Accurate eigenvalues and eigenfunctions for quantum-mechanical anharmonic oscillators

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Abstract. The representation of the Taylor expansion of the logarithmic-derivative of the wavefunction by means of a Padé approximant, followed by an appropriate quantization condition, proves a powerful way of obtaining accurate eigenvalues of the Schrödinger equation. In this paper we investigate in detail some of the interesting features of this approach, termed Riccati–Padé method (RPM), by means of its application to anharmonic oscillators. We analyse the occurrence of many roots in the neighborhoods of the physical eigenvalues in the weak-coupling regime, and also obtain accurate coefficients of the strong-coupling expansion. We finally investigate the global and the local accuracy of the RPM eigenfunctions.

1. Introduction

The Riccati–Padé method (RPM) proves a powerful tool for the calculation of accurate eigenvalues of the Schrödinger equation for separable problems [1–3]. It comprises the transformation of the second-order Schrödinger equation into a first-order Riccati differential equation for the logarithmic derivative of the eigenfunction. The power series expansion of the latter function is then represented by a Padé approximant and the eigenvalues are given by a quantization condition coming from the requirement that the approximant yields an additional coefficient of the Taylor expansion exactly. More precisely, the approximate eigenvalues are determined by the roots of Hankel–Hadamard determinants, which are polynomial functions of the energy eigenvalue. The number of roots of the Hankel–Hadamard determinants grows rapidly with the order of the determinant. Some of these roots correspond to physical eigenvalues, but others are spurious. One puzzling feature of the RPM is the concentration of roots in the neighbourhood of the actual eigenvalues. Remark also that in the general case the RPM does not define an approximation method in the standard sense of the word, because it does not construct an approximation sequence for any single eigenvalue.

For certain problems the RPM is useful in order to determine tight upper and lower bounds to the eigenvalues [1–3]. Furthermore, the RPM converges so fast that it is possible to calculate accurate coefficients of the strong coupling expansion for anharmonic oscillators and other perturbed systems [4]. This is a remarkable property of the RPM because it is well known that the accurate calculation of the coefficients of the strong-coupling expansion is an extremely difficult task [5, 6].

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In addition to all this, the RPM gives exact results for solvable or quasi-solvable quantum-mechanical problems because an eigenfunction for any such problem is typically a polynomial multiplied by the exponential of another polynomial and therefore its logarithmic derivative is a rational function [7].

The purpose of this paper is a further study of the RPM. In section 2 we summarize the main equations of the RPM to make the paper self-contained and to introduce the notation used throughout. In section 3 we obtain the coefficients of the weak-coupling expansion for anharmonic oscillators and discuss the appearance of an increasing number of roots of the Hankel–Hadamard determinants close to the selected eigenvalue. We also calculate highly accurate coefficients of the strong coupling expansion for the same models. In section 4 we investigate the form of the RPM eigenfunctions and estimate their global and local accuracy. Finally in section 5 we summarize the most relevant properties of the RPM and indicate further applications of this method.

2. The Riccati–Padé method

In what follows we specialize in the eigenvalue equation

$$\Psi'' = \left(V(x) + l(l+1)/x^2 - E\right)\Psi \tag{1}$$

which applies to many separable quantum-mechanical problems. If $l = 0, 1, \ldots$ is the angular momentum quantum number and $x \geqslant 0$ then equation (1) corresponds to the radial equation for a central-field model. In this case $\Psi(x)$ vanishes as x^{l+1} at origin. For a one-dimensional model we have $l(l+1) = 0$ and $-\infty < x < \infty$. In particular if $V(x)$ is parity invariant then $l = -1$ and $l = 0$ give rise to the even and odd solutions, respectively.

The first step in the RPM is the transformation of the Schrödinger equation (1) into a Riccati equation for the function $f(x)$ defined as

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

where $g(x)$ has been introduced to cancel out known singularities of $\Psi'(x)/\Psi(x)$. Differentiation of (2) with respect to x and substitution of the Schrödinger equation leads to

$$f' = f^2 - 2\frac{g'}{g}f + \frac{g''}{g} + E - V - \frac{l(l+1)}{x^2}. \tag{3}$$

The choice $g(x) = x^{l+1}$ removes the last term in (3) and there remains

$$f' = f^2 - 2\frac{l+1}{x}f + E - V. \tag{4}$$

For present purposes it suffices to consider a parity invariant potential of the form

$$V(x) = \sum_{j=0}^{K} v_j x^{2j}, \tag{5}$$

defined in terms of a set of coupling constants $v_0, \ldots, v_K$. Obviously v_0 may be taken zero without loss of generality. We will consider the domain $-\infty < x < \infty$ and $v_K > 0$ to ensure the existence of bound states.

