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Investigating a Hybrid Perturbation-Galerkin Technique using Computer Algebra

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A two-step hybrid perturbation-Galerkin method is investigated using computer algebra. The technique is applicable to a variety of differential equation type problems which involve a scalar parameter. An approximate solution is sought in the form of a sum where each term consists of the product of two functions. The first is a function of the independent field variable(s) x, and the second is a function of the parameter λ. In step one the functions of x are determined by forming a perturbation expansion in λ. In step two the functions of λ are determined through the use of the classical Bubnov-Galerkin method. This hybrid technique has the potential of overcoming some of the drawbacks of the perturbation and Bubnov-Galerkin methods applied separately, while combining some of the good features of each. In order to help investigate some of the properties of the approximate solutions generated by the hybrid technique, the technique is applied with the aid of computer algebra to a simple two-point boundary-value problem where the radius of convergence is finite and to a quantum eigenvalue problem where the radius of convergence is zero. For both problems the hybrid solutions are useful well beyond the radius of convergence associated with the perturbation expansion. Furthermore, for the first problem we demonstrate convergence for all values of the parameter. The role of computer algebra in applying and studying the hybrid technique is discussed.

1. Introduction

Perturbation solutions to differential equations type problems have been useful in a wide variety of applications and it has long been realized how useful computer algebra can be in forming perturbation expansions. Typically, however, the algebra becomes more and more tedious as higher and higher order terms are computed, and frequently the computational effort rises so fast from term to term that even with computational assistance very few terms can be computed. Such luxuries as determining the radius of convergence of the expansion are rarely allowed, let alone situations where the expansion parameter can be modified to increase in effect the radius of convergence (Andersen & Geer, 1982). Thus for cases where higher order terms may have a significant effect it is important to make as much use as possible of the information contained in the lower order terms. The hybrid perturbation-Galerkin method studied herein seems to greatly extend the power and usefulness of the perturbation method without adding significantly to the computational effort.

The hybrid technique was apparently first studied by Ahmed K. Noor and collaborators. Their series of papers (Noor, Andersen & Peters, 1980; 1981; 1979; 1984) combine the

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perturbation method, the Galerkin method (Galerkin, 1915), and the finite element method (or other discretization techniques) to attack a variety of structural mechanics problems. Their "reduced-basis method" allows some non-linear problems requiring thousands of degrees of freedom after discretization to be computed using non-linear systems of equations with only four to ten unknowns. Noor and collaborators have also applied the same general principles *sans* discretization to some thermal and structures problems (Noor, 1985; Noor & Balch, 1984; Noor, Balch & Shibut, 1984). We refer to the technique as the hybrid perturbation-Galerkin technique because without discretization we do not think in terms of having a large basis to reduce.

We believe the hybrid technique can be adapted to a wide variety of problem areas. Previous work by the present authors demonstrates applications to slender-body problems for potential flow and for electrostatic potential (Geer & Andersen, 1989*a*), to a slider bearing problem (Geer & Andersen, 1989*b*), to a natural frequency calculation (Geer & Andersen, 1990), and to classes of linear second-order two-point boundary-value problems exhibiting boundary layer phenomena (Geer & Andersen, 1990). It has also been reported by the authors that for problems which are amenable to perturbation expansions about two or more values of a parameter, the perturbation functions developed in these expansions may be combined in one Galerkin step to yield an approximate solution useful over an extended range of the parameter (Geer & Andersen, 1989*b*; 1990). An earlier version of this work was published in (Andersen & Geer, 1988).

Computer algebra can play an important role in applying the hybrid technique, a primary use being in carrying out the perturbation analysis which leads to the trial functions needed in the later Galerkin step. In fact, it seems likely to the authors that many of the perturbation solutions currently being generated by computer algebra can be markedly improved by application of the hybrid method. Even in the case of discretized problems, computer algebra has played a significant role in generating the required numerical programs (Noor & Andersen, 1981).

Despite the achievement of very good results by Noor and his coauthors and by the present authors, and despite the applications being drawn from a diverse set of problems, more effort is needed: to establish the general properties of the technique; to determine the range of problems for which the technique, as presently formulated, can be beneficial; and to find modifications of the technique which will allow the technique to be applied successfully to an even wider range of problems. This leads us to a second use of computer algebra, which is for the analysis of convergence properties of the technique. While the number of problems which are simple enough to be amenable to such analysis may be small, it is hoped that this type of analysis will shed light on the rates of convergence and the regions of convergence that can be expected for problems not amenable to such thorough analysis.

The purpose of this paper is two-fold, (i) to describe some aspects of the hybrid technique to a readership which appreciates the power and capability (and limitations) of computer algebra, and more importantly (ii) to explore how computer algebra may be used to investigate the form and the convergence properties of solutions generated by the technique.

In section 2 we give a brief description of the method. In section 3 we analyse a simple two-point boundary-value problem whose exact solution is known. We demonstrate that the hybrid solutions converge for all values of the perturbation parameter even though the perturbation radius of convergence is finite. Section 4 gives a treatment of a well-known quantum-mechanical one-dimensional anharmonic oscillator problem. For this problem

the perturbation radius of convergence is known to be zero, but the hybrid solutions seem to converge for all values of the perturbation parameter. We end with a discussion and some concluding remarks in section 5.

2. Description of the Method

The method used in this study is a two-step hybrid analysis technique which is based upon perturbation expansions and the Galerkin method. We suppose that we have a differential equation with independent variable x which involves a scalar parameter λ and that we desire the solution to this equation for a particular value or range of values of λ.

In the first step a perturbation solution is developed with λ as the expansion parameter. The perturbation solution takes the form of a sum of terms, where each term consists of a perturbation function (a function of x) times a gauge function (a pre-assigned function of λ). The expansion may be singular or regular. For a regular expansion the set of gauge functions consists simply of $\{1, \lambda, \lambda^2, \lambda^3, \dots\}$. The drawbacks of the perturbation method are that (i) frequently the radius of convergence in λ is finite, (ii) even within the radius of convergence the rate of convergence may be slow and a large number of terms may be required to gain the desired accuracy, and (iii) considerable computational effort may be expended computing higher order terms.

In the second step we retain the perturbation functions but replace the gauge functions by new amplitudes which depend on λ, which we will determine by a Galerkin technique. In the Galerkin technique one seeks an approximate solution in the form of a linear combination of specified (known) trial functions (functions of x) with unknown coefficients (or amplitudes) which are functions of λ. This techniques can work very well if a good set of trial functions is chosen. However, if a large set of trial functions is used, the computational effort can be unduly large since the matrices involved tend to be full rather than sparse (as in the finite element or finite difference methods). The essence of the hybrid approach is that the trial functions for the Galerkin step are chosen to be the perturbation functions computed in the first step. This provides a basis which clearly is relevant for small values of λ. We demonstrate that the hybrid solutions can be dramatically better than the perturbation solutions and that a set of perturbation functions can be useful as trial functions far outside the radius of convergence for the perturbation calculation in which they originate. In the absence of contrary indications, it seems reasonable to use the same set of functions as both trial and test functions. This is what is meant by the Bubnov-Galerkin designation.

