Calculation of bound states and resonances in perturbed Coulomb models

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Abstract

We calculate accurate bound states and resonances of two interesting perturbed Coulomb models by means of the Riccati-Padé method. This approach is based on a rational approximation to a modified logarithmic derivative of the eigenfunction and produces sequences of roots of Hankel determinants that converge towards the eigenvalues of the equation.
1 Introduction

In a most interesting series of papers Killingbeck et al [1–3] and Killingbeck
[4, 5] have shown that perturbation theory and the Hill-series method are
suitable tools for the calculation of bound states and resonances of simple
quantum–mechanical models. In order to obtain the complex eigenvalues
that correspond to unstable states they resort to a complex parametrization
of the methods that they call “complexification ”.

Another approach that proves useful for the accurate calculation of bound
states and resonances is the Riccati–Padé method (RPM) based on a rational
approximation to a modified (or regularized) logarithmic derivative of the
eigenfunction [6–15]. In this paper we apply the RPM to the interesting
perturbed Coulomb problems discussed recently by Killingbeck [5] with the
purpose of challenging the recently developed asymptotic iteration method
[16–22].

In Section 2 we outline the main features of the RPM. In Section 3 we dis-
cuss a perturbed Coulomb model with interesting bound states. In Section 4
we calculate the resonances for a slightly modified model with continuum
states. Finally, in Section 5 we draw conclusions on the performance of the
RPM.

2 The Riccati–Padé method (RPM)

Suppose that we want to obtain sufficiently accurate solutions to the eigen-
value equation

\[ \psi''(x) + Q(x)\psi(x) = 0, \quad Q(x) = E - V(x) \]  \hspace{1cm} (1)
where $Q(x)$ can be expanded as

$$Q(x) = \sum_{j=0}^{\infty} Q_j x^{\beta j - 2}$$  \hspace{1cm} (2)

about $x = 0$. We transform the linear differential equation (1) into a Riccati one for the modified logarithmic derivative of the eigenfunction:

$$f(x) = \frac{s}{x} - \frac{\psi'(x)}{\psi(x)}$$  \hspace{1cm} (3)

On substituting (3) into (1) we obtain

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

We choose $s(s-1) = -Q_{-2}$ in order to remove the pole at origin, and, as a result, the expansion

$$f(x) = x^{\beta - 1} \sum_{j=0}^{\infty} f_j x^{\beta j}$$  \hspace{1cm} (5)

for the solution to the Riccati equation (4) converges in a neighbourhood of $x = 0$. Notice that if we substitute the expansions (2) and (5) into the Riccati equation (4), we easily obtain the series coefficients $f_j$ as a function of $E$ and the known potential parameters $Q_j$.

We rewrite the partial sums of the expansion (5) as rational approximations $x^{\beta - 1}[N + d/N](z)$, where $z = x^{\beta}$, in such a way that

$$[N + d/N](z) = \frac{\sum_{j=0}^{N+d} a_j z^j}{\sum_{j=0}^{N} b_j z^j} = \sum_{j=0}^{2N+d+1} f_j z^j + O(z^{2N+d+2})$$  \hspace{1cm} (6)

In order to satisfy this condition the Hankel determinant $H^d_D$, with matrix elements $f_{i+j+d-1}$, $i, j = 1, 2, \ldots, D$, vanishes. Here, $D = N + 1 = 2, 3, \ldots$ is the determinant dimension and $d = 0, 1, \ldots$. The main assumption of the Riccati–Padé method (RPM) is that there is a sequence of roots $E^{[D,d]}$ of
\( H_D^d(E) = 0 \) for \( D = 2, 3, \ldots \) that converges towards a given eigenvalue of equation \( (\Pi) \). Comparison of sequences with different \( d \) values is useful to estimate the accuracy of the converged results.

Notice that we do not have to take the boundary conditions explicitly into account in order to apply the RPM; the approach selects them automatically. In addition to the answers expected from physical considerations, the RPM also yields unwanted solutions as shown below.

3 Model with bound states

From the ansatz \( \varphi(r, \lambda) = r \exp(-r - \lambda r^2) \) and the equation \( \varphi''(r, \lambda)/[2\varphi(r, \lambda)] = V(r, \lambda) - E(\lambda) \) we derive a potential–energy function \( V(r, \lambda) = -1/r + 2\lambda r + 2\lambda^2 r^2 \) if \( E(\lambda) = -1/2 + 3\lambda \). For \( \lambda > 0 \) \( \varphi(r, \lambda) \) and \( E(\lambda) \) are a pair of eigenfunction and eigenvalue of the Schrödinger equation with the potential \( V(r, \lambda) \). For \( \lambda < 0 \) \( E(\lambda) = -1/2 + 3\lambda \) is not an eigenvalue of the Schrödinger equation because the corresponding eigenfunction \( \varphi(r, \lambda) \) is not square integrable. Curiously enough, \( e(\lambda) = -1/2 - 3\lambda \) is close to the ground–state eigenvalue of the Schrödinger equation

\[
\psi''(r) + 2[E - V_1(r)]\psi(r) = 0, \quad V_1(r) = -\frac{1}{r} - 2\lambda r + 2\lambda^2 r^2, \quad \lambda > 0 \quad (7)
\]

when \( \lambda \) is sufficiently small. Killingbeck [5] calculated the energy shift \( \Delta(\lambda) = E(\lambda) - e(\lambda) \) very accurately for several values of \( \lambda \) by means of the Hill–series method.