In this case the solution of the Riccati equation can be expanded in a Taylor series about the origin

$$f(x) = x\sum_{j=0}^{\infty} f_j x^{2j} \tag{6}$$

the coefficients of which can be obtained recursively in terms of the energy according to

$$f_n = \frac{1}{n + 2l + 3} \left[\sum_{j=0}^{n-1} f_j f_{n-j-1} + E\delta_{n0} - v_n \right]. \tag{7}$$

This set of equations for $n = 0, 1, \ldots$, is a hierarchy of equations for the amplitudes f_n which may be solved sequentially in terms of the (unknown) energy eigenvalue E and of the values of the coupling constants defining the potential. For the case $v_0 = 0$ the first equation is simply $f_0 = E$.

The next step is the representation of the Taylor expansion for $f(x)/x$ by means of a rational function or Padé approximant

$$[M/N](x^2) = \sum_{j=0}^{M+N} f_j x^{2j} + \mathrm{O}(x^{2(M+N)+2}) \tag{8}$$

where $[M/N](x^2)$ is the quotient of a polynomial of degree M and a polynomial of degree N, both in x^2.

The coefficients f_j as well as the coefficients which determine the Padé approximant depend on the energy E which is so far undetermined. The main assumption of the RPM is that one obtains a good approximation to the energy if the left-hand side of (8) also yields the coefficient f_{M+N+1} exactly. This requirement leads to a quantization condition of the form [1–3]

$$H_D^d(E) = 0 \qquad D = 2, 3, \ldots \qquad d = 0, 1, \ldots \tag{9}$$

where $H_D^d(E)$ is the determinant of the matrix with elements $f_{i+j+d-1}$, $i, j = 1, 2, \ldots, D$. The dimension D of the determinant and the displacement d which appears in the definition of the matrix are related to M and N by $M = D + d - 1$ and $N = D - 1$.

For a given value of d the roots of H_D^d form sequences that converge rapidly to the actual eigenvalues as D increases. It has been proved that the roots of $H_D^0(E)$ and $H_D^1(E)$ are, respectively, the lower and upper bounds that tightly bracket the eigenvalues of the Schrödinger equation with $V(x) = w^2 x^2 + \lambda x^4$ [3]. For other anharmonic oscillators the situation is more complicated [3]. The RPM applies to the ground as well as to the excited states but the accuracy of the approximate eigenvalues decreases with the quantum number [2, 3]. A fascinating and altogether puzzling feature of the RPM is the occurrence of an increasing number of roots in the neighbourhood of the actual eigenvalue. In order to select a convergent sequence of roots one simply looks for a zero of $H_{D+1}^d(E)$ in the neighbourhood of the chosen zero of $H_D^d(E)$. The determinants of low order have few widely separated roots and therefore the physical ones can easily be recognized [1–3].

3. Weak-coupling expansion for the anharmonic oscillators

For concreteness we concentrate on the anharmonic oscillators

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \lambda x^{2K} \tag{10}$$

where $\lambda > 0$.

Any eigenvalue $E(\lambda)$ of this Hermitian operator can be formally expanded in a Taylor series about $\lambda = 0$ leading to what is called the weak-coupling expansion

$$E(\lambda) = \sum_{j=0}^{\infty} E_j \lambda^j \tag{11}$$

where E_0 is one of the harmonic oscillator eigenvalues, $E_0 = 2n + 1$, $n = 0, 1, \ldots$. The series in the right-hand side of (11) is divergent and the equality means that it is asymptotic to $E(\lambda)$ [8].

The calculation of the coefficients E_j of the weak-coupling expansion by means of the RPM is straightforward: one simply expands $H_D^d(E)$ in a Taylor series about $\lambda = 0$ and collects the coefficients. Their roots give the perturbation corrections E_j hierarchically for $j = 0, 1, 2, \ldots$. Here we have used the computer-algebra language REDUCE to obtain an analytic expression for $H_D^d(E, \lambda)$.

