NASA Contractor Report 181750

ICASE REPORT NO. 88-65

ICASE

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Contract Nos. NAS1-18107, NAS1-18605
November 1988

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NASA Langley Research Center, Hampton, Virginia 23665

Operated by the Universities Space Research Association

National Aeronautics and
Space Administration

Langley Research Center
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INVESTIGATING A HYBRID PERTURBATION-GALERKIN TECHNIQUE USING COMPUTER ALGEBRA

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Abstract

A two-step hybrid perturbation-Galerkin method is presented for the solution of a variety of differential equations type problems which involve a scalar parameter. The resulting (approximate) solution has the form of a sum where each term consists of the product of two functions. The first function 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. The resulting hybrid method 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 particular, the results can be useful well beyond the radius of convergence associated with the perturbation expansion. The hybrid method 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 method apparently converges for an infinite range of the parameter λ. The results obtained from the hybrid method are compared with approximate solutions obtained by other methods, and the applicability of the hybrid method to broader problem areas is discussed.

[1]Research for the first author was partially funded through NASA cooperative Agreement NCC1-40.

[2]Research for the second author was supported under the National Aeronautics and Space Administration under NASA Contract Nos. NAS1-18107 and NAS1-18605 while he was in residence at the Institute for Computer Applications in Science and Engineering (ICASE), NASA Langley Research Center, Hampton, VA 23665.

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. However, typically 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 in effect increase the radius of convergence [1]. Thus for cases where higher order terms may have a significant effect it is important to make as much use of the information contained in the lower order terms as possible. The hybrid perturbation-Galerkin method described 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 [8,9,10,12,13] combine the perturbation method, the Galerkin method [3], and the finite element method (or other discretization techniques) to attack a variety of structural mechanics problems. Their "reduced-basis method" allows some nonlinear problems requiring thousands of degrees of freedom after discretization to be computed using nonlinear 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 [7,11]. We refer to the same general principle as the hybrid perturbation-Galerkin technique because in using the technique without discretization we do not think in terms of having large bases 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 which result in singular perturbation expansions [4]. In this paper the main problem concerns a well-known quantum eigenvalue problem, namely the perturbed one-dimensional harmonic oscillator. This problem in first order perturbation theory is treated or referred to in many different elementary quantum mechanics texts. Other work yet to be published involves boundary layer problems and problems in which the perturbation expansion is made at two or more values of the expansion parameter.

In Section 2 we give a general description of the method. In Section 3 we analyze a simple two-point boundary value problem to illustrate the technique. Section 4 gives a treatment of the quantum anharmonic oscillator problem followed by 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 a perturbation expansion technique followed by a Bubnov-Galerkin or variational technique. 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 over terms, where each term consists a perturbation function (a function of x) times a gauge function (a preassigned function of λ). The expansion may be singular or regular. For a regular expansion the set of gauge functions consists simply of $\{1, \lambda, \lambda^2, \lambda^3, \ldots\}$. The drawbacks of the perturbation method are i) that frequently the radius of convergence in λ is finite, ii) that 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) that considerable computational effort may be expended computing higher order terms.

In the second step we will keep the perturbation functions but replace the gauge functions by new amplitudes which depend on λ. In the Bubnov-Galerkin or variational technique one seeks an approximate solution in the form of a linear combination of specified (known) coordinate functions (functions of x) with unknown coefficients (or amplitudes) which are functions of λ. This technique can work very well if a good set of coordinate functions is chosen. If a large set of coordinate functions is used, the computational effort can be 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 coordinate 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 results can be dramatically better than the perturbation results and that a set of coordinate functions can be useful far outside the radius of convergence for the perturbation calculation in which they originate.

3. A Simple Example

To introduce the method we consider the following simple two-point boundary value problem: The differential equation,

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

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

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

The exact solution to this problem, which is

$$V = y + 1 - \frac{2\left(1 - e^{\lambda(y+1)}\right)}{1 - e^{2\lambda}} \tag{3.3}$$

exhibits boundary layer behavior near $y = 1$ for large positive values of λ and near $y = -1$ for large negative values of λ. The center 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 [2].

We look for an approximate solution of the form

$$V = \sum_{j=1}^{n} v_j(y)\, \delta_{j,n}(\lambda). \tag{3.4}$$

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

Step 1:

To take step one first, the solution to (3.1) together with (3.2) is written in the form

$$V \cong \sum_{j=1}^{n} v_j(y)\, \lambda^j + O(\lambda^{n+1}). \tag{3.5}$$

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 v_j serve to determine the v_j's. Each v_j is a polynomial in y of degree $j + 1$, and thus they collectively span an n-dimensional space. The first few terms are

$$\begin{aligned} v_1 &= y^2 - 1, \\ v_2 &= y\,(y^2 - 1)/3, \\ v_3 &= (y^2 - 1)(y^2 - 1)/12, \\ v_4 &= y\,(y^2 - 1)(3y^2 - 7)/180, \\ v_5 &= (y^2 - 1)(y^4 - 4y^2 + 3)/360. \end{aligned} \tag{3.6}$$

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 tests 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 $\lambda = \pm m\pi i$ for positive integer values of m. The convergence 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.

