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New approach to separable bounded quantum-mechanical models

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Abstract

We develop an approach to the treatment of separable bounded quantum-mechanical models by the straightforward modification of a successful method for unbounded ones. We apply a new approach to a simple example and show that it provides solutions to both the bounded and unbounded types of models simultaneously.

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1. Introduction

The Riccati–Padé method (RPM) yields accurate eigenvalues of separable quantum-mechanical models [1–7]. The approach is based on a rational approximation to a modified logarithmic derivative of the eigenfunction and the best fit occurs when the eigenvalue is a root of a Hankel determinant [1–7].

The roots of the Hankel determinant approach the energies of bound states and resonances as the determinant dimension increases. The RPM does not require an explicit specification of the boundary condition and the approach commonly selects the physical one automatically for each problem. The resulting eigenvalues always correspond to the correct asymptotic behaviour at infinity [1–7]. As far as we know the RPM is the only approach that applies exactly in the same form to both bound states and resonances.

If the potential-energy function has poles at two points, then the roots of the Hankel determinant approach the eigenvalues of the problem with Dirichlet boundary conditions at such coordinate values [5, 6]. We call these boundary conditions 'natural'.

In some cases one is interested in that the eigenvalue equation satisfies 'artificial' boundary conditions [8–10]. For this reason, in this paper we propose a modification of the RPM to treat Dirichlet boundary conditions at arbitrary coordinate locations. In section 2 we introduce the RPM for one-dimensional models and suggest how to force the desired boundary conditions. In particular, we concentrate on a linear potential that has proved useful for the treatment

of some physical problems [8, 9]. In section 3 we show results for the chosen eigenvalue equation. In section 4 we discuss alternative approaches and in section 5 we summarize the main features of the RPM and draw some conclusions.

2. The method

We introduce the RPM by means of a simple one-dimensional problem of the form

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

that depends on an adjustable parameter that is necessary to satisfy the other boundary condition which we will specify below. For example, in the case of a dimensionless Schrödinger-like equation $Q(x) = E - V(x)$, where the energy E is the adjustable parameter. For concreteness we restrict to this case from now on.

In order to apply the RPM we define the modified logarithmic derivative [3]

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

where the function $g(x)$ is chosen so that $f(x)$ is analytic at $x = 0$ and therefore can be expanded in a Taylor series

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

Note that the coefficients f_j depend on E when $Y(x)$ is a solution to equation (1) with $Q(x) = E - V(x)$. The RPM is based on the transformation of the power series (3) into a rational function or Padé approximant that satisfies

$$[M/N](x) = \frac{\sum_{j=0}^{M} a_j x^j}{\sum_{j=0}^{N} b_j x^j} = \sum_{j=0}^{M+N+1} f_j x^j + O(x^{M+N+2}), \tag{4}$$

where $M = N + d, d = 0, 1, \ldots$. Note that this rational ansatz has just $M + N + 1$ adjustable parameters a_j and b_j to fit the first $M + N + 2$ coefficients of the Taylor series (3). The additional requirement determines the value of E as a root of the Hankel determinant:

$$H_D^d(E) = |f_{i+j+d+1}(E)|_{i,j=0,1,\ldots N} = 0, \tag{5}$$

where $D = N + 1$ is the dimension of the Hankel matrix [1, 2]. Each Hankel determinant is a polynomial function of E and we expect that there is a sequence of roots $E^{[D,d]}$, $D = 2, 3, \ldots$ that converges towards the value of E consistent with the second boundary condition.

The main reason for choosing the rational approximation (4) to the modified logarithmic derivative of the eigenfunction $f(x)$ is that it provides the exact solution for the harmonic oscillator [2], hydrogen atom, and other exactly solvable problems, as well as upper and lower bounds for some models that are not exactly solvable [1].

Commonly, the Hankel quantization condition (5) provides the eigenvalues consistent with the bound states ($Y(x \to \infty) = 0$) or the resonances embedded in the continuum (outgoing or incoming waves). The RPM automatically selects the eigenvalues that are consistent with such 'natural' boundary conditions [1–5, 7].