3. A Simple Example

To illustrate the method and show some convergence properties we consider first the following simple two-point boundary value problem. The differential equation

$$\ddot{U} - \lambda \dot{U} + \lambda = 0, \tag{3.1}$$

is to hold for x in the range $[-1, 1]$ with boundary conditions

$$U(-1) = U(1) = 0. \tag{3.2}$$

The exact solution to this problem, which is

$$U = 1 + x - \frac{2(1 - e^{\lambda(x+1)})}{1 - e^{2\lambda}} \tag{3.3a}$$

$$= \frac{\cosh(\lambda) - \cosh(\lambda x) + x \sinh(\lambda) - \sinh(\lambda x)}{\sinh(\lambda)}, \tag{3.3b}$$

exhibits boundary-layer behaviour near $x = 1$ for large positive values of λ and near $x = -1$ for large negative values of λ. The centre portion of the function approximates a straight line with slope equal to one in the limit of large absolute value of λ. Exact solutions for a number of values of λ are shown in Figure 1. A generalization of this problem has been studied by Ferguson (1986).

We look for an approximate solution of the form

$$\tilde{U} = \sum_{j=1}^{n} u_j(x) \delta_{j,n}(\lambda), \tag{3.4}$$

where in the first step the u_j are computed from a (regular) perturbation expansion about $\lambda = 0$ and in the second step the $\delta_{j,n}$ will be computed using the Bubnov-Galerkin method.

STEP 1.

In step 1 the solution to (3.1) together with (3.2) is written in the form

$$U = \sum_{j=1}^{n} u_j(x) \lambda^j + O(\lambda^{n+1}). \tag{3.5}$$

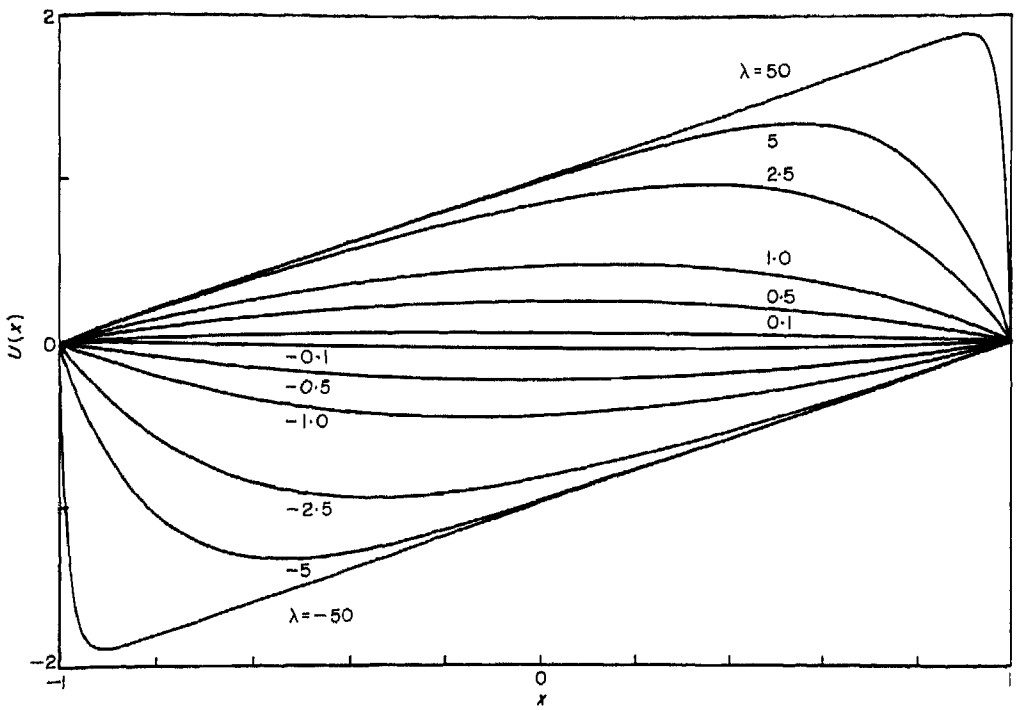

Figure 1. Solutions of the simple two-point boundary value problem for several values of the parameter λ.

This is substituted into (3.1), the differentiation is distributed onto the various terms, the left hand side is expressed in the form of a power series in λ, and the coefficient of each power of λ is set to zero. The immediate result is a set of second order differential equations independent of the parameter λ. These equations, plus the imposition of the boundary conditions on each u_j, serve to determine the u_j. Each u_j is a polynomial in x of degree $j+1$, and thus they collectively span an n-dimensional space. The first few terms are

$$\begin{aligned} u_1 &= (1-x^2)/2, \\ u_2 &= x(1-x^2)/6, \\ u_3 &= (1-x^2)(-1+x^2)/24, \\ u_4 &= x(1-x^2)(-7+3x^2)/360, \\ u_5 &= (1-x^2)(3-4x^2+x^4)/720, \\ u_6 &= x(1-x^2)(31-18x^2+3x^4)/15120. \end{aligned} \tag{3.6}$$

It is traditional to stop the calculation at this point. If the computation has been done for sufficiently large values of n, an analysis using the ratio or root test will show that the radius of convergence of the perturbation series is π. This may have been anticipated from the exact solution since the denominator is zero for $\lambda = m\pi i$ for non-zero integer values of m. Convergence of the perturbation solution is limited to λ in the range $(-\pi, \pi)$, even though the singularity occurs on the imaginary λ axis. The error of the perturbation solution may be measured by the L_2 norm of the difference of the perturbation solution for fixed n and the exact solution (3.3) divided by the L_2 norm of the exact solution. In Figure 2 the logarithm of this perturbation solution relative error is plotted vs. $\log(\lambda)$ for several different even values of n. As to be expected, the higher the value of n the more abruptly the error norm rises as the radius of convergence is reached.

The quantities in (3.6) may also be obtained by expanding (3.3) in a Taylor series in λ about $\lambda = 0$. By forming separate Taylor series expansions for the numerator and denominator in (3.3b) and by using (3.5) it can be shown that

$$\sum_{i=0}^{n-1} \frac{u_{2n-2i-1}(x)}{(2i+1)!} = \frac{1-x^{2n}}{(2n)!} \tag{3.7}$$

and

$$\sum_{i=0}^{n-1} \frac{u_{2n-2i}(x)}{(2i+1)!} = \frac{x(1-x^{2n})}{(2n+1)!}. \tag{3.8}$$

These formulae can serve as recursion relations for evaluating the $u_j(x)$ and will also be useful in the discussion of step 2.

STEP 2.

In step two, the u_j for $j = 1, 2, \ldots, n$ serve as trial (or interpolation) functions for the Bubnov-Galerkin method. The approximation (3.4) with the u_j known and the $\delta_{j,n}$ unknown is substituted into the left-hand side of (3.1). We would like, of course, for this quantity, the residual, to be zero for all values of x in the range $[-1, 1]$. Since this is impossible, we settle for n conditions which serve to force the residual to be small. There are many different criteria which can serve this purpose, but we choose the Bubnov-Galerkin criterion, which states that the residual is orthogonal to each of the trial functions,

