 + \lambda C(2,0,0)r^2\Phi_0 = 0
\end{aligned}
\tag{20}
$$

where $C(0,0,0) = \frac{2}{3}$, $C(0,2,0) = C(2,0,0) = -2\sqrt{5}/15$, and $C(2,2,0) = \frac{10}{21}$.

Table 1 shows results for the ground state obtained by applying the Riccati–Padé method to one ($l = 0$) and two equations, and the corresponding values determined numerically. For completeness, this table also includes the numerical integration of 10 coupled equations and an accurate variational approach [14, 15]. For the values of λ considered in table 1, the two-channel approach is acceptable (although the contribution of higher l channels is nonnegligible) and the Riccati–Padé method yields satisfactory results suggesting that the method may be of practical utility.

4.4. A system with no bound states

The last example, given by the functions

$$
\begin{aligned}
Q_{11}(x) &= -2(x^2\mathrm{e}^{-x} + E - \epsilon_1) \\
Q_{12}(x) &= -15x^2\mathrm{e}^{-x} \\
Q_{22}(x) &= 15x^2\mathrm{e}^{-x} + 2(E - \epsilon_2) \\
\epsilon_1 &= 0 \\
\epsilon_2 &= 0.1
\end{aligned}
\tag{21}
$$

does not support bound states. Unlike the cases studied above, here the coupling potentials are transcendental functions of the coordinate.

Table 1. Energy of the lowest state with $m = 0$ for the Zeeman effect in hydrogen.

Method	$\lambda = 0.045$	$\lambda = 0.125$
One equation RPM	−0.425 409 9762	−0.323 840 2978
One equation numeric	−0.425 409 98	−0.323 840 3
Two equations RPM	−0.427 429 9	−0.330 92
Two equations numeric	−0.427 429 88	−0.330 920 2
Ten equations numeric	−0.427 462 23	−0.331 168 9
Variational [14, 15]	−0.427 462 29	−0.331 168 9

This model has been used to test new approaches for the calculation of resonance energies and widths [16, 17]. In this case the Riccati–Padé method converges less rapidly than in the previous examples. From determinants of order $D = 12$ (with $d = 0$ and $d = 1$) we obtain $E = E_R + i\Gamma/2 = 4.7681 - 0.0007i$ in agreement with previous calculations [16, 17].

5. Summary

The results shown throughout this paper suggest that the Riccati–Padé method applies to coupled-channel equations. The relevant features of the method are: simplicity, the same straightforward quantization condition for both bound and quasibound states, and in many cases a remarkable rate of convergence. However, it remains to be proved that the approach is practical for the treatment of many coupled-channel equations as one encounters in typical physical problems. The calculation of the appropriate root of a given system of Hankel determinants appears to be the most difficult task because of satellite roots that increase in number as D increases.

Acknowledgments

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