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A higher-order finite-difference approximation with Richardson's extrapolation to the energy eigenvalues of the quartic, sextic and octic anharmonic oscillators

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Abstract

In this paper, we present highly accurate numerical results for the lowest four energy eigenvalues of the quartic, sextic and octic anharmonic oscillators over a wide range of the anharmonicity parameter λ . Also, we provide illustrative graphs describing the dependence of the eigenvalues on λ . Our computation is carried out by using higher-order finite-difference approximation, involving the nine-and-ten-point differentiation formulas. In addition, we apply Richardson's extrapolation method in our calculation for the purpose of achieving a maximum numerical precision. The main advantage of utilizing the finite-difference approach lies in its simplicity and capability to transform the time-independent Schrödinger equation into an eigenvalue matrix equation. This allows the use of numerical matrix algebra for obtaining several eigenvalues and eigenvectors simultaneously without consuming much of the computer time. The method is illustrated in a simple pedagogical way through which the close relation between differential and algebraic eigenvalue problems are clearly seen. The findings of our computations via MATLAB are tested on a number of accurate results derived by different methods.

Keywords: higher-order finite-difference approximation, Richardson's extrapolation, anharmonic oscillators

1. Introduction

The exact eigenvalues and eigenfunctions of the time-independent Schrödinger equation can be obtained analytically in closed form only for a handful of potentials, and in most cases one has to resort to either numerical analysis or approximation techniques such as perturbation theory, variational methods or Wentzel–Kramers–Brillouin approximation [1]. Outside the range of applicability of the approximation methods, which are restricted by limiting conditions, numerical computation is a feasible and strategic alternative. The finite-difference method (FDM) [2] is an efficient and practical computational algorithm for solving differential equations numerically, especially when applied to the two-point boundary-value problems in ordinary differential equations. This method converts the one dimensional time-independent Schrödinger equation into a system of linear algebraic equations for the unknown values of the eigenfunctions at evenly spaced mesh points. This system of linear equations can be easily expressed in the form of an eigenvalue matrix equation which can be solved by diagonalization for both the eigenvalues and eigenvectors simultaneously, using any familiar software package such as MATLAB, MAPLE or MATHEMATICA.

In this article, we focus our attention on a high-precision numerical eigenvalue determination of the quantum anharmonic oscillators that are not yet exactly solvable, namely those defined by the dimensionless Hamiltonians:

$$\hat{H}^{(m)}(\lambda) = -\frac{d^2}{dx^2} + x^2 + \lambda x^{2m}, \quad (1)$$

where $m = 2, 3, 4$ corresponds to the quartic, sextic and octic anharmonic oscillators, respectively, and $\lambda \geq 0$. This problem is of considerable interest from both physical and mathematical points of view. It is considered as the most popular theoretical laboratory for examining the validity of various approximation techniques [3], and has above all some important applications in molecular physics [4] and quantum field theory [5, 6]. Several authors have worked on the calculation of the energy spectra of the anharmonic oscillators using many different methods [3, 6–11]. However, a discussion of these methods is beyond the scope of the present paper.

The usual Rayleigh–Schrödinger perturbation theory gives a divergent series [6] for the energy spectra of such oscillators for any value of the coupling constant λ . Therefore, resummation methods such as Padé approximation [7] and Borel’s technique [8] were introduced to extract the energy spectra from the divergent Rayleigh–Schrödinger perturbative expansions. However, the accuracy of the Padé and Borel summation procedures of the perturbatively divergent series decreases for large values of λ , and requires the knowledge of a large number of the expansion coefficients. Thus, the need arises to consider a relatively simple, time-saving and more effective alternative method which can produce the energy spectra with high accuracy.

Biswas *et al* [9] used the Hill determinant method to calculate non-perturbatively some of the lowest energy eigenvalues of the quartic, sextic and octic anharmonic oscillators for various λ in the range $0 < \lambda \leq 100$. Their results for moderately large values of λ and/or for energy levels with quantum numbers $n > 0$, especially for the sextic and octic anharmonicity, suffer from severe round-off errors [10] even with the use of double precision arithmetic. Banerjee [10, 11], on the other hand, modified the Hill determinant method by introducing a (λ, n) –dependent scaling parameter α to the set of basis functions in the series expansion of the trial wave function postulated by Biswas *et al* [9] as a solution to the anharmonic-oscillator problem. This allowed, for a given amount of computational labour, much greater accuracy to all energy eigenvalues [11] in a very wide range of λ .