As examples we show the determinants corresponding to $D = 2$

$$H_2^0(E, \lambda) = \frac{1}{4725} \left[(E^2 - 1)^2 (E^2 - 25) + 162 E(E^2 - 1)\lambda - 189\lambda^2 \right] \quad (12)$$

and to $D = 3$

$$\begin{aligned}
H_3^0(E, \lambda) = \frac{1}{46414974375} [&(E^2 - 1)^3 (E^2 - 25)^2 (E^2 - 81) \\
&+ 6E(E^2 - 1)^2 (E^2 - 25)(143E^2 - 779)\lambda \\
&- 9(E^2 - 1)(403181E^4 - 460846E^2 - 8575)\lambda^2 \\
&+ 4374E(2281E^2 - 2401)\lambda^3 - 6751269\lambda^4]
\end{aligned} \quad (13)$$

corresponding to the quartic oscillator ($K = 2$ in (10)) and for a displacement $d = 0$.

The roots of $H_D^d(E, 0)$ yield E_0 for the lowest-lying states. In equations (12) and (13) we see that $E_0 = 1$ is a double root ($D = 2$) or a triple root ($D = 3$). Analogously $E_0 = 5$ is a simple root ($D = 2$) or a double root ($D = 3$), and so on. This pattern of occurrence of the unperturbed solutions is general and for a given dimension D of the determinant the ground state appears D times, the first even parity excited state is present $D - 1$ times, and so on. The scheme is obviously independent of the parameter K of the anharmonic perturbation, because we are dealing with the zero-order term ($\lambda = 0$).

To obtain the perturbative corrections one first substitutes $E_0 + \lambda E_1$ for E in the determinant H_D^d and obtains E_1 from the roots of the resulting equation for $\lambda = 0$. Then one proceeds exactly in the same way substituting $E_j + \lambda E_{j+1}$ for E_j in the function of E_j and λ derived in the previous step. The process is equivalent to calculating the weak-coupling series as $E_0 + \lambda(E_1 + \lambda(E_2 + \lambda(E_3 + \cdots)))$ and saves much memory which is one of the weak points of the algebraic manipulation of analytic expressions by means of computer algebra.

In table 1 we show the resulting weak-coupling expansions corresponding to all the roots of the Hankel determinants of dimension 2, 3 and 4, of the quartic anharmonic oscillator obtained with $d = 0$ by means of the method previously described. We have included the coefficients of the expansion up to, and including, the first appearance of an incorrect coefficient. Note that, in addition to the quoted solutions, there also exist other unphysical roots of negative energy. If the pair (E, λ) is a solution of the determinantal equation $H_D^d(E, \lambda) = 0$, the pair $(-E, (-1)^{K+1}\lambda)$ is also a solution of the same equation. This is a consequence of the transformation of the Hamiltonian under the change $x \to ix$.

Table 1 shows that the multiplicity of a given root E_j decreases with j and increases with D. This fact clearly indicates that one should expect many roots with different degrees of accuracy in the neighbourhood of a given eigenvalue. These roots become more closely packed as D increases and/or λ decreases. Comparing the results in table 1 with independent calculations of the perturbation corrections leads to the conclusion that repeated coefficients are always exact. For a sufficiently large order j only two single roots E_j are obtained, one of which may be exact, but there does not seem to be a way of selecting it. The number of

Table 1. Weak-coupling expansion for the quartic anharmonic oscillator, for displacement $d = 0$ and for several values of the dimension D of the Hankel determinant.

E_0	E_1	E_2	E_3	E_4	E_5	E_6	E_8
$D = 2$							
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{1227}{256}$				
1	$\frac{21}{8}$						
5	$-\frac{27}{8}$						
$D = 3$							
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{333}{64}$	$-\frac{30885}{1024}$	$\frac{3656529}{16384}$		
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{3609}{512}$				
1	$-\frac{81}{32}$						
5	$\frac{39}{4}$	$-\frac{615}{16}$	$\frac{150237}{512}$				
5	$\frac{1101}{16}$						
9	$-\frac{2481}{32}$						
$D = 4$							
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{333}{64}$	$-\frac{30885}{1024}$	$\frac{916731}{4096}$	$-\frac{65518401}{32768}$	$\frac{21784330359}{1048576}$
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{333}{64}$	$-\frac{30885}{1024}$	$\frac{7468983}{32768}$		
1	$\frac{3}{4}$	$-\frac{21}{16}$	$\frac{261}{2048}$				
1	$\frac{363}{64}$						
5	$\frac{39}{4}$	$-\frac{615}{16}$	$\frac{20079}{64}$	$-\frac{3576255}{1024}$	$\frac{1533961719}{32768}$		
5	$\frac{39}{4}$	$-\frac{615}{16}$	$\frac{37131979500}{1024}$				
5	$-\frac{9771}{64}$						
9	$\frac{123}{4}$	$-\frac{3249}{16}$	$\frac{4801221}{2048}$				
9	$\frac{47013}{64}$						
13	$-\frac{40965}{64}$						