Step 2:

In step two, the v_j for $j = 1, 2, \ldots, n$ serve as coefficient (or interpolation) functions for the Bubnov-Galerkin method. The approximation (3.4) with the v_j's known and the $\delta_{j,n}$'s unknown are 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 y 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 says that the residual is orthogonal to each of the coefficient functions v_j. The result is a linear system of n equations

$$\sum_{j=1}^{n} a_{i,j}(\lambda)\, \delta_{j,n} = b_i(\lambda), \qquad (i = 1, 2, \ldots, n) \tag{3.7}$$

where

$$\begin{aligned} a_{i,j}(\lambda) &= \int_{-1}^{1} v_i(y)\, [\tilde{v}_j(y) - \lambda \dot{v}_j(y)]\, dy, \\ b_i &= \lambda \int_{-1}^{1} v_i(y)\, dy. \end{aligned} \tag{3.8}$$

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

$$\delta_{1,2} = \frac{60\,\lambda}{60 + \lambda^2}, \qquad \delta_{2,2} = \frac{60\,\lambda^2}{60 + \lambda^2}. \tag{3.9}$$

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

$$\delta_{i,n} = \frac{\sum_{j=0}^{\lfloor (n-i)/2 \rfloor} \beta_{j,n}\, \lambda^{2j+i}}{\Delta_n} \tag{3.10}$$

where

$$\Delta_n = \sum_{i=0}^{\lfloor n/2 \rfloor} \beta_{i,n} \lambda^{2i}, \qquad \beta_{i,n} = \frac{(2n-2i+1)!!}{(2i+1)!!\, i!} \prod_{j=1}^{i} (n-i-j+1). \tag{3.11}$$

We have no proof of this formula, but it has been verified through $n = 15$.

We measure the error of the hybrid approximation by computing the relative L_2 norm of the approximate solution (3.6) compared with the exact solution (3.3). In Figure 2, the log of the error of the hybrid solution is also plotted vs. λ 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 $|\lambda|$. In comparing the errors of the hybrid solutions with those of the perturbation solutions we see that for given values of n the hybrid solution are always more accurate. Further, while the radius of convergence has a dramatic effect of the perturbation solutions, there is no trace of an effect on the hybrid solutions.

It was mentioned above that the denominator of the exact solution (3.1) has zeros for $\lambda = \pm m\pi i$ for positive integers m. It is interesting to note that these singularities are reflected in the $\delta_{j,n}$'s. Since the $\delta_{j,n}$'s are rational functions of λ^2, their singularities must correspond to the zeros of their denominators, the Δ_n's. The zeros of the Δ_n's, which are all purely imaginary, are plotted in Figure 3 for several low values of n. We see that as n gets larger and larger the roots approach integer multiples of πi.

For purposes of investigating convergence properties we have made extensive use of computer algebra. For less trivial problems, we may be forced to use numerical quadrature in computing the coefficients in the Galerkin equations, the $a_{i,j}$'s and b_j's introduced above. In that case it may be appropriate also to solve the system of Galerkin equations, similar to (3.7), numerically. In fact, for some problems it may be necessary to discretize the system of differential equations and to perform even the perturbation expansion numerically. Thus the mix of symbolic and numerical computation is problem dependent. However, the basic results seem to hold that *i*) the perturbation results can be dramatically improved by use of the second step in the hybrid method, and *ii*) the radius of convergence limitations of the perturbation method do not extend to the hybrid method. We should add that for this problem the perturbation step has provided very little information. The perturbation functions v_j all contain a factor of $y^2 - 1$ due to the boundary conditions; and the set of functions

$$w_j = (y^2 - 1)\, y^j \tag{3.12}$$

spans the same function space as the v_j's. Moreover, the w_j's can be written upon in-

spection of the problem and without any computation. However, for many other problems the perturbation step plays a significant role in determining a small but appropriate set of coordinate functions to use as input for the Galerkin technique. In such problems a wild guess as to a set of basis functions might require a very large number of coefficients in the Galerkin equations to be determined in order to obtain the accuracy desired.

4. Quantum One-Dimensional Anharmonic Oscillator

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

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

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

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

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

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

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

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

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 our sample problem we choose the case

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

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

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

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 $\lambda \neq 0$, we believe that closed form solutions do not exist. Many elementary quantum mechanics textbooks discuss procedures for quantum perturbations and apply them to this problem for sake of illustration. Step one follows a standard procedure.

Step 1:

Let

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

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

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

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

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

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

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

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

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

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

Now multiply both sides by $\phi_n(x)$ where $n \neq m$, integrate over all x, use the completeness conditions on the $\phi_m(x)$, and use (4.12) to get

$$\psi_{m,1}=\sum_{n\neq m}\frac{\int_{-\infty}^{\infty}\phi_n(x)\,x^4\,\phi_m(x)\,dx}{e_m-e_n}\phi_n(x). \tag{4.17}$$

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

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

which can be written as

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

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

$$\psi_{m,i}=\sum_{n\neq m}\frac{\int_{-\infty}^{\infty}\phi_n(x)\,f_{m,i}}{e_n-e_m}. \tag{4.22}$$

The summations indicated in this procedure, while nominally over an infinite number of terms, are in practice 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 [6] or Mathematica [14] 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!

The fact that the radius of convergence is zero can be demonstrated by performing ratio and root tests on the series $E_{m,i}$ $(i = 1, 2, \ldots)$. But this situation may have been anticipated by observing that for any value of λ less than zero the solutions to (4.4) and (4.5) change drastically. We suddenly have all continuum states and no bound states.

Before proceeding with step two it should be noted that the total wavefunction $\psi_m(x)$ 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

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

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

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

which may be written in the form

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

where

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

Nontrivial 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.