Our computation is based mainly on the FDM and Richardson's extrapolation [2]. We begin by discretizing the Schrödinger equation on a mesh of points that are equally spaced by a small distance h in a finite interval $|x| \leq L$. Then, we employ the so-called nine-point central difference formula [12] for the second-order derivative in the Schrödinger equation at all mesh points except the first three interior neighbours to the boundary points $x = \pm L$, where we apply therein partly one-sided ten-point difference formulas. Here, the truncation errors of all the aforementioned difference formulas are consistent in being proportional to h^8 , and L is chosen appropriately to render the values of the eigenfunctions outside the interval $(-L, L)$ considerably close to zero. After the discretization and algebraic manipulation, we obtain an eigenvalue matrix equation which we solve numerically in MATLAB [13, 14] for both the energy eigenvalues and eigenvectors.

The special case $\lambda = 0$ is analytically solvable for infinite L as it corresponds to the simple harmonic oscillator (SHO). Hence, it is useful for testing our numerical calculations and estimating the values of L that are suitable cutoffs for mimicking the oscillator problem in an unbounded domain. So, by considering the case $\lambda = 0$ for various values of L we found that our results for any small h converge accurately to the exact analytical solutions of the unbounded SHO as L approaches small values in the range $5 \leq L \leq 8$.

Barakat and Rosner [15] studied the pure quartic oscillator bounded by infinitely high potentials at $x = \pm L/2$, using the power series method. They showed that by gradually increasing L the first lowest eigenvalues of the bounded oscillator converge rapidly to the values of their counterpart in the unbounded domain. This result was confirmed and extended by Chaudhuri and Mukherjee [16] to include the potentials λx^{2m} and $\mu x^2 + \lambda x^4$ that are confined to $|x| \leq L$ for real values of μ and positive values of λ , where m is a positive integer. In this respect, we show that the energy eigenvalues of the Hamiltonians $\hat{H}^{(m)}(\lambda)$, defined on the bounded region $|x| \leq L$, converge very rapidly to the values of their counterparts in the unbounded domain for all $\lambda \geq 0$ as L approaches a small number such as 8.

One way of increasing the order of accuracy of the FDM results is by using Richardson's extrapolation. It is an excellent method to use for improving accuracy and convergence of the eigenvalues obtained from FDM, provided that their error term is expressible as a polynomial or power series in h . Our chief goal is to investigate directly the effectiveness of Richardson's extrapolation in reducing the error and increasing the accuracy of the energy eigenvalues of the quartic, sextic and octic anharmonic oscillators over a wide range of λ . To the best of our knowledge, there are not many research works on using Richardson's extrapolation for enhancing the eigenvalue approximations in quantum mechanics.

The accuracy of our results for various values of λ is checked by the scaled Hill determinant method [11], and tested on a number of highly accurate results available from different methods. Our results for the eigenvalues are confirmed to be precise and accurate to eleven decimal places. Furthermore, the dependence of the energy eigenvalues of the anharmonic oscillators on the coupling parameter λ is provided graphically by the higher-order FDM. Although the methodological content of this paper has been focused on the time-independent Schrödinger equation for anharmonic oscillators, it can also be applied to similar two-point boundary value problems in ordinary differential equations.

This paper is organized in six sections including the introduction. In section 2, the method of undetermined coefficients for deriving the finite difference formulas for derivatives of any order is fully described. In section 3, we present the discretization of the one-dimensional Schrödinger equation on a grid of equispaced points, and show how it is reformulated in a matrix form that can be solved numerically by the so-called implicitly restarted Arnoldi (IRA) method [17] with the use of MATLAB. In section 4, we describe the

method of Richardson's extrapolation for boosting the accuracy of the energy eigenvalues computed by the IRA method through the finite difference approach. Finally, we devote sections 5 and 6 to our results, discussion and conclusion.