coefficients of the weak-coupling expansion correctly obtained depends on the dimension of the Hankel determinant D, the value of the displacement and the unperturbed level considered. In the case of the quartic oscillator, and for $d = 0$, the leading power of λ of a given determinant is $2D - 2$, and this is at most the highest coefficient of the weak-coupling expansion for the ground state to be obtained correctly. This fact may be checked by looking at table 1, and comparing the expansion of the ground state with the weak-coupling expansion obtained by standard perturbation theory methods.

This application of the RPM may be regarded as an improvement of the standard logarithmic perturbation theory [9] for separable problems in the sense that our method

enables one to treat the ground and excited states simultaneously. The reason for this is that a Padé approximant explicitly accounts for the nodes of the excited states. On the other hand, in the standard logarithmic perturbation theory, one introduces the nodes of the excited states explicitly into the eigenfunction and then expands them in a Taylor series about $\lambda = 0$. The application of the RPM just outlined is particularly useful for the treatment of the ground state for which it yields more perturbation corrections exactly. To generate a scheme that favours an excited state with quantum number $n > 0$ one simply chooses $g(x)$ in (2) equal to the Hermite polynomial $H_n(x)$.

The RPM is not only capable of generating many terms of the perturbative expansion. It also provides an implicit equation for the energy for all values of the coupling constant, like those shown in equations (12) and (13). Actually, the expansions quoted in table 1 are not convergent for all values of λ, because of the presence of branch points in the function $E = E(\lambda)$ defined by the equation $H_D^d(E, \lambda) = 0$. The accurate determination of the branch points is difficult, due to the high powers of E in in the Hankel determinants, but they clearly appear in a *map of roots* for a given dimension D. Figure 1 shows the map of roots corresponding to the quartic anharmonic oscillator for $D = 2$, $D = 3$ and $D = 4$. The criterion by which to construct these figures is rather complex and requires some explanation. The figure shows dots for many pairs (E, λ) with $|\lambda| < 1$, which solve the corresponding Hankel determinant. For $|\lambda| > 1$ we instead plot $(E/|\lambda^{1/3}|, 1/\lambda)$, so as to fit the region of large values of E and λ into a reasonable scale. This procedure gives rise to an artificial discontinuity at $|\lambda| = 1$. The collection of individual pairs (E, λ) finally draws some lines which represent the evolution of a given solution for varying values of λ. Every figure has a centre of symmetry showing the occurrence of the pairs (E, λ) and $(-E, -\lambda)$. The region of physical interest is the upper right corner, corresponding to positive values of the energy and coupling constant. It is very helpful to analyse this figure concurrently with the weak-coupling expansions of table 1. For example, in the case $D = 2$, stemming from the point $(E = 1, \lambda = 0)$, there are two branches, one with the correct slope $E_1 = 3/4$ and the other with the incorrect value of $E_1 = 21/8$. The good branch is smooth up to $\lambda = \infty$, which means that even at the lowest order we obtain a root with the proper asymptotic behaviour $\lambda^{1/3}$ (the coefficients of the strong-coupling expansions will be analysed in the next section). The other branch goes upwards and finally connects with the other unperturbed solution $(E = 5, \lambda = 0)$. Going to negative values of λ from the point $(E = 1, \lambda = 0)$ there appears a loop (almost impossible to distinguish in the figure) its tip being another branch point. The condition $d\lambda/dE = 0$ determines all the square-root-type branch points of $E(\lambda)$.