If the potential-energy function exhibits poles, then the RPM automatically selects Dirichlet boundary conditions at the corresponding coordinate points. For example, when $V(x) = V_0 \sec(x)^2$ the RPM selects the boundary conditions $Y(\pm\pi/2) = 0$ [5], and $Y(\pm R) = 0$ when $V(x) = a^2x^2/(1 - x^2/R^2)^2$ [6].

In some cases one wants to force boundary conditions that are not related to singular points in the potential-energy function [8–10]. Suppose that we are interested in the differential equation (1) with the boundary conditions $Y(0) = Y(1) = 0$. We can force such 'artificial' boundary conditions by means of a properly chosen function $g(x)$ in equation (2). In fact, the function $g(x) = x(1-x)$ introduces poles at $x = 0$ and $x = 1$ into the differential equation for $f(x)$ that we can rewrite as

$$x(1-x)f'(x) + 2(1-2x)f(x) - x(1-x)f(x)^2 - x(1-x)Q(x) + 2 = 0. \tag{6}$$

In this way we expect to obtain the eigenvalues consistent with those boundary conditions.

For simplicity we consider

$$Q(x) = \epsilon - \lambda x. \tag{7}$$

A motivation for this choice is that the resulting differential equation and boundary conditions are related to a simple model for the study of electrons in a crystal under the effect of an electric field [8]. The Schrödinger equation

$$-\frac{\mathrm{d}^2\Phi(X)}{\mathrm{d}X^2} + eFX\Phi(X) = E\Phi(X), \qquad \Phi(0) = \Phi(L) = 0 \tag{8}$$

provides the stationary states and energy levels of an electron of mass m and charge e in a box of impenetrable walls at $X = 0$ and $X = L$ (that mimics the finite size of the crystal) under the effect of an electric field of strength F [8]. This extremely simple model has also been useful in the study of the tail of the density of states of a disordered system in the presence of an electric field [9]. By means of the change of variables $X = Lx$ and $\Phi(Lx) = Y(x)$ one obtains the differential equation (1) with the coefficient (7) where $\lambda = 2mL^3Fe/\hbar^2$ and $\epsilon = 2mL^2E/\hbar^2$.

Another reason for the choice of such an example is that one can write its solutions exactly in terms of the Airy functions $Ai(z)$ and $Bi(z)$:

$$Y(x) = N\left[Bi\left(-\frac{\epsilon}{\lambda^{2/3}}\right)Ai\left(\frac{\lambda x-\epsilon}{\lambda^{2/3}}\right) - Ai\left(-\frac{\epsilon}{\lambda^{2/3}}\right)Bi\left(\frac{\lambda x-\epsilon}{\lambda^{2/3}}\right)\right], \tag{9}$$

where N is a normalization factor, and the dimensionless eigenvalues $\epsilon_n, n = 0, 1, \ldots$, are given by the quantization condition

$$Bi\left(-\frac{\epsilon}{\lambda^{2/3}}\right)Ai\left(\frac{\lambda-\epsilon}{\lambda^{2/3}}\right) - Ai\left(-\frac{\epsilon}{\lambda^{2/3}}\right)Bi\left(\frac{\lambda-\epsilon}{\lambda^{2/3}}\right) = 0. \tag{10}$$

3. Results

The application of the RPM is straightforward: we obtain as many coefficients $f_j(\epsilon)$ as necessary from the differential equation for $f(x)$, construct the Hankel determinants $H_D^d(\epsilon)$, $D = 2, 3, \ldots$, and calculate their roots. We expect these roots to converge towards the eigenvalues of the differential equation with the Dirichlet boundary conditions mentioned above.

Table 1 shows sequences of roots of the Hankel determinants $H_D^0(\epsilon)$ that already converge towards the exact eigenvalues given by equation (10) when $\lambda = 1$. As in previous applications of the RPM we appreciate that the rate of convergence of the Hankel sequences decreases as the energy increases because the denominator of the rational approximation (4) requires greater values of N to accommodate the increasing number of zeros of the solution $Y(x)$.