Our interest in this model stems from the fact that \( 1/r - \varphi'(r, -\lambda) / \varphi(r, -\lambda) = 1 - 2\lambda r \) is an exact rational function and therefore \( e(\lambda) \) will always be a root of the Hankel determinants even though it does not correspond to
a square–integrable eigenfunction if $\lambda > 0$. This unwanted solution will appear as an exact multiple root of the Hankel determinant, very close to the physical one when $\lambda$ is close to zero.

If $\lambda < 2/27$ the potential–energy function \(^{(7)}\) exhibits three stationary points: a minimum at $r_1 < 0$, a maximum at $r_2 \geq 4$ and a shallow minimum at $r_3 > 4$. On the other hand, there is only a minimum at $r_1 < 0$ when $\lambda > 2/27$. Obviously, only the stationary points at $r > 0$ make sense from a physical point of view, and we expect the RPM to yield better results in the latter case. The expansion of the solution to the Riccati equation about $r = 0$ will require many terms in order to take into account the shallow minimum that will move away from origin as $\lambda$ decreases. In this case we expect to face the necessity of Hankel determinants of greater dimension in order to obtain the shift to a given accuracy as $\lambda$ decreases. This unfavourable situation is an interesting test for the RPM that has not been applied to this kind of problems before.

The Hankel determinants are polynomial functions of $\Delta$ and $\lambda$. For example, $H_D^0(\Delta, \lambda) = \Delta^{D-1}P_D(\Delta, \lambda)$ and, therefore, the approximation to the energy shift is given by a root of $P_D(\Delta, \lambda) = 0$ that approaches the multiple root $\Delta = 0$ as $\lambda$ decreases. Table \(\square\) shows $\Delta(\lambda)$ for some values of $\lambda$ calculated with determinants of dimension $D \leq 20$. In order to estimate the last stable digit we compared the sequences of roots with $d = 0$ and $d = 1$. As expected from the argument above, the accuracy decreases as $\lambda$ decreases if we do not increase the maximum value of $D$ consistently, but in all cases we have verified that there is a sequence of roots of the Hankel determinants that converge towards the ground–state eigenvalue. Present results agree
with those calculated by Killingbeck by means of the Hill–series method [5].

4 Model with no bound states

It has already been shown that the RPM is a most efficient tool for the calculation of resonances in the continuum of simple quantum–mechanical models [11, 14, 15]. However, for completeness in what follows we consider the potential–energy function

\[ V_2(r) = -\frac{1}{r} + 2\lambda r - 2\lambda^2 r^2 \]  

(8)

that is closely related to the preceding one but does not support bound states because it is unbounded from below as \( r \to \infty \). In this case we expect unstable or resonant states with complex eigenvalues that correspond to tunnelling from the Coulomb well.

Table 2 shows present results obtained from Hankel sequences with \( D \leq 20 \). As in the preceding example we compared sequences with \( d = 0 \) and \( d = 1 \) in order to estimate the last stable digit. Our results agree with those reported by Killingbeck [5], except for \( \lambda = 0.08 \). While the first digits of the imaginary part of our eigenvalue agree with those in Killingbeck’s Table 3 [5], the real part is completely different. The disagreement is due to a misprint in Killingbeck’s Table 3 for that particular entry. In fact, we have found that the real part of the eigenvalue reported by Killingbeck for \( \lambda = 0.08 \) corresponds to \( \lambda = 0.05 \) instead, as shown in present Table 2.
5 Conclusions

We have shown that the RPM is suitable for the accurate calculation of bound states and resonances of perturbed Coulomb problems. The first model, equation (7), considered in this paper exhibits interesting features that were not faced in previous applications of the RMP [6–15]. A shallow minimum that moves forward from origin as the potential parameter $\lambda$ decreases makes it necessary to resort to Hankel determinants of increasing dimension in order to obtain eigenvalues of a given accuracy. On the other hand, we had already proved that the RPM is suitable for the calculation of resonances in the continuum, and we simply confirmed this strength of the approach by means of the second model chosen above.

The applicability of the RPM is not restricted to eigenvalue equations. We have recently applied it to several ordinary nonlinear differential equations [23]. Since most of them are not Riccati equations we called this variant of the method Padé–Hankel, but the strategy is basically the same outlined in this paper.

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Table 1: Energy shift $\Delta(\lambda)$ for the ground–state energy of the perturbed Coulomb model (7)

| $\lambda$ | $\Delta(\lambda)$ |
|-----------|-------------------|
| 0.10      | 3.41730960373299 $10^{-2}$ |
| 0.09      | 2.31341988422733 $10^{-2}$ |
| 0.08      | 1.4212168993068 $10^{-2}$ |
| 0.07      | 7.546639486534 $10^{-3}$  |
| 0.06      | 3.1738752354 $10^{-3}$   |
| 0.05      | 8.93101948 $10^{-4}$    |
| 0.04      | 1.1819718 $10^{-4}$    |

Table 2: Resonance for the 1s state of the perturbed Coulomb model (8)

| $\lambda$ | Re$E$ | Im$E$ |
|-----------|-------|-------|
| 0.10      | $-0.27519233330828482428$ | 1.3918964850900 $10^{-8}$ |
| 0.09      | $-0.29265795893536614770$ | 7.9213310722 $10^{-10}$ |
| 0.08      | $-0.31105186469292522577$ | 2.094858859 $10^{-11}$ |
| 0.05      | $-0.372260539194895485$   | $-$ $-$ |