Once this simple case has been understood, one may try to analyse the vicinity of $(E = 1, \lambda = 0)$ for $D = 4$ in figure 1. There are four roots at this point. One of the roots goes upwards passing through the point $(E = 5, \lambda = 0)$. The weak-coupling expansion for this root is displayed in the fourth line of the $D = 4$ block in table 1. The other three roots go together with increasing values of λ, but one of them starts to separate at about $\lambda = 1$. This corresponds to the third line of the referred block of table 1. Finally, the other two remaining roots go up to $\lambda = \infty$ almost indistiguishably from one another, their relative difference being less than one part in ten thousand. These two roots correspond to the expansions quoted in the first two lines of the block $D = 4$ in table 1.

Similar comments may be put forward for the branches emerging from other physical solutions, like those corresponding the first even-parity excited state related to the unperturbed solution $(E = 5, \lambda = 0)$. For $D = 3$ there is a single branch with the correct behaviour for large values of λ. For $D = 4$ there are two branches clearly separated in the figure.
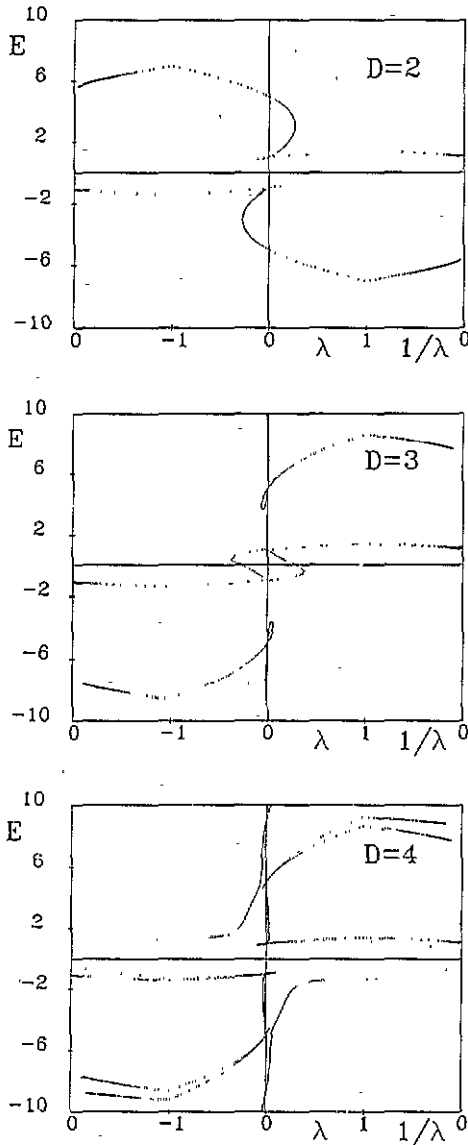
Figure 1. The map of roots corresponding to the quartic anharmonic oscillator $x^2 + \lambda x^4$ for displacement $d = 0$ and for dimension of the Hankel determinant $D = 2, 3$ and 4.

4. Strong-coupling expansion for the anharmonic oscillators

In addition to the weak-coupling series just discussed the eigenvalues of the anharmonic oscillator (10) satisfy a strong-coupling expansion of the form [8]

$$E(\lambda) = \lambda^{1/(K+1)} \sum_{j=0}^{\infty} e_j \lambda^{-2/(K+1)}. \tag{14}$$

The accurate calculation of the coefficients e_j is much more difficult because the exact eigenfunctions and eigenvalues of the operator $-\mathrm{d}^2/\mathrm{d}x^2 + x^{2K}$ are unknown. However, the strong-coupling expansion for some anharmonic oscillators has been calculated by means of a matrix method based on the use of the basis set of eigenfunctions of the harmonic oscillator [5] and more accurately through a properly renormalized perturbation series [6]. The RPM

proves to be useful for the calculation of highly accurate coefficients of the strong-coupling expansion for the anharmonic oscillators and other problems [4].

The accuracy of the strong-coupling coefficients e_j determined by any of those methods decreases rapidly with K. For this reason we deem it necessary to compare the coefficients e_j for the ground state of the anharmonic oscillators with $K = 3, 4$ and 5 previously obtained [6] with an accurate calculation by means of the RPM. For the coefficient e_0 of the quartic oscillator one may also consider the most accurate value determined up to now [10] by using a special method of diagonalization with extended precision—up to 200 digits. The procedure is similar to that for the weak-coupling expansion except that in this case one considers the potential $x^{2K} + \xi x^2$ and then directly substitutes the strong-coupling series for E into the Hankel–Hadamard determinants. From the resulting expansion in power series of the parameter $\xi = \lambda^{-2/(K+1)}$ one easily obtains the coefficients e_j. The details of the calculation have been given elsewhere [4]; here we only present results and indicate any difference with respect to that previous application.