2. Finite difference formulas for numerical differentiation

In this section, we give a short overview of the method of undetermined coefficients [18] which is a very practical and intuitive approach for deriving the finite difference formulas for numerical differentiation. In this approach, we approximate a derivative of order s of a function $f(x)$ at a reference point x by a linear combination of the function's values at a finite set of equally spaced mesh points:

$$h^s f^{(s)}(x) + O(h^{s+p}) = \sum_{n=n_1}^{n_2} C_n^{(s)} f(x + nh), \quad C_n^{(s)} = C_n^{(s)}(n_1, n_2), \quad (2)$$

where h is the distance between the adjacent mesh points, called the step size, $C_n^{(s)}$ denotes the expansion coefficients to be determined for every choice of (n_1, n_2) , and p is a positive integer denoting the order of the truncation error $O(h^p)$ for $f^{(s)}(x)$. Since the differentiation formula (2) depends on $(n_2 - n_1 + 1)$ distinct mesh points, it is usually called an $(n_2 - n_1 + 1)$ -point formula for approximating $f^{(s)}(x)$. Now, if we expand $f(x + nh)$ in (2), for $n \neq 0$, by Taylor's theorem as:

$$f(x + nh) = \sum_{k=0}^{s+p-1} \frac{n^k h^k}{k!} f^{(k)}(x) + \frac{n^{s+p}}{(s+p)!} h^{s+p} f^{(s+p)}(\xi_n), \quad (3)$$

we obtain:

$$\begin{aligned} h^s f^{(s)}(x) + O(h^{s+p}) &= \sum_{k=0}^{s+p-1} \left(\sum_{n=n_1}^{n_2} n^k C_n^{(s)} \right) \frac{h^k}{k!} f^{(k)}(x) \\ &\quad + \frac{h^{s+p}}{(s+p)!} \sum_{n=n_1}^{n_2} n^{s+p} C_n^{(s)} f^{(s+p)}(\xi_n), \end{aligned} \quad (4)$$

where ξ_n lies between the mesh points x and $x + n h$. This suggests that

$$f^{(s)}(x) = \frac{1}{h^s} \left(\sum_{n=n_1}^{n_2} C_n^{(s)} \right) f(x) + \frac{1}{h^s} \sum_{k=1}^{s+p-1} \left(\sum_{n=n_1}^{n_2} n^k C_n^{(s)} \right) \frac{h^k}{k!} f^{(k)}(x), \quad (5)$$

and

$$O(h^p) = \frac{h^p}{(s+p)!} \sum_{n=n_1}^{n_2} n^{s+p} C_n^{(s)} f^{(s+p)}(\xi_n). \quad (6)$$

For this to be true, the coefficients $C_n^{(s)}$ must satisfy the following constraint:

$$\sum_{n=n_1}^{n_2} C_n^{(s)} = 0, \quad \sum_{n=n_1}^{n_2} n^k C_n^{(s)} = s! \delta_{s,k}, \quad (7)$$

where $\delta_{s,k}$ is the Kronecker delta and $k = 1, 2, \dots, s + p - 1$. This condition yields a set of $s + p$ linear equations in $(n_2 - n_1 + 1)$ unknowns, namely all the coefficients $C_n^{(s)}$. To have a unique solution to (7), we simply restrict the number of unknowns to $s + p$, i.e.

$s + p = n_2 - n_1 + 1$. The coefficients of the standard forward and backward difference formulas for approximating $f^{(s)}(x)$ can be obtained from (7) by letting $(n_1, n_2) = (0, s + p - 1)$ and $(n_1, n_2) = (-s - p + 1, 0)$ respectively. Moreover, the coefficients of the familiar central difference formulas [12] can be determined from (7) by taking $(n_1, n_2) = (-N, N)$ and $k = 1, 2, \dots, 2N$ with the restriction that $N = \lfloor (s + p - 1)/2 \rfloor$ and p is even, where $\lfloor z \rfloor$ denotes the greatest integer less than or equal to the real number z .