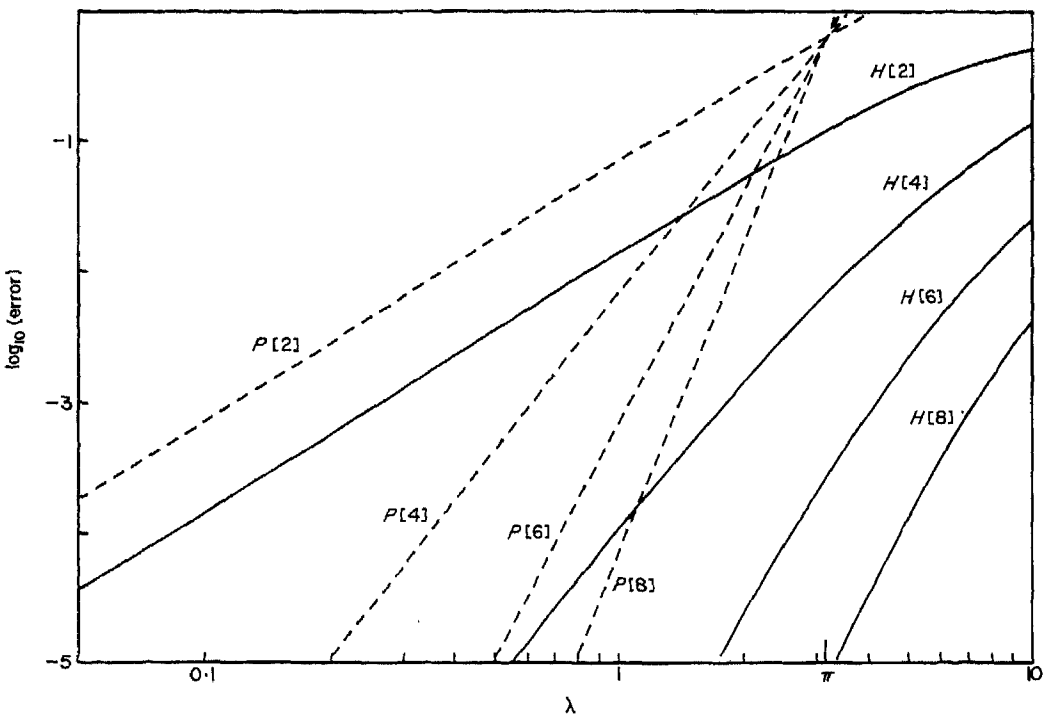

Figure 2. Comparison of errors for perturbation and hybrid solutions showing the dependence on the number of terms n and the parameter λ. The perturbation solutions are labelled $P[n]$ and the hybrid solutions $H[n]$, where n is the number of terms used in the expansion. The radius of convergence of the perturbation expansion equals π.

i.e. to the set of perturbation functions $u_j(x)$ in the case of the hybrid technique. The result is a linear system of n equations

$$\sum_{j=1}^{n} a_{i,j}(\lambda)\delta_{j,n} = b_i(\lambda) \qquad (i = 1, 2, \ldots, n), \tag{3.9}$$

where

$$\begin{aligned} a_{i,j}(\lambda) &= \int_{-1}^{1} u_i(x)[\ddot{u}_j(x) - \lambda u_j(x)]\, dx, \\ b_i &= -\lambda \int_{-1}^{1} u_i(x)\, dx. \end{aligned} \tag{3.10}$$

For example, for $n = 2$, the $\delta_{i,n}$ are given by

$$\delta_{1,2} = \frac{15\lambda}{15+\lambda^2}, \qquad \delta_{2,2} = \frac{15\lambda^2}{15+\lambda^2}. \tag{3.11}$$

The use of computer algebra allowed us to determine that $\delta_{i,n}$ for $i = 1$ through n and for any value of n has the form

$$\delta_{i,n} = \frac{\sum_{j=0}^{\lfloor (n-i)/2 \rfloor} \beta_{j,n}\lambda^{2j+i}}{\Delta_n}, \tag{3.12}$$

where

$$\Delta_n = \sum_{i=0}^{\lfloor n/2 \rfloor} \beta_{i,n}\lambda^{2i}, \qquad \beta_{i,n} = \frac{(2n-2i+1)!!}{(2n+1)!!(2i+1)!!i!} \prod_{j=1}^{i} (n-i-j+1). \tag{3.13}$$

We have no proof of this formula, but it has been verified through $n = 15$. The $\delta_{i,n}$, as is typical for the hybrid method, satisfy the relation

$$\delta_{i,n} = \lambda^i + O(\lambda^{n+1}) \tag{3.14}$$

for small λ. Thus the n-term hybrid solution agrees with the n-term perturbation solution in the limit that $|\lambda|$ goes to zero. On the other hand, for large $|\lambda|$ the difference between the hybrid and perturbation solutions is very significant.

We measure the error of the hybrid approximation by computing the L_2 norm of the relative error between the approximate solution (3.4) and the exact solution (3.3). In Figure 2, the log of the error of the hybrid solution is also plotted vs. $\log(\lambda)$ for a number of even values of n. We see that $n = 2$ gives a reasonable approximation for $|\lambda|$ less than about 0·5. Use of higher and higher values of n allows reasonable results for higher and higher values of $|\lambda|$. Thus $n = 6$ gives approximately the same error at $|\lambda| = 7{\cdot}0$ as $n = 2$ gives at $|\lambda| = 0{\cdot}5$. In comparing the errors of the hybrid solutions with those of the perturbation solutions we see that for any given value of n the hybrid solution are always more accurate than the perturbation solution on which it is based. Further, while the radius of convergence has a severely limiting effect on the perturbation solutions, there is no trace of such an effect on the hybrid solutions.

It was mentioned above that the denominator of the exact solution (3.1) has zeros for $\lambda = m\pi i$ for non-zero integers m. It is interesting to note that these singularities are reflected in the $\delta_{j,n}$. Since the $\delta_{j,n}$ are rational functions of λ^2, their singularities must correspond to the zeros of their denominators, the Δ_n. The zeros of the Δ_n, which are all purely imaginary, are plotted in Figure 3 for several low values of n. We see that as n increases the roots approach integer multiples of πi. Also, by using (3.13) and the identity $(2i+1)!!2^i i! = (2i+1)!$, we find for $n \gg i$ that

$$\beta_{i,n} = \frac{1}{(2i+1)!} - \frac{i(4i-3)}{2n(2i+1)!} + O(n^{-2}). \tag{3.15}$$

Since the Taylor series expansion for $\sinh(\lambda)/\lambda$ is

$$\frac{\sinh(\lambda)}{\lambda} = \sum_{i=0}^{\infty} \frac{1}{(2i+1)!} \lambda^{2i}, \tag{3.16}$$

we conclude that

$$\lim_{n\to\infty} \Delta_n(\lambda) = \sinh(\lambda)/\lambda \tag{3.17}$$

for all λ.

To complete the demonstration that we have convergence for all λ we need to show that $\Delta_n \sum_{i=1}^{n} \delta_{i,n} u_i(x)$ converges to the numerator of (3.3b) for all λ. The numerator may be partitioned into even and odd functions of x. Thus, it needs to be shown for all λ that

$$\lim_{n\to\infty} \sum_{i=0}^{(n-1)/2} \left(\sum_{j=0}^{(n-1)/2-i} \beta_{j,n}\lambda^{2i+2j+1} \right) u_{2i+1}(x) = \frac{\cosh(\lambda) - \cosh(\lambda x)}{\lambda} \tag{3.18}$$