Table 2. Strong-coupling coefficients for the ground state of the anharmonic oscillators with $V(x) = x^2 + \lambda x^{2K}$

	$K = 2$	$K = 3$	$K = 4$	$K = 5$
e_0	1.060 362 090 484 183	1.1448 024 537 970 7	1.225 820 113 82	1.298 843 702
$10^{-1}e_1$	3.620 226 487 886 77	3.079 203 037 329 6	2.771 189 343 36	2.566 473 842
$10^{-2}e_2$	$-$3.451 026 272 321	$-$1.854 166 431 932 19	$-$1.263 228 426 95	$-$0.966 539 384
$10^{-3}e_3$	5.195 302 710 91	1.559 742 195 768	0.750 441 570 6	0.454 884 85
$10^{-4}e_4$	8.308 344 463 08	$-$1.239 011 743 119	$-$0.385 978 159 7	$-$0.174 023 06

The accuracy of the computed coefficients decreases with K merely because the convergence of the method with increasing D becomes slower. One of the reasons for this is that the coefficients of f_n with $n < K$ do not carry information about x^{2K}. Therefore, if we use the same value of the displacement d for all the oscillators the amount of that information in a Hankel–Hadamard determinant of a given order decreases with K. It seems preferable to change d accordingly. One can easily study the effect of this parameter on the velocity of convergence. The choices $d = K - 1$ or $d = K - 2$ yield sufficiently accurate results as shown in table 2; they confirm and considerably improve (particularly for $K = 5$) those obtained by means of the renormalized series [6]. The calculation was carried out by means of REDUCE in *floating* or *rounded* mode with a precision of 100 digits and the accuracy of the coefficients was estimated by comparing the roots of the Hankel–Hadamard determinants with $D = 10$ and $D = 11$, and with $d = K - 1$ and $d = K - 2$. We may state loosely that for an increase of one in the dimension of the Hankel determinant we obtain two more exact digits for the expansion coefficients. To obtain a precision similar to that reported in [10] we should use matrices of very large dimension which would be very costly to evaluate in terms of computer time. Note, however, that the RPM also produces the coefficients of the expansion in fractional powers of the coupling constant, and not just the leading term as in [10]

5. Eigenfunctions

Previous investigations of the RPM have proved that it produces remarkably accurate eigenvalues [1–4]. However, nothing has been said about the eigenfunctions except that the RPM yields exact solutions for solvable or quasi-solvable problems [1, 3, 7]. According to

(2) the approximate eigenfunctions are of the form

$$\Psi(x) = g(x)\exp\left[-\int^x f(t)\,dt\right]. \tag{15}$$

To facilitate the discussion we restrict ourselves to the ground state ($g(x) = 1$) of the anharmonic oscillators with potential-energy function $V(x) = x^{2K}$. The asymptotic behaviour of the solution of the Riccati equation $f = x^K$ can be exactly reproduced by the Padé approximant provided that K is odd and $d = (K-1)/2$.

To obtain the wavefunction one has to construct the Padé approximant (8) from the expansion of $f(x)$ and for the desired eigenvalue. Then the approximant is introduced in (15) and the integration is carried out. To this end the change of variable $y = x^2$ considerably simplifies the algebraic procedure.

The calculation of the expectation value of the Hamiltonian is a good test of the *global* quality of the obtained wavefunctions. By numerical integration we have found that $\langle H \rangle$ is a better approximation to the energy than the root of the corresponding Hankel–Hadamard determinant. Furthermore, as D increases the eigenfunction satisfies the virial theorem $-\langle d^2/dx^2 \rangle = K\langle r^{2K} \rangle$ with increasing accuracy. Both tests show that the RPM gives good global approximations to the eigenfunctions. A much more demanding test is the calculation of $H\Psi/\Psi$ which reveals the local accuracy of the RPM eigenfunction. For $V(x) = x^{2K}$ we simply have

$$\frac{H\Psi}{\Psi} = f' - f^2 + x^{2K}. \tag{16}$$

Again, when using this equation, one has to substitute the Padé form for $f(x)$.