The results of table 1 show that the present modification of the RPM, consisting in the explicit insertion of the zeros of $Y(x)$ as poles into the Riccati equation for $f(x)$, enables one to apply the approach to models with Dirichlet boundary conditions.

Table 1. First four eigenvalues of the bounded model ($d = 0$).

D	ϵ_0	ϵ_1
2	9	
3	10.2	
4	10.36	
5	10.367 9	35
6	10.368 48	39.3
7	10.368 506	39.89
8	10.368 507 13	39.97
9	10.368 507 161	39.978
10	10.368 507 161 827	39.9787
11	10.368 507 161 8362	39.978 74
12	10.368 507 161 836 336	39.978 7445
13	10.368 507 161 836 3371	39.978 744 77
14	10.368 507 161 836 337 126	39.978 744 7892
15	10.368 507 161 836 337 127	39.978 744 789 86
16	10.368 507 161 836 337 127	39.978 744 789 882
Exact	10.368 507 161 836 337 127	39.978 744 789 883 354 325
D	ϵ_2	ϵ_3
8	81	
9	88	
10	89.1	
11	89.3	144
12	89.321	156
13	89.3259	157.9
14	89.3266	158.31
15	89.326 628	158.39
16	89.326 6340	158.411
Exact	89.326 634 542 478 746 080	158.413 789 814 310 048 71

The Hankel determinants are polynomial functions of the eigenvalues and display many more roots than those that we choose to build the sequences that converge towards the actual eigenvalues of the given problem. One of the features of the RPM is that an increasing number of roots cluster around the eigenvalues as D increases. For the simple example chosen here there are only two roots that approach a given eigenvalue as D increases (at least for $D \leqslant 16$). Figure 1 shows $\log\left|\epsilon_0^{\text{approx}}(D) - \epsilon_0^{\text{exact}}\right|$ for these two sequences when $d = 0$.

In the present case the Hankel determinants exhibit other roots than those mentioned above. They correspond to the 'natural' boundary condition $Y(x \to \infty) = 0$ with eigenvalues given exactly by the quantization condition $Ai(-\epsilon/\lambda^{2/3}) = 0$. The choice of $g(x)$ suggests that we are looking for a solution of the form $Y(x) = x(1-x)\,\mathrm{e}^{-\int f(x)\,\mathrm{d}x}$, but the RPM also selects a solution of the form $Y(x) = x\,\mathrm{e}^{-\int \tilde{f}(x)\,\mathrm{d}x}$ with the 'natural' boundary condition at infinity. The rational approximation to $\tilde{f}(x) = f(x) + 1/(1-x)$ absorbs and removes the pole at $x = 1$ and produces sequences of roots that converge towards the solutions of the unbounded problem ($0 \leqslant x < \infty$). Table 2 shows some of these eigenvalues for $\lambda = 1$. Curiously, more roots cluster around a given eigenvalue of the unbounded model than of the bounded one. Figure 2 shows $\log\left|\epsilon_0^{\text{approx}}(D) - \epsilon_0^{\text{exact}}\right|$ for all the sequences that appear when $D \leqslant 16$ and $d = 0$.

The function $g(x) = x$ is more convenient for the 'natural' boundary conditions and, consequently, the sequences of roots of the Hankel determinants exhibit a greater convergence

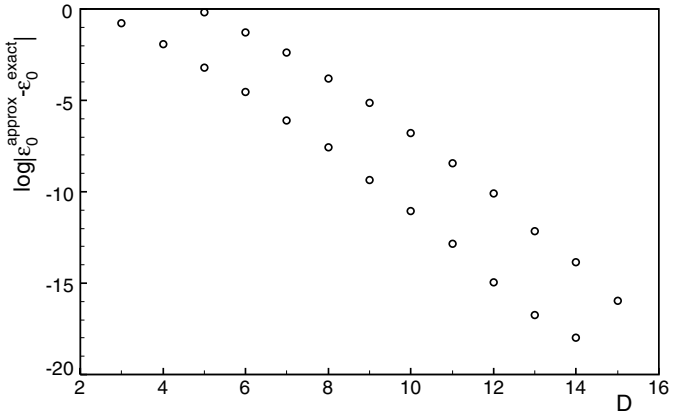

Figure 1. Sequences of roots of the Hankel determinants for the lowest eigenvalue of the bounded model ($d = 0$).