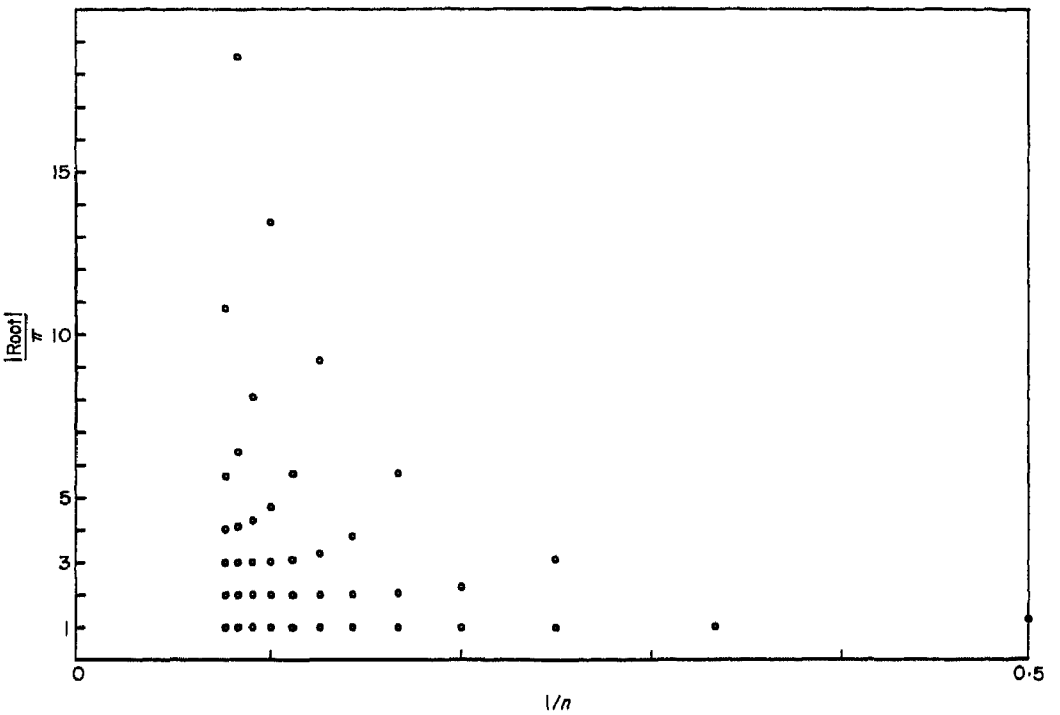

Figure 3. Absolute values of the roots of the denominators of the hybrid solutions as dependent on the number of terms n. All roots are purely imaginary and approach $m\pi i$ for non-zero values of m as n increases.

and

$$\lim_{n\to\infty} \sum_{i=1}^{n/2} \left(\sum_{j=0}^{n/2-i} \beta_{j,n} \lambda^{2i+2j} \right) u_{2i}(x) = \frac{x \sinh(\lambda) - \sinh(\lambda x)}{\lambda}. \tag{3.19}$$

That these relations hold is indicated by the fact that

$$\sum_{i=0}^{(n-1)/2} \left(\sum_{j=0}^{(n-1)/2-i} \beta_{j,\infty} \lambda^{2j} \right) \lambda^{2i+1} u_{2i+1}(x) = \sum_{k=1}^{(n+1)/2} \frac{(1-x^{2k})\lambda^{2k-1}}{(2k)!} \tag{3.20}$$

and

$$\sum_{i=1}^{n/2} \left(\sum_{j=0}^{n/2-i} \beta_{j,\infty} \lambda^{2j} \right) \lambda^{2i} u_{2i}(x) = \sum_{k=1}^{n/2} \frac{x(1-x^{2k})\lambda^{2k}}{(2k+1)!}, \tag{3.21}$$

where the right hand sides of (3.20) and (3.21) are the truncated Taylor series expansions of the right hand sides of (3.18) and (3.19), respectively. Equations (3.20) and (3.21) follow directly from (3.7) and (3.8).

More specifically, using the expression (3.15) we see that for any fixed value of λ and x

$$\Delta_n(\lambda) = \sinh(\lambda)/\lambda + O(n^{-1}) \tag{3.22}$$

and

$$\Delta_n(\lambda) \sum_{i=1}^{n} \delta_{i,n} u_i(x) = \frac{\cosh(\lambda) - \cosh(\lambda x)}{\lambda} + \frac{x \sinh(\lambda) - \sinh(\lambda x)}{\lambda} + O\left(\frac{1}{n}\right). \tag{3.23}$$

Thus, we can write

$$\tilde{U} = U + O(n^{-1}), \tag{3.24}$$

which gives us an indication of the rate of convergence of $\tilde{U}$ to U as n increases.

4. Quantum One-Dimensional Anharmonic Oscillator

The second problem we study is of a very different nature. The classical harmonic oscillator (mass on a weightless spring without damping) satisfies the equation

$$m\ddot{x} = -kx. \tag{4.1}$$

Throughout time the sum E of the kinetic energy $T = m\dot{x}^2/2$ and the potential energy $V_0 = kx^2/2$ remains constant, i.e.

$$T + V_0 = \frac{m\dot{x}^2}{2} + \frac{kx^2}{2} = E. \tag{4.2}$$

Any small modification which makes the forcing term (the right hand side of (4.1)) non-linear results in an anharmonic oscillator. We then write the energy equation (4.2) as

$$\frac{m\dot{x}^2}{2} + \frac{kx^2}{2} + V = E. \tag{4.3}$$

The quantum one-dimensional anharmonic oscillator satisfies the non-dimensionalized Schrödinger equation

$$(H_0 + V(x))\psi(x) = \left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} + V(x)\right]\psi(x) = E\psi(x) \tag{4.4}$$

with

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1. \tag{4.5}$$

We assume that $x^2/2 + V(x)$ goes to positive infinity as $|x|$ becomes infinite. Then, the only solutions are bound states with

$$\psi(\pm\infty) = 0, \tag{4.6}$$

and E has a discrete spectrum.

For purposes of this study we choose the case

$$V(x) = \lambda x^4 \quad \text{with } \lambda > 0. \tag{4.7}$$

The solutions consist of energy eigenvalues $E_m(\lambda)$ and their corresponding wavefunctions (eigenfunctions) $\psi_m(x, \lambda)$ for $m = 0, 1, 2, \ldots$.

For the harmonic oscillator, $\lambda = 0$, the solutions are

$$\begin{aligned} E_m(0) &= e_m = m + \tfrac{1}{2}, \\ \psi_m(x, 0) &= \phi_m(x) = h_m(x)\, e^{-x^2/2}, \end{aligned} \tag{4.8}$$

where the Hermite polynomial of degree m, $h_m(x)$, is given by

$$h_m(x) = \frac{(-1)^m}{\sqrt{2^m m!\sqrt{\pi}}} e^{x^2} \left(\frac{d}{dx}\right)^m e^{-x^2}. \tag{4.9}$$

The ϕ_m alternate between being even and odd functions of x. It can easily be shown that

$$\int_{-\infty}^{\infty} \phi_m(x)\phi_n(x)\,dx = \delta_{m,n}, \tag{4.10}$$

where $\delta_{m,n}$, in this equation only, represents the Kronecker δ function. For $\lambda \neq 0$, closed form solutions apparently do not exist.

This quantum mechanical one-dimensional perturbed harmonic oscillator problem (4.4–4.7) is well known and detailed analyses have been given by several authors, most notably by Bender & Orszag (1978), Bender & Wu (1962; 1969; 1971; 1973), and Simon (1970). Many elementary quantum mechanics textbooks discuss procedures for quantum perturbations and apply them to this problem. Step 1 follows a standard procedure.

STEP 1.

Let the wave function for the mth energy state be

$$\psi_m(x,\lambda) = \sum_{i=0}^{n-1} \lambda^i \psi_{m,i}(x) + O(\lambda^n), \qquad \psi_{m,0} = \phi_m, \tag{4.11}$$

with

$$\int_{-\infty}^{\infty} \phi_m(x)\psi_{m,i}(x)\,dx = 0 \qquad (i = 1, 2, \ldots, n-1) \tag{4.12}$$

and let the energy of that state be

$$E_m(\lambda) = \sum_{i=0}^{n-1} \lambda^i E_{m,i} + O(\lambda^n), \qquad E_{m,0} = e_m. \tag{4.13}$$

Then substitute (4.11) and (4.13) into the differential equation

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} + \lambda x^4 - E_m(\lambda)\right)\psi_m(x,\lambda) = 0, \tag{4.14}$$

expand in powers of λ, set the coefficients of λ^i to zero, and solve for $E_{m,i}$ and $\psi_{m,i}(x)$.