Figure 2 shows this quantity for various values of K and for various values of the dimension of the Hankel–Hadamard determinant used to compute the approximate eigenvalue. As shown in figure 2, this quantity is almost constant for $K = 2, 3, 4$ and 5 in a wide interval of values of x. Closer inspection of the values of Ψ reveals that the quantity defined in (16) deviates appreciably from E only when Ψ is vanishingly small. This fact proves that the RPM eigenfunctions are suitable for the calculation of accurate expectation values or matrix elements as indicated above. To give a more precise idea of the *flatness* of (16) we mention that $H\Psi(x)/\Psi(x)$ deviates from $H\Psi(0)/\Psi(0)$ by as much as one part in 10^7 at $x = 2$ and one part in 10^5 at $x = 3$, for $D = 6$. It also follows from figure 2 that the interval in which $H\Psi/\Psi$ is relatively constant decreases as K increases. This deterioration of the eigenfunction is partly counterbalanced, with respect to the calculation of expectation values, by the fact that its asymptotic behaviour $\exp[-|x|^{K+1}/(K+1)]$ makes Ψ vanish faster as K increases.

The form of the eigenfunction depends mainly on the roots of the denominator of the Padé approximant. For example, in the case $K = 2$ the singular points of the approximants with $d = 0$ are simple poles on the imaginary axis and as a result the eigenfunctions are of the form

$$\Psi_{K=2}(x) = \prod_{j=1}^{D-1}(1 + p_j x^2)^{q_j}\exp(-cx^2) \tag{17}$$

where c, p_j and q_j are positive. Notice that the RPM eigenfunctions do not have the proper exponential dependence for large values of x for $K = 2$, as argued above. For $K = 3$ and $K = 5$ the RPM eigenfunctions have the appropriate exponential behaviour provided that the displacement is $d = (K-1)/2$. In these cases the poles of the Padé approximants may be complex and they give rise to terms of the form $\tan^{-1}(p_j x^2 + q_j)$ in the exponential part of the eigenfunction. These unexpected terms are bounded and therefore have no effect on the
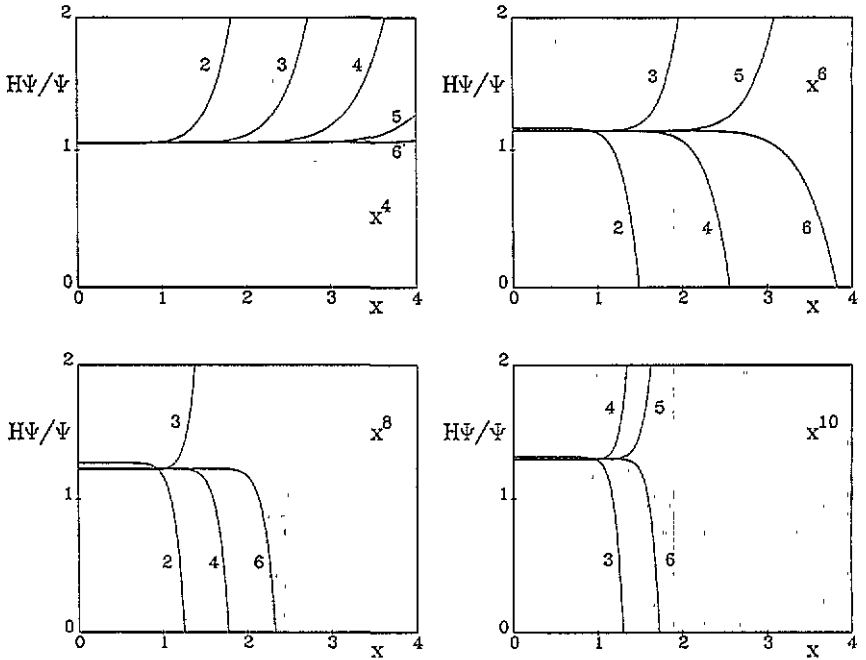
Figure 2. The value of $H\Psi(x)/\Psi(x)$ computed in the RPM for the potentials x^{2K}, $K = 2, 3, 4$ and 5, corresponding to various values of the dimension D of the Hankel determinant.

exponential behaviour at large values of x. However, they are partly responsible for the high accuracy of the eigenfunction for small and moderate values of the coordinate. Samples of RPM eigenfunctions are shown in table 3. For large values of x the Padé approximant to $f(x)$ behaves asymptotically as $a_{N+d}x^{2d+1}/b_N$. Therefore for K odd and $d = (K - 1)/2$ this approximant will give the exact asymptotic behaviour of the eigenfunction provided that a_{D+d-1}/b_{D-1} is close to unity. In table 4 we show this ratio for $K = 2$ and $K = 5$ and for several values of the order of the determinant D. As expected the RPM gives the asymptotic behaviour more closely for $K = 3$ than for $K = 5$.