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 λ-$\tilde{E}_{m,n}$ 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 [5]. 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

$$\int_{-\infty}^{\infty} |\, \tilde{\psi}_{m,n}(x, \lambda)\, |^2\, dx = 0. \tag{4.30}$$

While the Taylor series of the energy eigenvalues as a function of λ may agree, 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. As in the previous problem we do not yet have a mathematical proof, but the empirical evidence in favor of convergence is strong.

Consider first the energy eigenvalues. 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 for $n = 2$ 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. One 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 order 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.

5. Concluding Remarks

In this study we have treated two sample linear problems to exhibit some of the behavior of the hybrid method. The first is a simple two-point boundary value problem with a known exact solution. The perturbation method exhibits a radius of convergence equal to π. The hybrid method converges faster and appears to converge for all values of λ. In common with the perturbation method, accurate solutions can be achieved with a small number of terms for small λ. 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 algebraic formula for the solution of the resulting Galerkin equations for any order. Thus, a proof of convergence may not be difficult to obtain.

The second problem is an eigenvalue problem where the eigenvalues and eigenfunctions are perturbed. This 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 can be achieved with a

small number of terms for small λ, and more and more terms are needed as λ increases. A future publication will demonstrate that a numerical solution can be found 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. Again computer algebra has allowed us to work without round-off error and thus to get more "pure" comparisons.

Computer algebra has been used here primarily to investigate convergence properties. However, computer algebra can be expected to play a major role in more practical calculations, particularly in the perturbation step.

The improvements brought about by step two of the hybrid method are considerable, and yet the computational effort of step two typically is not as great as for step one.

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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:

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

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

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

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

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

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

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

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

FIGURE CAPTIONS

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

2. Comparison of errors for the perturbation and hybrid techniques showing the dependence on the number of terms n and the parameter λ. The radius of convergence, R_c, of the perturbation expansion equals π.

3. Roots of the denominator of the (approximate) hybrid solution as dependent on the number of terms n. This shows that for large n that the singularities are located at $\pm m\pi i$ for positive integer m.

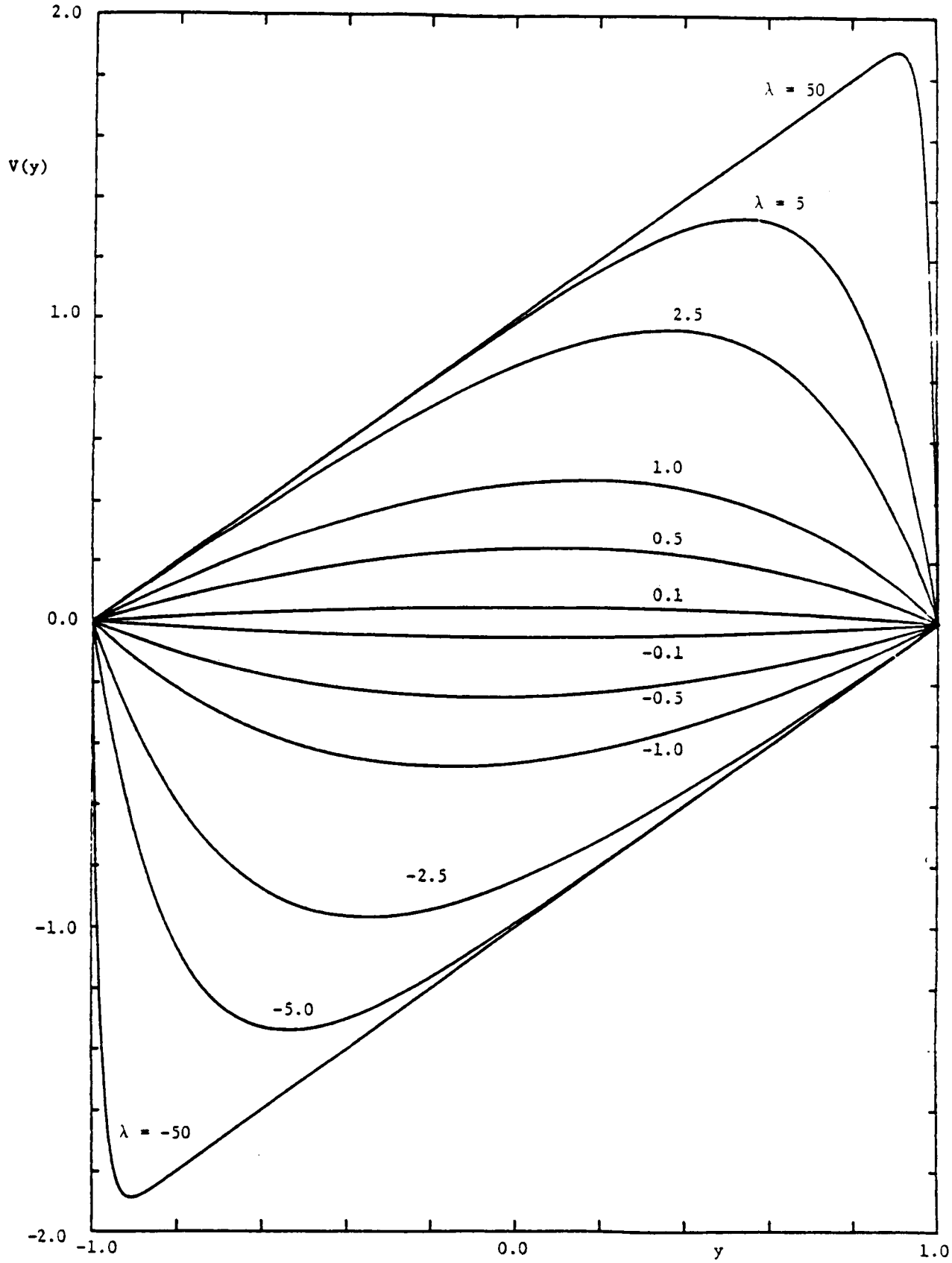
4. Comparison of hybrid results for the ground state ($m = 0$) energy with perturbation and numerical results. The number of terms used in the expansion is n. Hybrid results – solid lines; perturbation results – dashed lines; numerical ("exact") results – circles. Perturbation and hybrid results are the same for $n = 1$. The perturbation results have zero radius of convergence.