More specifically, the computation of the perturbation terms is as follows. The coefficient of λ^1 in the expansion is

$$\left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{x^2}{2} - E_{m,0}\right)\psi_{m,1}(x) = (-x^4 + E_{m,1})\psi_{m,0}(x). \tag{4.15}$$

Multiply both sides of (4.15) by $\phi_m(x)$, integrate over all x, use the normalization condition on $\phi_m(x)$ to obtain

$$E_{m,1} = \int_{-\infty}^{\infty} x^4 \phi_m^2(x)\,dx. \tag{4.16}$$

Now multiply both sides of (4.15) by $\phi_k(x)$ where $k \neq m$, integrate over all x, use the completeness conditions on the $\phi_m(x)$, and then use (4.12) to obtain

$$\psi_{m,1} = \sum_{k \neq m} \frac{\int_{-\infty}^{\infty} \phi_k(\bar{x})\bar{x}^4\phi_m(\bar{x})\,d\bar{x}}{e_m - e_k}\phi_k(x). \tag{4.17}$$

Only a finite number of terms in the summation contribute, and, consequently, $\psi_{m,1}$ has the form of the exponential, $\exp(-x^2/2)$, times a polynomial in x.

To compute higher order terms in the perturbation expansion, note that setting the coefficient of λ^i in the expansion of (4.14) to zero results in

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}-E_{m,0}\right)\psi_{m,i}=(-x^4+E_{m,1})\psi_{m,i-1}(x) + \sum_{j=2}^{i-1} E_{m,j}\psi_{m,i-j}(x)+E_{m,i}\psi_{m,0}(x) \tag{4.18}$$

which can be written as

$$\left(-\frac{1}{2}\frac{d^2}{dx^2}+\frac{x^2}{2}-e_m\right)\psi_{m,i}=f_{m,i}(x)+E_{m,i}\psi_{m,0}(x), \tag{4.19}$$

where $f_{m,i}$ is at this stage a known quantity given by

$$f_{m,i}(x)=(-x^4+E_{m,1})\psi_{m,i-1}(x)+\sum_{j=2}^{i-1} E_{m,j}\psi_{m,i-j}(x). \tag{4.20}$$

Multiply both sides of (4.20) by $\phi_m(x)$ and integrate over all x. The left hand side vanishes and, consequently,

$$E_{m,i}=-\int_{-\infty}^{\infty}\phi_m(x)f_{m,i}(x)\,dx=\int_{-\infty}^{\infty}\phi_m(x)x^4\psi_{m,i-1}(x)\,dx. \tag{4.21}$$

The quantity $\psi_{m,i}(x)$ evaluates to

$$\psi_{m,i}=\sum_{k\neq m}\frac{\int_{-\infty}^{\infty}\phi_k(\bar{x})f_{m,i}(\bar{x})\,d\bar{x}}{e_k-e_m}\phi_k(x). \tag{4.22}$$

The summations indicated in this procedure, while nominally over an infinite number of terms, are for this problem all finite. For this reason, and since all the integrals cited above can be evaluated in closed form, the calculations can, in principle, be carried out to any order without any loss of accuracy. With the use of a computer algebra system such as MACSYMA (1988) or Mathematica (Wolfram, 1988) it is relatively easy to get eight or ten terms. However, by itself a high order perturbation computation is not very useful for this problem since the expansion has a radius of convergence in λ which is zero!

An indication that the radius of convergence is zero can be obtained by performing ratio and root tests on the series $E_{m,i}$ $(i=1,2,\ldots)$. This may have been anticipated, since for $\lambda<0$ we suddenly have only continuum states and no bound states. The zero radius of convergence was previously observed by a number of authors, see for example, Bender & Wu (1969), Reid (1967) and Simon (1970), and thus is not new to this study.

Before proceeding with step 2 it should be noted that the total wavefunction $\psi_m(x,\lambda)$ as computed by this procedure has not yet been normalized (see (4.5)). The renormalization can be carried out as the last step in the perturbation calculation. However, it is not needed at all if we go on to step two of the hybrid method.

STEP 2.

Despite the lack of convergence, we proceed to step two. For n terms in the approximation let the wavefunction which is a perturbation of $\phi_m(x)$ be

$$\tilde{\psi}_{m,n}(x)=\sum_{j=0}^{n-1}\psi_{m,j}(x)\delta_{m,j,n}(\lambda) \tag{4.23}$$

and let its associated energy eigenvalue be $\tilde{E}_{m,n}$. The Galerkin orthogonality conditions become

$$\int_{-\infty}^{\infty} \psi_{m,i}(x)\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\tilde{\psi}_{m,n}(x)+\left(\frac{x^2}{2}+\lambda x^4-\tilde{E}_{m,n}\right)\tilde{\psi}_{m,n}(x)\right]\mathrm{d}x=0 \qquad (i=0,1,\ldots,n-1), \tag{4.24}$$

which may be written in the form

$$\sum_{j=0}^{n-1}(B_{m,i,j}+\lambda C_{m,i,j}-\tilde{E}_{m,n}D_{m,i,j})\delta_{m,j,n}=0 \qquad (i=0,1,\ldots,n-1), \tag{4.25}$$

where

$$\begin{aligned} B_{m,i,j} &= \int_{-\infty}^{\infty}\psi_{m,i}(x)\left[\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{x^2}{2}\right)\psi_{m,j}(x)\right]\mathrm{d}x, \\ C_{m,i,j} &= \int_{-\infty}^{\infty}\psi_{m,i}(x)x^4\psi_{m,j}(x)\,\mathrm{d}x, \\ D_{m,i,j} &= \int_{-\infty}^{\infty}\psi_{m,i}(x)\psi_{m,j}(x)\,\mathrm{d}x. \end{aligned} \tag{4.26}$$

Non-trivial solutions are allowed only for

$$\det(\mathbf{B}_{m,n}+\lambda\mathbf{C}_{m,n}-\tilde{E}_{m,n}\mathbf{D}_{m,n})=0, \tag{4.27}$$

where **B**, **C** and **D** are symmetric n by n matrices. Consider first the case of $n=1$. Then the matrices **B**, **C** and **D** are all 1 by 1 matrices. The quantity **B** evaluates to e_m; **D** is unity because of the normalization of the ϕ_m; and **C** evaluates to $\frac{3}{4}(1+2m+2m^2)$, resulting in

$$\tilde{E}_{m,1}=\frac{1+2m}{2}+\frac{3\lambda(1+2m+2m^2)}{4}. \tag{4.28}$$

For $n=2$ the left hand side of (4.27) evaluates to a polynomial in m, λ, and $\tilde{E}_{m,n}$ which is of total degree 2 in λ and $\tilde{E}_{m,n}$. There are two solutions, but the one which is of interest is the one which passes through $\tilde{E}_{m,n}=m+\frac{1}{2}$ at $\lambda=0$. The form of $\tilde{E}_{m,2}$ is

$$\tilde{E}_{m,2}=\frac{a(m)+b(m)\lambda}{e(m)}-\sqrt{\left[\frac{c(m)+d(m)\lambda}{e(m)}\right]^2+\frac{[c(m)\lambda]^2}{128e(m)}}, \tag{4.29}$$

where $a(m)$, $b(m)$, $c(m)$, $d(m)$ and $e(m)$ are all polynomials in m with integer coefficients. See the Appendix for further details. The authors believe that (4.29) and the contents of the Appendix are new results which are presented for the first time in this paper and its earlier version (Andersen & Geer, 1988).