Since our computation involves the use of the nine-point central difference formula for the second order derivative $f''(x)$ with the truncation error $O(h^8)$, we will illustrate the derivation of this formula via (7). By taking $(n_1, n_2) = (-4, 4)$ and $k = 1, 2, \dots, 8$ for the case $(s, p) = (2, 8)$, it follows from (7) that the unknown coefficients $C_n^{(2)}$ for the central difference formula satisfy the matrix equation:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -4 & -3 & -2 & -1 & 0 & 1 & 2 & 3 & 4 \\ 16 & 9 & 4 & 1 & 0 & 1 & 4 & 9 & 16 \\ -64 & -27 & -8 & -1 & 0 & 1 & 8 & 27 & 64 \\ 256 & 81 & 16 & 1 & 0 & 1 & 16 & 81 & 256 \\ -1024 & -243 & -32 & -1 & 0 & 1 & 32 & 243 & 1024 \\ 4096 & 729 & 64 & 1 & 0 & 1 & 64 & 729 & 4096 \\ -16384 & -2187 & -128 & -1 & 0 & 1 & 128 & 2187 & 16384 \\ 65536 & 6561 & 256 & 1 & 0 & 1 & 256 & 6561 & 65536 \end{pmatrix} \begin{pmatrix} C_{-4} \\ C_{-3} \\ C_{-2} \\ C_{-1} \\ C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 2 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad (8)$$

where C_n denotes $C_n^{(2)}$ for $n = 0, \pm 1, \pm 2, \pm 3, \pm 4$. This equation has the unique solution $(C_0, C_{\pm 1}, C_{\pm 2}, C_{\pm 3}, C_{\pm 4}) = (-14350, 8064, -1008, 128, -9)/5040$. This result complies with the general coefficient formula for $N = 4$:

$$C_0^{(2)} = -2 \sum_{n=1}^N C_n^{(2)}, \quad C_n^{(2)} = (-1)^{n+1} \frac{2!}{n^2} \frac{(N!)^2}{(N-n)!(N+n)!}, \quad (9)$$

where $n = \pm 1, \pm 2, \dots, \pm N$, provided by Khan and Ohba [19] for the central difference approximation to $f''(x)$, and also agrees with the result reported by Fornberg [12].

Using the values of these coefficients in (2), we obtain the value of the second-order derivative at a reference point $x = x_0$ in the form:

$$f''(x_0) = \frac{1}{5040 h^2} (-9f_{-4} + 128f_{-3} - 1008f_{-2} + 8064f_{-1} - 14350f_0 + 8064f_1 - 1008f_2 + 128f_3 - 9f_4) - O(h^8), \quad (10)$$

where $f_n = f(x_0 + nh)$ and $O(h^8)$ stands for the truncation error whose upper bound can be estimated from (6) by solely assuming the continuity of $f^{(10)}(x)$, yielding:

$$|O(h^8)| \leq \frac{1957}{992250} M h^8, \quad (11)$$

where M is a positive number such that $|f^{(10)}(\xi)| \leq M$ for any ξ between $x_0 - 4h$ and $x_0 + 4h$. The accuracy of the central difference approximation in (10) is of the order eight, meaning the truncation error is proportional to h^8 . When the function value $f(x)$ at either side of the reference point x_0 is not available, then we use a one-sided difference approximation with the same order of accuracy as explained in the next section. We have checked and

confirmed the outcomes of (7) for the coefficients of the finite difference formulas of $f^{(s)}(x)$ by comparing them with those given by Li [20] for various s and p .

3. The matrix formulation of the Schrödinger equation

In this section we will present how to apply the numerical method of higher-order finite-difference approximation to the solution of the one-dimensional eigenvalue problem of the quantum anharmonic oscillators, defined by the Schrödinger equation in the dimensionless form [3, 9]:

$$-\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x) = E\psi(x), \quad (12)$$

where $\psi(x)$ is the eigenfunction corresponding to the eigenvalue E , and $V(x)$ is the confining anharmonic potential:

$$V(x) = x^2 + \lambda x^{2m}, \quad (13)$$

with λ being a positive coupling parameter. Here, $m = 2, 3, 4$ corresponds to the quartic, sextic and octic anharmonic oscillator, respectively. Since $V(x)$ approaches infinity as $x \rightarrow \pm\infty$, the eigenfunctions $\psi(x)$ converge appreciably to zero for considerably large $|x|$. This allows us to restrict the infinite domain of $\psi(x)$ to a sufficiently large but finite interval $[-L, L]$ beyond which $\psi(x)$ is negligibly small, and hence one has the so-called two-point boundary value problem. This paves the way for the numerical computation [21] of the differential equation (12) under the Dirichlet boundary conditions $\psi(\pm L) = 0$.