5. Comparison of the hybrid results with numerical results for the four lowest states. Hybrid results – solid lines; numerical ("exact") results – circles. The accuracy becomes less as the energy level increases.

6. Comparison of the ground state ($m = 0$) wavefunctions for $\lambda = 1$ as computed by the perturbation method (dashed lines), the hybrid method (solid lines) and by a numerical shooting method (circles). Perturbation and hybrid results are the same for $n = 1$.

7. Comparison of the wavefunctions for the four lowest energy states for $\lambda = 1/2$ as computed by the hybrid method (various dashed and solid lines) and by a numerical shooting method (circles).

Figure 1.



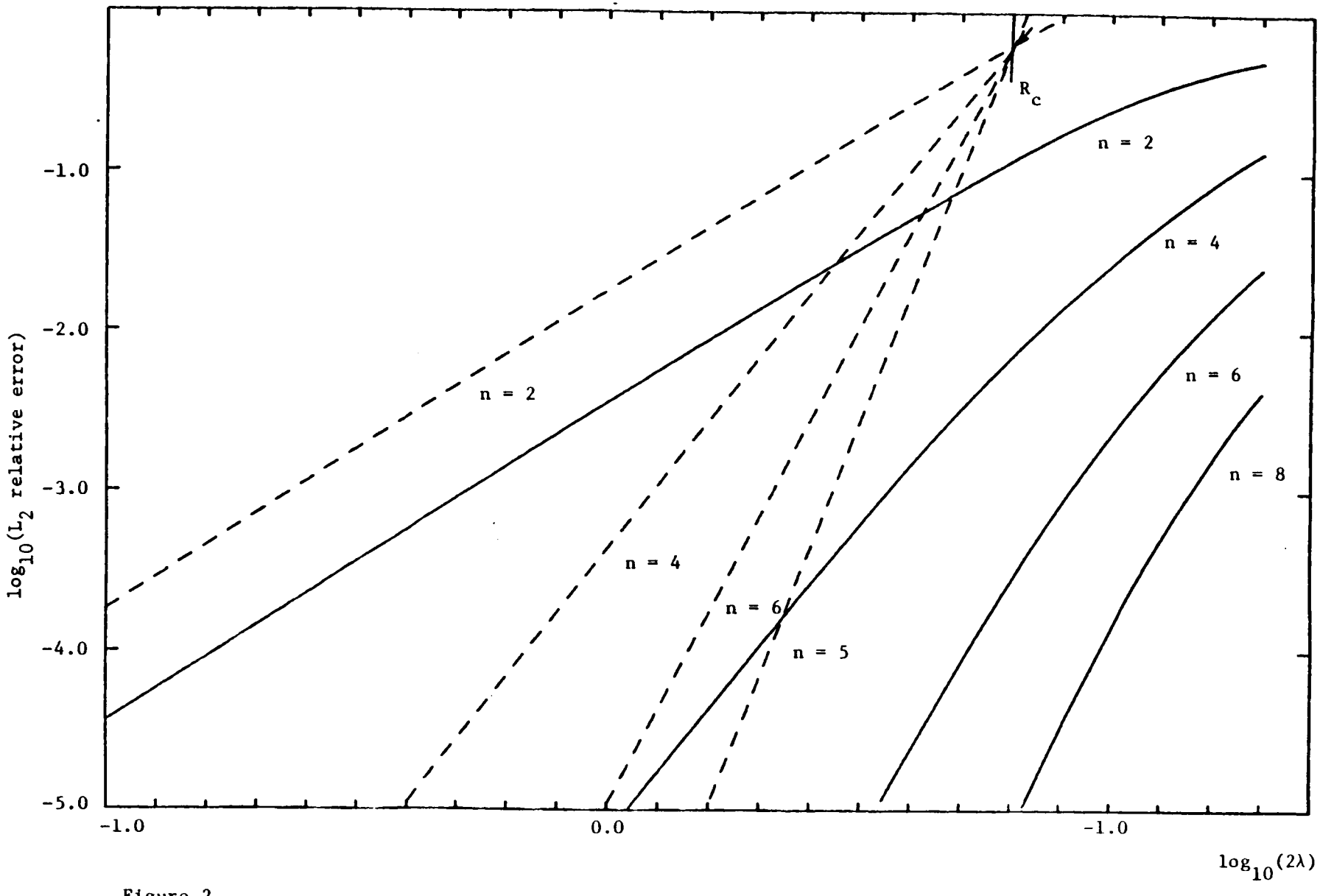

R_c
n = 2
n = 4
n = 6
n = 8
n = 2
n = 4
n = 6
n = 5
-1.0
-2.0
-3.0
-4.0
-5.0
-1.0
0.0
-1.0
$\log_{10}(L_2$ relative error)
$\log_{10}(2\lambda)$

Figure 2.