For higher values of n the left hand side of (4.27) evaluates to a polynomial of total degree n in λ and $\tilde{E}_{m,n}$. Thus (4.27) defines n curves in the $\lambda-\tilde{E}_{m,n}$ plane. However, the only curve of interest is the one which passes through the point $(0, e_m)$. Examination of a number of specific cases indicates that the Taylor series of $\tilde{E}_{m,n}$ as a function of λ agrees with the first $2n$ terms of the perturbation solution. This is gratifying though not completely surprising, because it is known that the first n wavefunctions from the perturbation expansion can be used to determine an energy value which is correct to the first $2n$ terms in the energy expansion (Löwdin, 1965). Thus the hybrid and perturbation methods give the same number of correct terms in the energy power series expansion.

Once the energy eigenvalue $\tilde{E}_{m,n}$ has been determined, we may find the eigenvector $\delta_{m,n}(\lambda)$ from which the wavefunction $\tilde{\psi}_{m,n}(x, \lambda)$ may be constructed. As the last step the normalization is determined by requiring that

$$\int_{-\infty}^{\infty} |\tilde{\psi}_{m,n}(x, \lambda)|^2 \, dx = 1. \tag{4.30}$$

Figure 4 shows the results of the perturbation and hybrid approaches in computing the ground state ($m = 0$) energy level as a function of λ. The perturbation result is the same as the hybrid result for $n = 1$. Using higher perturbation terms seems to be counterproductive for almost all values of λ on the scale shown, since at best only asymptotic convergence is exhibited. On the other hand, the hybrid results appear to be converging well for all λ to the numerically obtained solutions.

The numerical results were obtained by a shooting method and are presumed to be accurate to plotting accuracy. The initial point for the shooting method was a relatively large value of x with the requirement that the slope at the initial value of x be adjusted such that either the slope of ψ (in the case of even m) or ψ itself (in the case of odd m) be zero at the origin.

Figure 5 compares the hybrid results for the first four energy levels with numerical results. The errors always seem to diminish as the number of terms in the hybrid technique

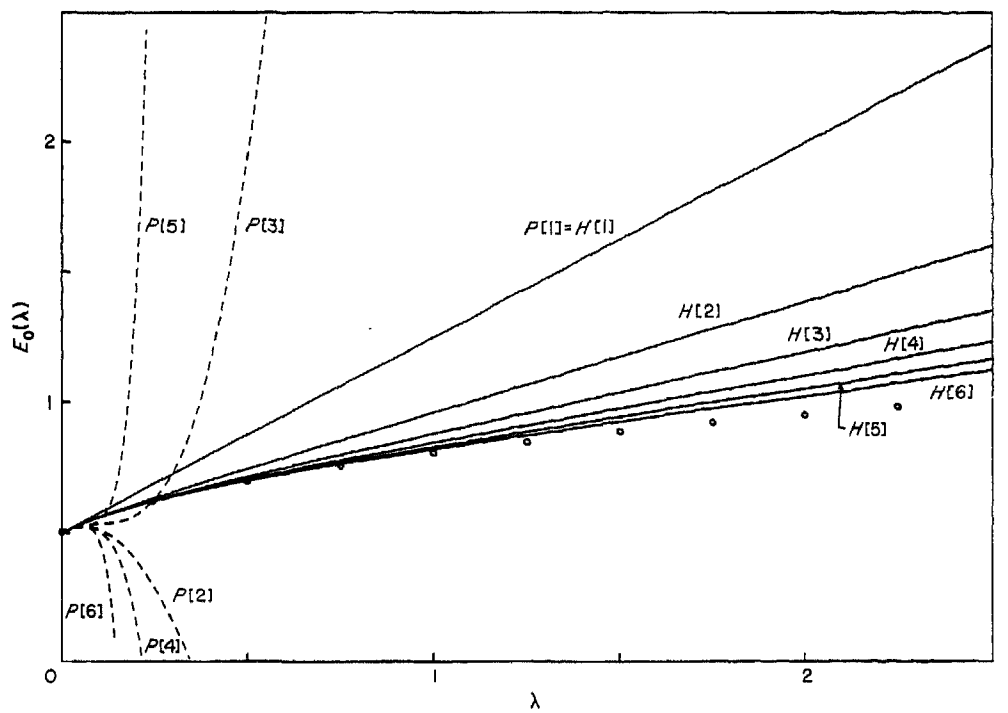

Figure 4. Comparison of hybrid solutions for the ground state ($m = 0$) energy with perturbation and numerical solutions. The hybrid results are labelled $H[n]$ and the perturbation results $P[n]$, where the number of terms in the expansion is n. The numerical ("exact") results are indicated by circles. The perturbation and hybrid solutions are the same for $n = 1$. The perturbation results have zero radius of convergence.

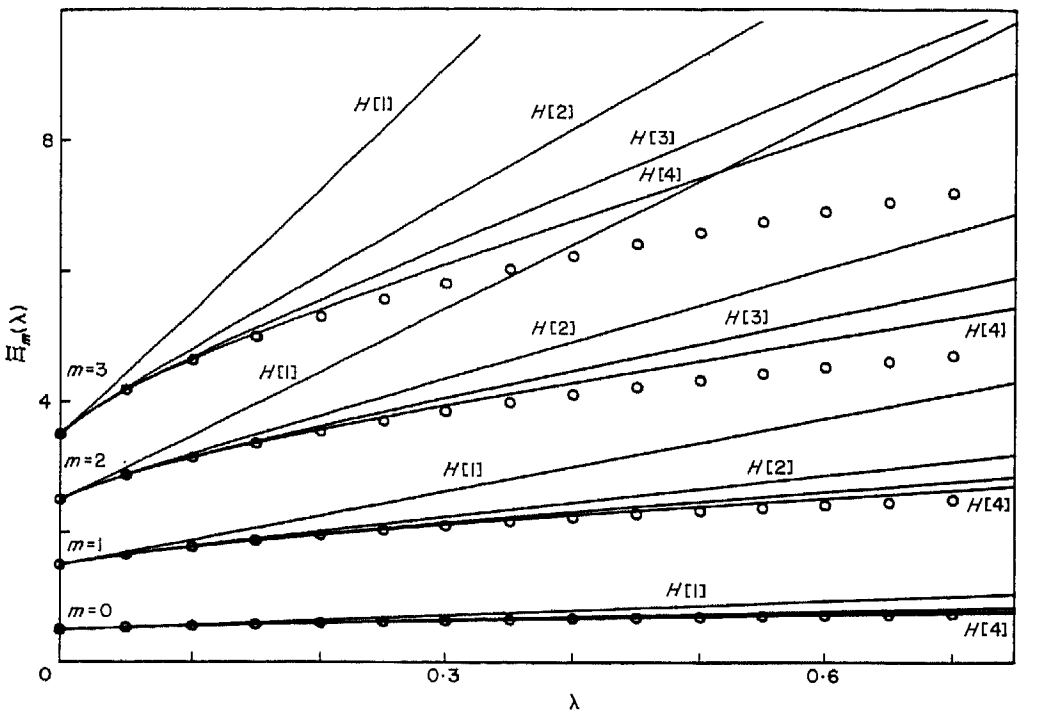

Figure 5. Comparison of the hybrid solutions with numerical solutions for the energies of the four lowest states. Hybrid solutions with n terms are labelled $H[n]$, and the numerical ("exact") solutions are indicated by circles. The accuracy decreases as the energy level increases.

is increased; and our work gives no hint of any limit to the range of convergence as λ is increased. It may be noted, however, that the number of hybrid terms needed for a given level of accuracy does increase with energy.