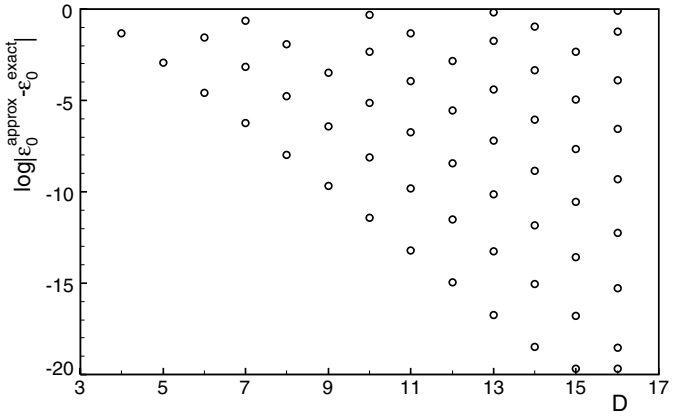

Figure 2. Sequences of roots of the Hankel determinants for the lowest eigenvalue of the unbounded model ($d = 0$).

rate. Figure 3 shows $\log\left|\epsilon_0^{\text{approx}}(D) - \epsilon_0^{\text{exact}}\right|$ for the optimal sequences for both choices of $g(x)$. When $g(x) = x(1-x)$ the rational approximation to $\tilde{f}(x)$ has to remove the wrong zero at $x = 1$ and, for this reason, the rate of convergence of the RPM is slightly smaller. Note that the solution $Y(x)$ that satisfies $Y(x) = Y(x \to \infty) = 0$ does not have a zero at $x = 1$.

4. Alternative approaches

We can also expand the solutions to the bounded model as

$$Y(x) = x(1-x)\sum_{j=0}^{\infty} c_j x^j \tag{11}$$

and try two alternative approaches. First we consider sequences of roots of the Hankel determinant $|c_{i+j+d+1}(\epsilon)|_{i,j=0,1,\ldots,N} = 0$ (approach A1) and, second the truncation condition

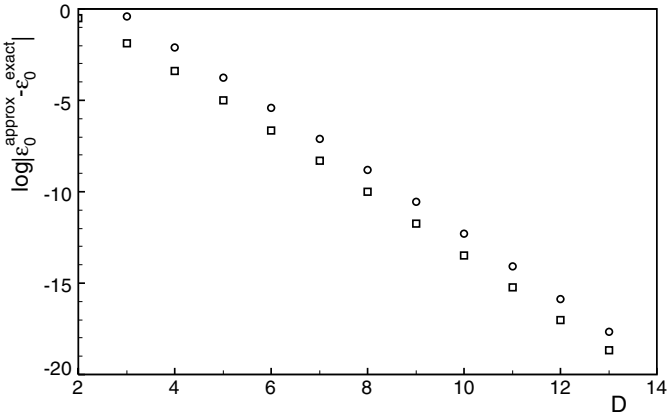

Figure 3. Sequences for the lowest eigenvalue of the unbounded model for $g(x) = x(1-x)$ (circles) and $g(x) = x$ (squares) ($d = 0$).

Table 2. First four eigenvalues of the unbounded model ($d = 0$).