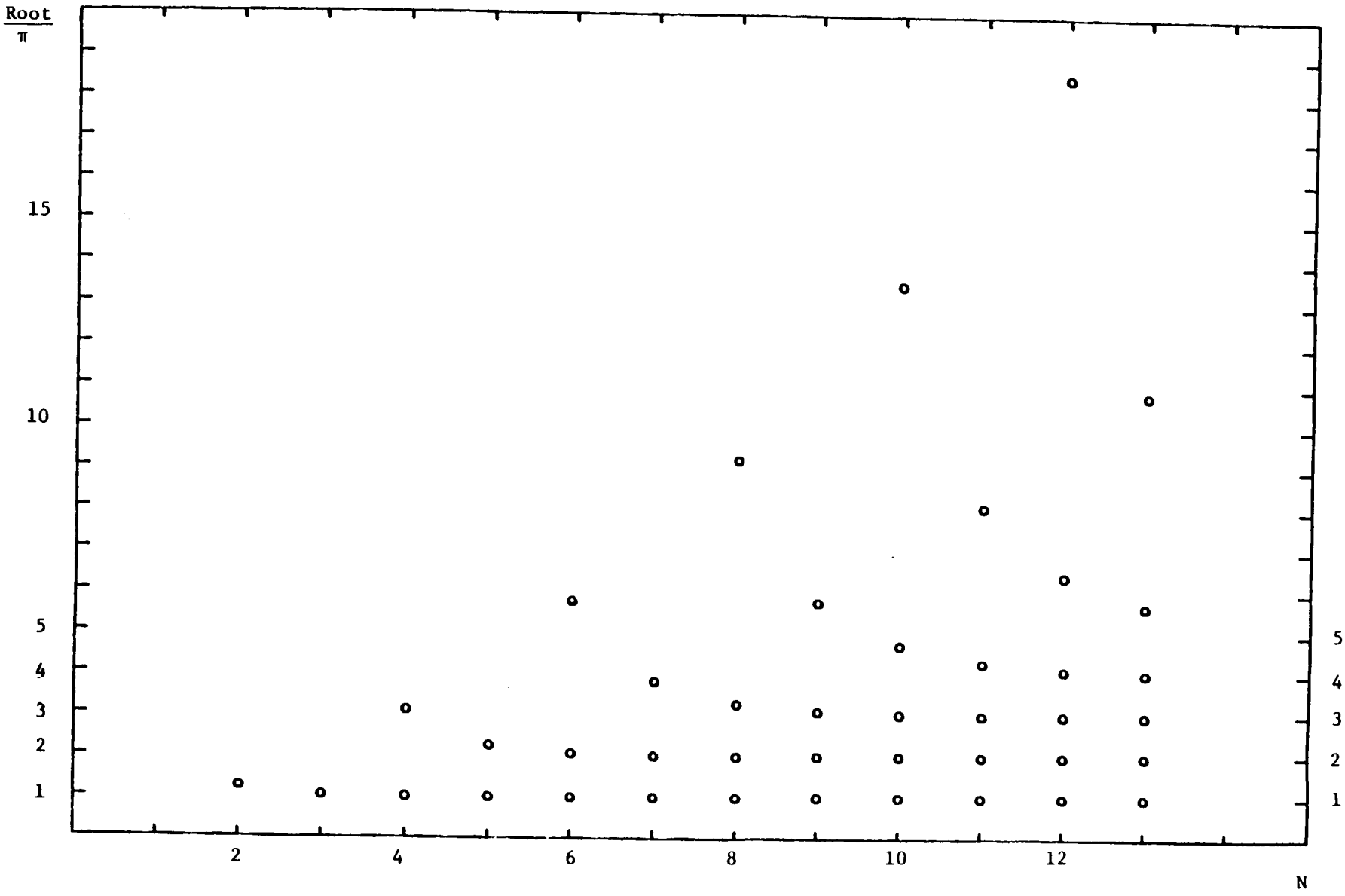


Figure 3.