Convergence of the wavefunctions is considerably slower. Some representative cases are shown in Figures 6 and 7.

While we are not able to predict how many hybrid terms are needed to gain a given level of accuracy for a given value of λ, the convergence is monotone and the difference in the results for $n-1$ terms and n terms seems to be a good indication.

Though the Taylor series of the energy eigenvalues as a function of λ may agree to order $2n$, there is a vast difference in the usefulness of the perturbation and hybrid results. The perturbation results, indeed, are virtually useless for the computation of energy eigenvalues and wave functions for any value of λ, while the hybrid results seem to converge to the exact solutions as the number of terms increases. With the aid of computer algebra, we can hope for insight which will someday lead to a proof of convergence.

5. Concluding Remarks

In the course of this study we have made extensive use of computer algebra. Both MACSYMA and Mathematica have been used. Computer algebra has been used here not only to evaluate the perturbation solutions and, at least partially, to perform the Galerkin step, but also to begin to explore the form the hybrid solutions take and their

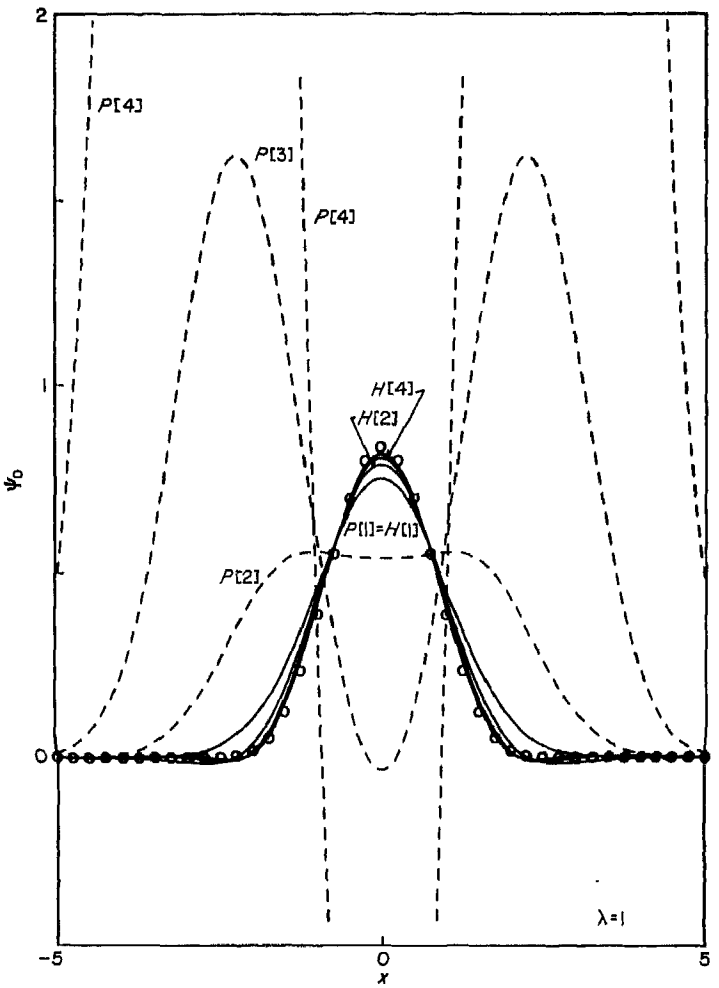

Figure 6. Comparison of the ground state ($m=0$) wavefunction solutions for $\lambda=1$ as computed by the perturbation method, the hybrid technique and an accurate numerical shooting method. The perturbation results are labelled $P[n]$ and the hybrid results $H[n]$, where n is the number of terms in the expansion. The numerical ("exact") results are indicated by circles. The perturbation and hybrid solutions are the same for $n=1$.

regions and rates of convergence. Also, by allowing us to perform some steps without round-off error, it allows us to separate round-off errors from errors intrinsic to the methods being explored.

In more practical problems, computer algebra can be expected to play a more restricted (but nevertheless important) role. It may be used in many non-discretized problems to generate the perturbation functions. For discretized problems it may be used to help formulate the needed numerical code (Noor & Andersen, 1981). For the Galerkin step computer algebra may be useful in formulating the integrands, but for many problems the required integrals will not have closed-form expressions. The solution of the linear or non-linear equations for the Galerkin amplitudes will typically require numerical methods. We conclude that the mix of algebraic and numerical computation is very much problem dependent.

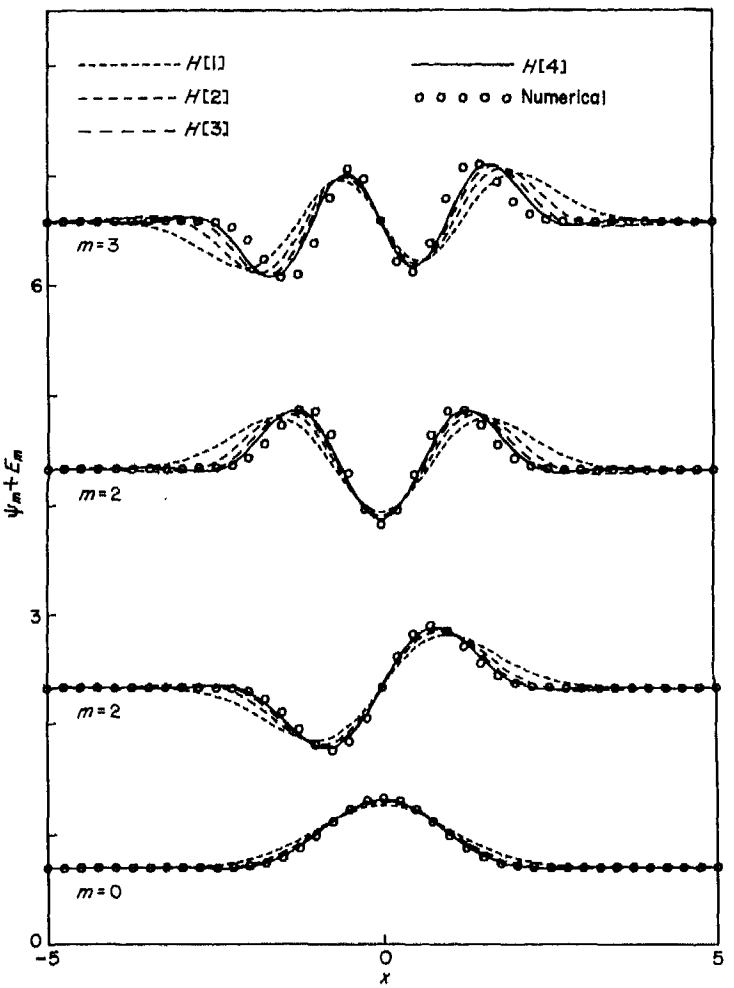

Figure 7. Comparison of the wavefunction solutions for the four lowest energy states for $\lambda = 1/2$ as computed by the hybrid technique and by an accurate numerical shooting method. The wave functions are displaced vertically by an amount equal to their energy levels.