D	ϵ_0	ϵ_1
4	2.29	
5	2.337	
6	2.338 08	4.0
7	2.338 1070	4.083
8	2.338 107 40	4.0878
9	2.338 107 4103	4.087 945
10	2.338 107 410 456	4.087 9493
11	2.338 107 410 459 70	4.087 949 441
12	2.338 107 410 459 766	4.087 949 4440
13	2.338 107 410 459 767 02	4.087 949 444 129
14	2.338 107 410 459 767 0382	4.087 949 444 130 93
15	2.338 107 410 459 767 0385	4.087 949 444 130 970
16	2.338 107 410 459 767 0385	4.087 949 444 130 970 60
Exact	2.338 107 410 459 767 0385	4.087 949 444 130 970 6166
D	ϵ_2	ϵ_3
8	5.1	
9	5.50	
10	5.520	
11	5.520 54	6.74
12	5.520 5591	6.785
13	5.520 559 81	6.7866
14	5.520 559 827	6.786 705
15	5.520 559 828 08	6.786 7080
16	5.520 559 828 0950	6.786 708 086
Exact	5.520 559 828 095 551 0591	6.786 708 090 071 758 9988

$c_M(\epsilon) = 0$ (A2). The convergence rate of these alternative methods is similar and smaller than the RPM. However, from a purely practical point of view the procedure A2 is preferable because the coefficients $c_j(\epsilon)$ are the simplest polynomials of the energy, which results in a faster derivation and calculation of their roots.

Some time ago Fernández and Castro [11] proposed another approach to the treatment of bounded systems which is related to that discussed here. When applied to the present model that approach consists of the ansatz

$$Y(x) = x(1-x)\exp\left(-\sum_{j=1}^{\infty} b_j x^j\right) \tag{12}$$

and the allowed energies are given by the roots of $b_M(\epsilon) = 0$ [11]. This approach does not appear to be successful but the roots of the Hankel determinant $|b_{i+j+d+1}(\epsilon)|_{i,j=0,1,\ldots,N} = 0$ exhibit a reasonable convergence rate (although not as great as the RPM one).

5. Discussion

Simple models of bounded quantum-mechanical systems have proved useful for the study of several physical phenomena [10] (and references therein). The modification to the RPM proposed here is suitable for bounding a system between impenetrable walls that force Dirichlet boundary conditions at their locations. The numerical results of the preceding section show that the convergence rate of the modified RPM is as remarkable as in the case of the unbounded and naturally bounded systems [1–7]. A curious feature of the present application of the RPM to a bounded model is that the approach also provides the eigenvalues of the unbounded one. This outcome is a consequence of the fact that the RPM automatically selects the correct asymptotic behaviour at infinity of the solution to the differential equation. In all the cases studied this asymptotic behaviour coincided with that required by physical reasons (vanishing at infinity, incoming or outgoing waves, etc) [1–5, 7].

In the particular case of the forced Dirichlet boundary conditions considered here, we have found that a straightforward truncation of the series requiring that a coefficient of sufficiently large order vanishes ($c_M(\epsilon) = 0$) leads to a more practical approach from a numerical point of view. However, we think that the remarkable features of the RPM discussed above justify the study of this approach.

The transformation of the Schrödinger equation into a Riccati one has proved suitable for the application of the quasilinearization method (QLM) to quantum mechanics [12–17]. Regarding the calculation of the complex eigenvalues that provide the position and width of the resonances of a quartic anharmonic oscillator, the RPM [4] proves to be more accurate than the QLM [17]. On the other hand, the QLM takes the asymptotic behaviour of the eigenfunctions into account explicitly and the RPM does not, because it is a local approximation. However, the RPM eigenfunctions are accurate in a wide neighbourhood of the origin as shown by the fact that the rational approximation to the modified logarithmic derivative satisfies the corresponding Riccati equation accurately [3].

The main ideas behind the RPM have recently proved useful for the treatment of two-point nonlinear equations [18] of interest in some fields of physics [19–21]. The resulting approach called the Hankel–Padé method (HPM) appears to be an alternative accurate tool for the determination of unknown parameters of the theory that are consistent with the desired asymptotic behaviour of the solution of the nonlinear differential equation [18].

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