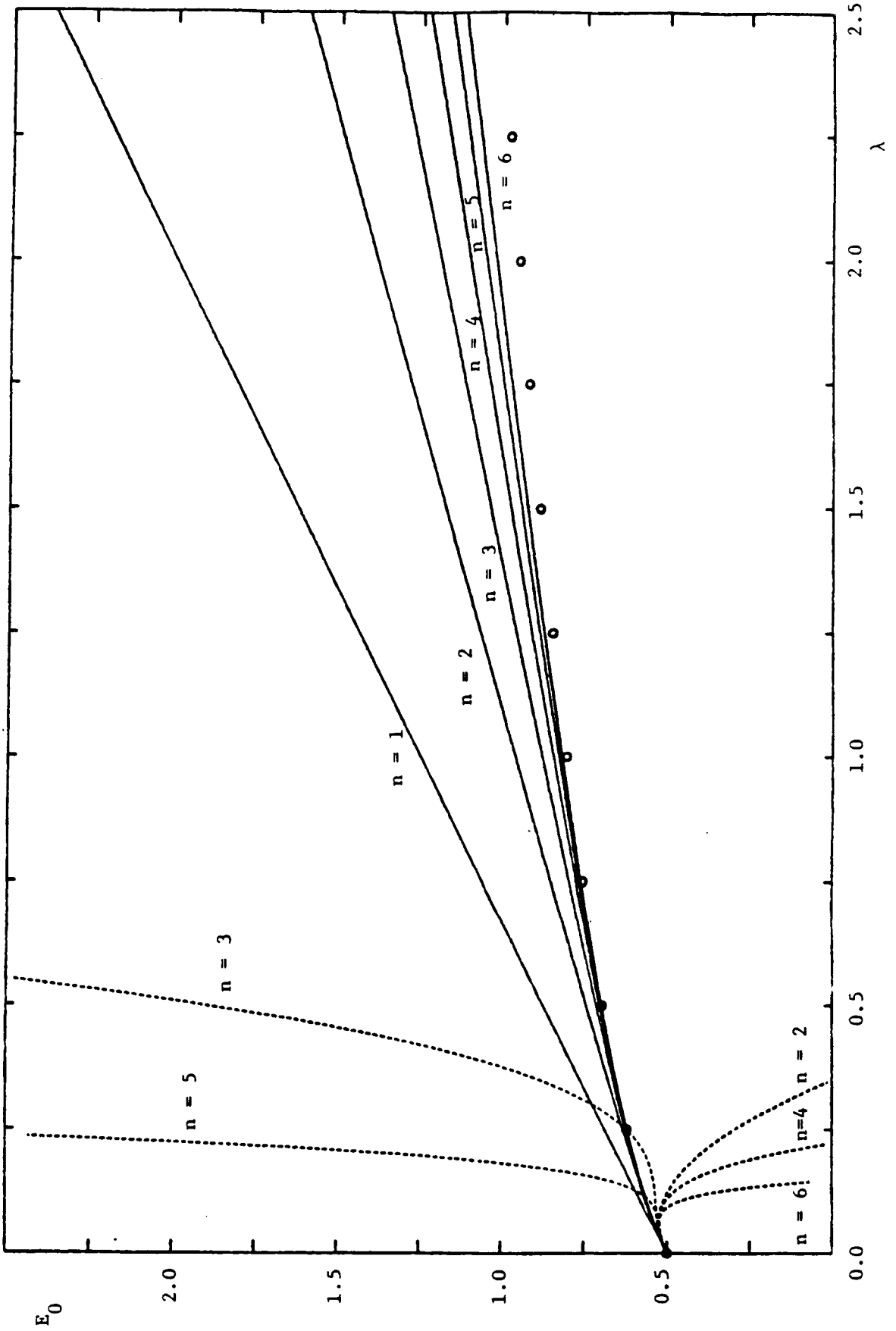


Figure 4.

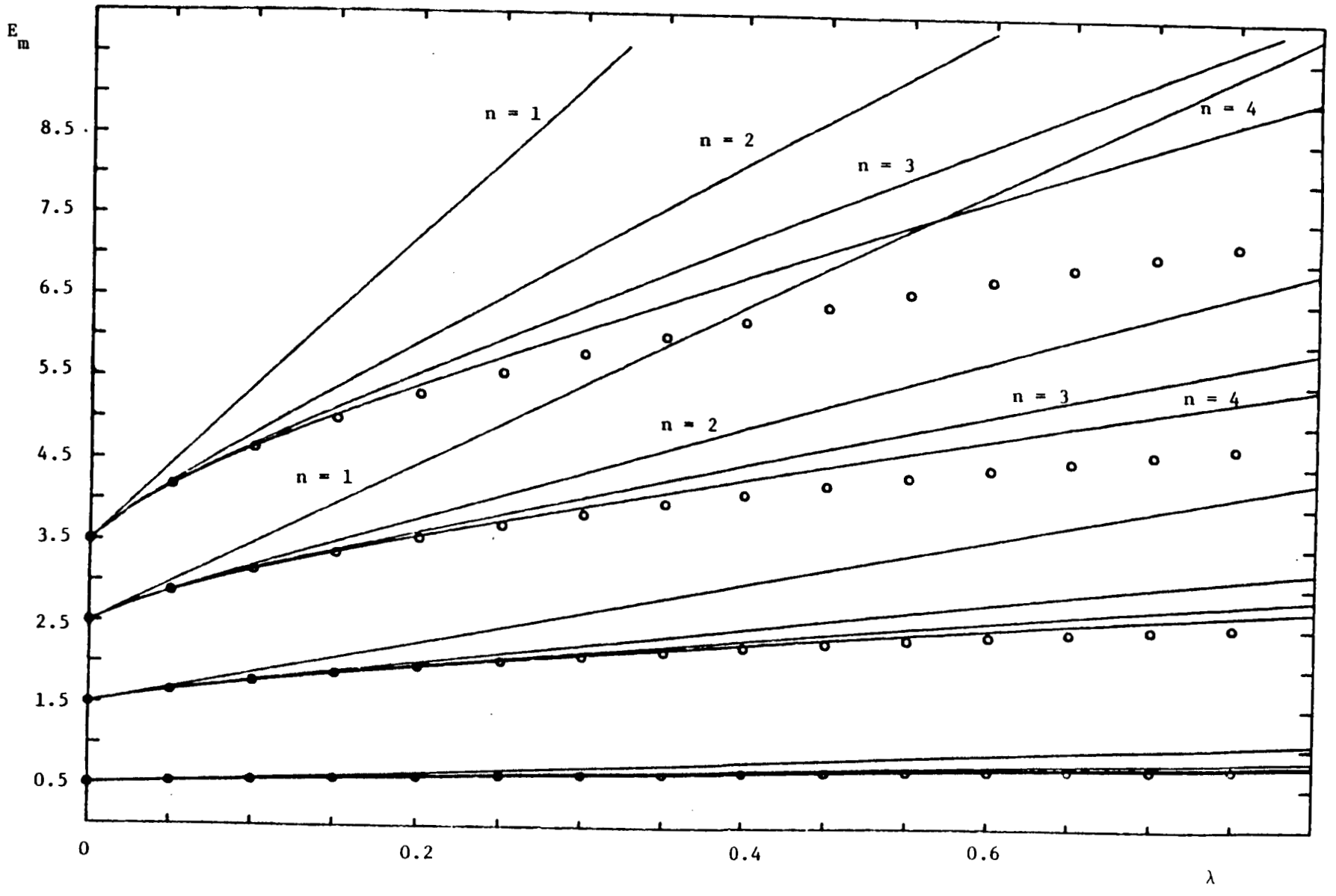


Figure 5.