It may be remarked that once a space of trial functions has been indicated by the perturbation step it may be useful to select a new (equivalent) set of basis functions for that space. A new set of basis functions may be selected to simplify subsequent steps or, as in the case of Gram-Schmidt orthonormalization, for example, to improve the conditioning of the Galerkin equations and thereby improve the accuracy of the hybrid solutions.

In the case of the simple two-point boundary-value problem of section 3, an alternate set of basis functions is

$$v_i = (1-x^2)x^i \qquad (i = 0, 1, 2, \ldots). \tag{5.1}$$

These basis functions each satisfy the boundary conditions and can be deduced with almost no computation. They span the same function space as the perturbation functions in (3.6).

For the quantum problem, the perturbation functions all lie in the space spanned by

$$\Psi_i(x) = e^{-x^2/2}x^i \qquad (i=0,1,2,\dots). \tag{5.2}$$

However, appropriate combinations of $\Psi_i(x)$ used to span only a small space of trial functions depend on the state, m, being perturbed and are only found by computing the perturbation functions.

For many other problems the perturbation step plays an even more significant role in determining a small but appropriate set of trial functions to use as input for the Galerkin technique. A trial function basis chosen by a wild guess might require the use of a very large system of Galerkin equations in order to obtain the accuracy desired. Further, the insight from obtaining a semi-analytic solution would be lost.

It has been observed that the Galerkin amplitudes, $\delta_{i,n}$, in section 3 are rational functions of λ. This is typical of linear two-point boundary-value problems which have homogeneous boundary conditions, which have polynomial dependence on the parameter λ, and which have regular perturbation expansions in λ. In this case there is a strong similarity with Padé solutions. For such problems the rational function dependence on λ arises because of the linearity of the equations in the Galerkin step.

As a parenthetical remark, we include an observation based on numerical empirical evidence. For the problem studied in section 3 it seems that

$$\lim_{n\to\infty} \delta_{i,n} = \lambda^i \tag{5.3}$$

for all λ. It will be interesting to see if this relation holds with any generality.

The rational function dependence on the expansion parameter is lost in the case of linear eigenvalue problems such as the quantum problem of section 4. However, the solutions to (4.25) through (4.27) are algebraic functions of the parameter λ. In the slender body problems studied in Geer & Andersen (1989*a*), it was found that the solutions for the $\delta_{i,n}$ involve terms like $\log\lambda$ and hence are transcendental functions of λ.

In this study we have examined two sample linear problems to explore some of the behaviour of the hybrid method. The first is a simple non-selfadjoint two-point boundary-value problem with a known exact solution. The perturbation method exhibits a finite radius of convergence. Within this radius the hybrid solutions converge faster than the perturbation solutions, and, while the convergence rate slows as λ increases, the hybrid technique is shown to converge for all values of λ. In common with the perturbation method, accurate solutions for very small λ can be achieved with a small number of terms. However, as the magnitude of λ increases, more and more terms must be used to achieve a given level of accuracy. Use of computer algebra has allowed us to give an explicit (recursive) formula for the hybrid solution for any number of terms n, and thus has led to a demonstration of convergence for all values of λ. It is hoped that the same approach can be applied to many other problems where the $\delta_{i,n}$ are rational functions of λ. The problem (3.1) and (3.2) has also been studied (using a different notation) in a previous publication (Geer & Andersen, 1989*a*).

The second problem is an eigenvalue problem where the eigenvalues and eigenfunctions are perturbed. This self-adjoint problem has simple solutions for $\lambda = 0$, but the perturbation method exhibits a zero radius of convergence. Empirical evidence suggests that the hybrid solutions converge for all positive values of λ. Once again, accurate answers for small λ can be achieved with a small number of terms, but more and more terms are needed as λ increases. A previous publication (Geer & Andersen, 1990) demonstrates that a perturbations solution (determined numerically) can be found which is valid in the limit of large

λ, and that this solution can be coupled with the expansion at $\lambda = 0$ to give much improved convergence properties. The use of multiple perturbation expansions promises to be a powerful tool, but we expect this to greatly complicate any studies of convergence rates and any proofs of convergence.

We conclude by observing that the hybrid technique promises frequently to be an improvement over the perturbation method since the accuracy is increased, the range of parameter for which useful solutions are obtained is often extended, and relatively little additional computational effort is required.

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Appendix

For the second order hybrid solution for the quantum anharmonic oscillator problem of section 4, we record the following results:

$$b_{m,0,0} = m + \tfrac{1}{2},$$
$$b_{m,0,1} = b_{m,1,0} = 0, \tag{A.1}$$
$$b_{m,1,1} = \frac{(1+2m)}{256}(828+966m+1031m^2+130m^3+65m^4),$$

$$c_{m,0,0} = \tfrac{3}{4}(1+2m+2m^2),$$
$$c_{m,0,1} = c_{m,1,0} = -\frac{(1+2m)}{8}(21+17m+17m^2), \tag{A.2}$$
$$c_{m,1,1} = \tfrac{3}{512}(3708+11838m+16747m^2+9948m^3+5299m^4+390m^5+130m^6),$$

$$d_{m,0,0} = 1,$$
$$d_{m,0,1} = d_{m,1,0} = 0, \tag{A.3}$$
$$d_{m,1,1} = \frac{156+422m+487m^2+130m^3+65m^4}{128}.$$

It follows that $\tilde{E}_{m,2}$ has the form (4.29) with

$$\begin{aligned} a &= 2(1+2m)(492+694m+759m^2+130m^3+65m^4), \\ b &= 3(1932+6286m+9195m^2+5948m^3+3299m^4+390m^5+65m^6), \\ c &= 32(1+2m)(21+17m+17m^2), \\ d &= 48(111+347m+472m^2+250m^3+125m^4), \\ e &= 4(156+422m+487m^2+130m^3+65m^4). \end{aligned} \tag{A.4}$$

The Taylor series expansion of (4.29) about $\lambda = 0$ is

$$\tilde{E}_{m,2} = \frac{a-c}{e} + \frac{b-d}{e}\lambda - \frac{c}{256}\lambda^2 + \frac{d}{256}\lambda^3 + O(\lambda^4), \tag{A.5}$$

which is in agreement with (4.28) since

$$\frac{a-c}{e} = b_{m,0,0} = m + \tfrac{1}{2} \tag{A.6}$$

and

$$\frac{b-d}{e} = c_{m,0,0} = \tfrac{3}{4}(1+2m+2m^2). \tag{A.7}$$

For $m=0$, 1, 2 and 3, (4.29) evaluates to

$$\begin{aligned}
\tilde{E}_{0,2} &= \frac{41}{26}+\frac{483\lambda}{52}-\sqrt{\left(\frac{14+111\lambda}{13}\right)^2+\frac{147\lambda^2}{26}},\\
\tilde{E}_{1,2} &= \frac{107}{42}+\frac{453\lambda}{28}-\sqrt{\left(\frac{22+261\lambda}{21}\right)^2+\frac{605\lambda^2}{14}},\\
\tilde{E}_{2,2} &= \frac{2915}{838}+\frac{43113\lambda}{1676}-\sqrt{\left(\frac{410+6693\lambda}{419}\right)^2+\frac{126075\lambda^2}{838}},\\
\tilde{E}_{3,2} &= \frac{707}{162}+\frac{445\lambda}{12}-\sqrt{\left(\frac{70+1485\lambda}{81}\right)^2+\frac{6125\lambda^2}{18}}.
\end{aligned} \tag{A.8}$$