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# Local approximation to the critical parameters of quantum wells

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ABSTRACT

We calculate the critical parameters for some simple quantum wells by means of the Riccati–Padé method. The original approach converges reasonably well for nonzero angular-momentum quantum number $l$ but rather too slowly for the $s$ states. We therefore propose a simple modification that yields remarkably accurate results for the latter case. The rate of convergence of both methods increases with $l$ and decreases with the radial quantum number $n$. We compare RPM results with WKB ones for sufficiently large values of $l$. As illustrative examples we choose the one-dimensional and central-field Gaussian wells as well as the Yukawa potential. The application of perturbation theory by means of the RPM to a class of rational potentials yields interesting and baffling unphysical results.



## 1. Introduction

The accurate calculation of the number of bound states supported by a finite quantum–mechanical potential well is of great physical and mathematical importance and for this reason there has been considerable interest in the derivation of upper and lower bounds[1–13]. Most of those bounds are given in terms of the potential-energy function. In a recent paper Liverts and Barnea [14] proceeded in a different way and proposed the calculation of the critical parameters for negative central-field quantum wells. To this end they applied two exact methods and the WKB approach, the latter for the estimation of the large-quantum number behaviour of the critical parameters. In this context a critical parameter is the value of a potential parameter for which an energy eigenvalue is exactly zero (what the authors call a transition state). As they pointed out, one can obtain the exact number of bound states from the tables of critical parameters, as well as other relevant information about the eigenvalue equation [14].

There are local and global methods for the calculation of eigenvalues and eigenfunctions. The former are based on the behaviour of the solution at a properly chosen coordinate point; for example, a power-series expansion. On the other hand, global approaches like the variational method take into account the whole coordinate interval (through expectation values of the associated linear operators, etc.). In principle, local methods are expected to be unsuitable for the calculation of critical parameters. Even the Riccati–Padé method (RPM) [15,16], based on Padé approximants, was shown to be impractical for the calculation of the eigenvalues of the Yukawa potential close to the zero-energy threshold (transition state) [15]. The purpose of this paper is to investigate in more detail whether those earlier results already prove that the RPM is actually useless for the calculation of critical parameters.

In Section 2 we outline the main ideas of the RPM. In Section 3 we briefly discuss the solutions of the Schrödinger equation with even-parity potential wells. In Section 4 we apply the approach to some simple one-dimensional models: the Pöschl–Teller potential, the Gaussian well and a rational potential. We calculate some critical parameters and the

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corresponding eigenfunctions for the first and third cases. In Section 5 we propose a modified version of the RPM that is more suitable for the calculation of critical parameters and apply it to the Gaussian well. Some of those results also apply to *s*-states of the analogous central-field model. In Section 6 we apply the modified RPM to the *s*-states of central-field models and choose the Yukawa potential as a suitable illustrative example. We also show that the original RPM is suitable for the calculation of critical parameters of states with $l > 0$. In Section 7 we discuss the application of perturbation theory to a model with a rational potential that is exactly solvable at threshold. In this case we discuss the appearance of spurious RPM eigenvalues. Finally, in Section 8 we summarize the main results and draw conclusions.

## 2. The Riccati–Padé method

We consider the eigenvalue equation

$$\psi''(x) + Q(E,x)\psi(x) = 0, \quad -\infty < x < \infty, \tag{1}$$

were $E$ is the eigenvalue. We assume that $\psi(x)$ can be expanded about the origin as

$$\psi(x) = x^s \sum_{j=0}^{\infty} c_j x^{\beta j}, \quad s, \beta > 0. \tag{2}$$

It is clear that

$$f(x) = \frac{s}{x} - \frac{\psi'(x)}{\psi(x)}, \tag{3}$$

can be expanded about the origin as

$$f(x) = x^{\beta-1} \sum_{j=0}^{\infty} f_j z^j, \quad z = x^\beta. \tag{4}$$

We approximate $f(x)$ by means of a rational function of the form $x^{\beta-1}[M/N](z)$ where

$$[M/N](z) = \frac{\sum_{j=0}^{M} a_j z^j}{\sum_{j=0}^{N} b_j z^j} = T(M+N+1,z) + O(z^{M+N+2}) \tag{5}$$

and

$$T(n,z) = \sum_{j=0}^{n} f_j z^j. \tag{6}$$

We choose $M \geqslant N$ and define $d = M - N$. It is not possible to satisfy the condition (5) unless $H_D^d = |f_{i+j+d-1}|_{i,j=1}^{D} = 0, D = N+1$. The coefficients $f_j$, and thereby the Hankel determinant $H_D^d$, depend on the eigenvalue $E$. Some of the roots $E^{[D,d]}$ of $H_D^d(E) = 0$ converge toward the eigenvalues of Eq. (1) as $D$ increases [15,16].

The ordinary Padé approximation to $f(x)$ is

$$[M/N](z) = \frac{\sum_{j=0}^{M} a_j z^j}{\sum_{j=0}^{N} b_j z^j} = T(M+N,z) + O(z^{M+N+1}). \tag{7}$$

If $z_0$ is a zero of the denominator then

$$z_0 = -\frac{b_{N-1}}{b_N} - \frac{b_{N-2}}{b_N z_0} - \cdots - \frac{b_0}{b_N z_0^{N-1}}. \tag{8}$$

Suppose that $E^*$ is a root of $b_N(E) = 0$ and that $b_{N-1}(E)$ does not vanish in the interval $(E^* - \epsilon, E^* + \epsilon)$ for a sufficiently small positive real number $\epsilon$. Therefore $|z_0| \to \infty$ as $E \to E^*$. The coefficient $b_N$ is proportional to the Hankel determinant $H_{N-1}^{d+1}(E)$ so that the Hankel condition $H_D^d(E) = 0$ is equivalent to moving a singularity of a rational approximation towards infinity [17]. It is also equivalent to moving a zero of the approximate $\psi(x)$ towards infinity. Consequently, it appears to be reasonable to assume that the Hankel condition is equivalent to selecting bound states that vanish at infinity.

The strategy just outlined applies to other nonlinear equations and for this reason Amore and Fernández [18] chose the more general name Padé–Hankel method which was later discussed by Abbasbandy and Bervillier [17]. However, for historical reasons we prefer to keep the original name RPM when the problem is a Riccati equation derived from the Schrödinger one [15,16].

## 3. Parity-invariant finite wells

The Riccati–Padé method is known to produce accurate eigenvalues for infinite wells or sufficiently deep finite ones [15,16]. The purpose of this section is to investigate to which extent it is possible to apply the RPM to shallow wells. To this end we consider the eigenvalue Eq. (1) with