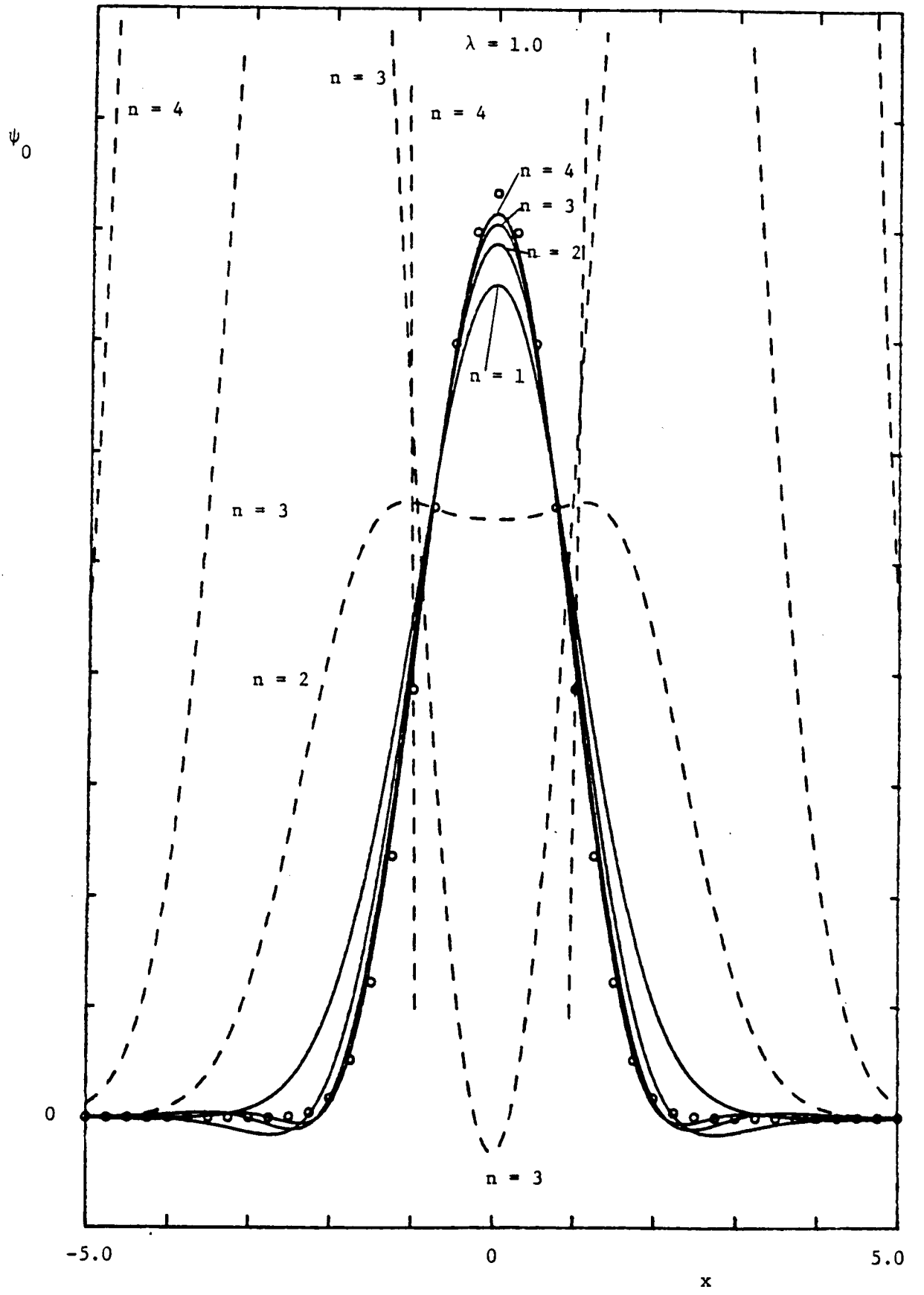


Figure 6.