Table 3. Unnormalized low-order RPM eigenfunctions for some anharmonic oscillators.

$V(x) = x^4$	$d = 0$	
$D = 2$		$\Psi = (x^2 + 8.07)^{11.98} \exp(-2.01x^2)$
$D = 3$		$\Psi = (x^2 + 28.42)^{90.61} (x^2 + 4.53)^{1.54} \exp(-4.06x^2)$
$V(x) = x^6$	$d = 1$	
$D = 2$		$\Psi = (x^2 + 4.71)^{-21.81} \exp(-0.36x^4 + 1.74x^2)$
$D = 3$		$\Psi = (x^4 + 5.68x^2 + 13.13)^{1.46}$
		$\times \exp[-0.23x^4 - 0.54x^2 - 3.87 \tan^{-1}(0.44x^2 + 1.26)]$
$V(x) = x^{10}$	$d = 2$	
$D = 3$		$\Psi = (x^4 + 3.16x^2 + 9.55)^{-9.73}$
		$\times \exp[-0.27x^6 + 0.52x^4 + 1.50x^2 + 3.81 \tan^{-1}(0.38x^2 + 0.59)]$

Table 4. Ratio a_{D+d-1}/b_{D-1} for $d = (K-1)/2$ when $K = 3$ and $K = 5$ in terms of D.

D	K = 2	K = 5
2	1.43	
3	0.91	1.63
4	1.03	−0.75
5	0.99	0.94
6	1.002	1.24
7	0.9995	0.94
8	1.0001	0.94
9	0.999 97	1.02

6. Further comments and conclusion

Throughout this paper we have confirmed that the RPM is suitable for the calculation of accurate eigenvalues of the Schrödinger equation for separable problems. The method proves to converge sufficiently fast to provide the strong-coupling expansion which is extremely difficult to obtain by other approaches. The RPM also provides a convenient implementation of the logarithmic perturbation theory to treat excited states.

One of the most important points of this paper is the study of the eigenfunctions. In general the RPM eigenfunctions are extremely accurate for small and moderate values of the coordinates which have the greatest effect on the calculation of quantum-mechanical properties. Because of their complicated form these eigenfunctions have to be used in numerical integration algorithms and in many cases they can be easily improved by the addition of a scaling parameter adjusted according to the variational theorem. For instance, the change of variables $x \to \alpha x$ leads to $-\langle d^2/dx^2 \rangle(\alpha) = -\alpha^{-2}\langle d^2/dx^2 \rangle(1)$ and $\langle x^{2K} \rangle(\alpha) = \alpha^{2K} \langle x^{2K} \rangle(1)$, so that one may obtain the parameter α and an improved ansatz from the variational theorem without any extra calculation.

A bizarre characteristic of the RPM is the *clustering* of solutions, i.e., the existence of several close roots of the Hankel determinant for a given value of the coupling constant λ. Clustering is a signal of being close to a physical root, but a decision has to be made as to which of these roots is the best one. In some specific cases, and for some specific levels, the RPM provides upper and lower bounds to the eigenvalues [1–3], but we have not found a general way of establishing this property. The best way of selecting the physical root requires the analysis of the corresponding wavefunction, constructed in the way described in section 5, by counting the number of nodes and/or checking the asymptotic behaviour. The procedure is costly but sure. In practice, however, it is simpler to follow a sequential method; for a given level and coupling constant, one determines the approximate eigenvalue by using the Hankel determinant of smaller dimension D. This root is used as input for a Newton–Raphson algorithm when solving the next determinant, of dimension $D + 1$, and so on.

For simplicity and concreteness we have restricted ourselves to anharmonic oscillators with polynomial potentials but we deem it worth mentioning that the RPM applies to other problems as well. For instance, the treatment of many spherically-symmetric potentials is straightforward [2, 4, 7].

Acknowledgments

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