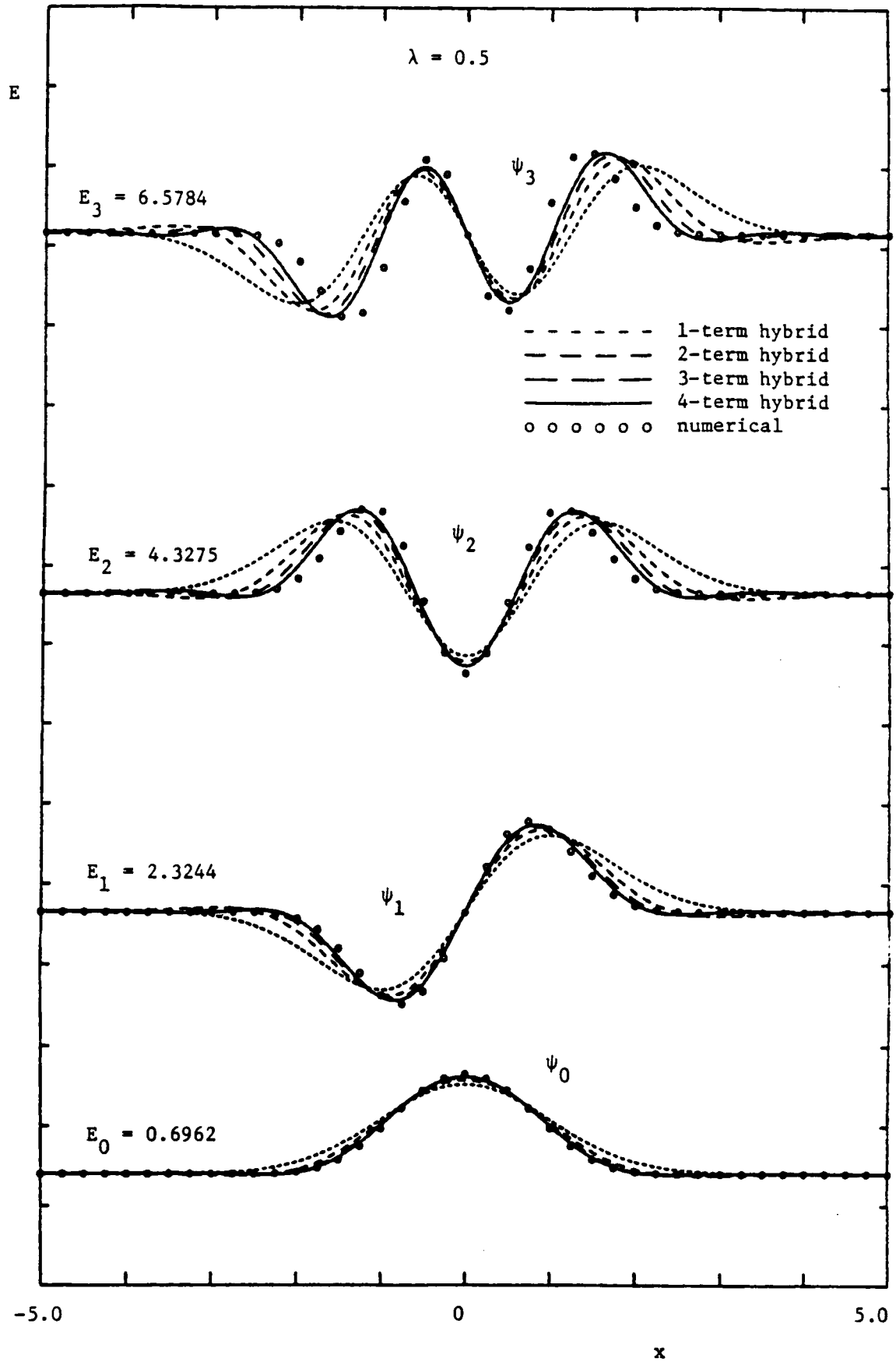

λ = 0.5
E
E3 = 6.5784
ψ3
1-term hybrid
2-term hybrid
3-term hybrid
4-term hybrid
numerical
E2 = 4.3275
ψ2
E1 = 2.3244
ψ1
ψ0
E0 = 0.6962
-5.0
0
5.0
x

Figure 7.

NASA

Report Documentation Page

1. Report No.	2. Government Accession No.	3. Recipient's Catalog No.
NASA CR-181750 ICASE Report No. 88-65		

4. Title and Subtitle

INVESTIGATING A HYBRID PERTURBATION-GALERKIN TECHNIQUE USING COMPUTER ALGEBRA

5. Report Date

November 1988

6. Performing Organization Code

7. Author(s)

Carl M. Andersen and James F. Geer

8. Performing Organization Report No.

88-65

10. Work Unit No.

505-90-21-01

9. Performing Organization Name and Address

Institute for Computer Applications in Science and Engineering
Mail Stop 132C, NASA Langley Research Center
Hampton, VA 23665-5225

11. Contract or Grant No.

NAS1-18107, NAS1-18605

13. Type of Report and Period Covered

Contractor Report

12. Sponsoring Agency Name and Address

National Aeronautics and Space Administration
Langley Research Center
Hampton, VA 23665-5225

14. Sponsoring Agency Code

15. Supplementary Notes

Langley Technical Monitor:
Richard W. Barnwell

Final Report

Submitted to the Proc. of Computer Algebraic Integration and the Solution of Differential Equations

16. Abstract

A two-step hybrid perturbation-Galerkin method is presented for the solution of a variety of differential equations type problems which involve a scalar parameter. The resulting (approximate) solution has the form of a sum where each term consists of the product of two functions. The first function 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. The resulting hybrid method 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 particular, the results can be useful well beyond the radius of convergence associated with the perturbation expansion. The hybrid method 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 method apparently converges for an infinite range of the parameter λ. The results obtained from the hybrid method are compared with approximate solutions obtained by other methods, and the applicability of the hybrid method to broader problem areas is discussed.

17. Key Words (Suggested by Author(s))

perturbation method, Galerkin technique, quantum theory, Schrödinger equation, computer algebra

18. Distribution Statement

59 - Mathematical and Computer Sciences (General)
70 - Physics (General)
Unclassified - unlimited

19. Security Classif. (of this report)	20. Security Classif. (of this page)	21. No. of pages	22. Price
Unclassified	Unclassified	26	A03