The numerical procedure for solving (12) by the FDM [2, 21] starts by partitioning the interval $[-L, L]$ over which the solution is sought into N equal subintervals $[x_i, x_{i+1}]$ of length h each, called the step size, where $h = 2L/N$ and x_i stands for the mesh points:

$$x_i = x_0 + ih, \quad i = 0, 1, 2, \dots, N, \quad (14)$$

with x_0 and x_N being the endpoints $-L$ and L , respectively. At the interior mesh points x_i for $i = 1, 2, \dots, N-1$, the second-order derivative $\psi''(x)$ in (12) is replaced by the finite-difference formulas defined in (2) to obtain a system of $N-1$ simultaneous linear equations in $N-1$ unknowns, namely $\psi_i = \psi(x_i)$. This system of equations is then reformulated as a matrix eigenvalue equation which can be solved algebraically for both the eigenvalues and eigenvectors simultaneously, using any familiar software package such as MATLAB, MAPLE or MATHEMATICA.

In our computation, we will consider the use of the central difference formula (10) with truncation error of order $O(h^8)$ for approximating the second-order derivative in (12) at the interior mesh points x_i for $i = 4, 5, \dots, N-4$. Since the central difference formula (10) for $\psi''(x)$ at a given reference point $x = x_i$ involves the values of $\psi(x)$ at the mesh points $x_{i\pm k} = x_i \pm kh$ for $k = 0, 1, 2, 3, 4$, it cannot be applied at the first three neighbouring mesh points to $\pm L$, namely x_i for $i = 1, 2, 3, N-3, N-2, N-1$. Hence, to overcome this difficulty we apply noncentral difference formulas at these points but with truncation errors of the same order as the central difference formula, i.e. $O(h^8)$. So, at the first three interior points on the left, namely x_1, x_2 and x_3 , we adopt for $\psi''(x)$ the approximations that follow from (2) and (7) by taking $(n_1, n_2) = (-1, 8), (-2, 7), (-3, 6)$ and $(s, p) = (2, 8)$:

Table 1. The coefficients of the ten-point finite difference formulas for the second-order derivatives $\psi''(x_i)$ and $\psi''(x_{N-i})$ given by (16) and (18), respectively, for $i = 1, 2, 3$.

i	$a_0^{(i)}$	$a_1^{(i)}$	$a_2^{(i)}$	$a_3^{(i)}$	$a_4^{(i)}$	$a_5^{(i)}$	$a_6^{(i)}$	$a_7^{(i)}$	$a_8^{(i)}$	$a_9^{(i)}$
1	3044	2135	-28 944	57 288	-65 128	51 786	-28 560	10 424	-2268	223
2	-223	5274	-7900	-2184	10 458	-8932	4956	-1800	389	-38
3	38	-603	6984	-12 460	5796	882	-952	396	-90	9

$$\psi''(x_i) = \frac{1}{h^2} \sum_{n=-i}^{9-i} C_n^{(2)} \psi(x_i + nh) - \frac{h^8}{10!} \sum_{n=-i}^{9-i} n^{10} C_n^{(2)} \psi^{(10)}(\xi_n), \quad i = 1, 2, 3, \quad (15)$$

which can be rewritten as:

$$\psi''(x_i) = \frac{1}{5040h^2} \sum_{k=0}^9 a_k^{(i)} \psi_k - \tau_i, \quad a_k^{(i)} = 5040 C_{k-i}^{(2)}, \quad i = 1, 2, 3, \quad (16)$$

where the coefficients $a_k^{(i)}$ are obtained from (7) with the help of MAPLE and their values are listed in table 1, and $\psi_k = \psi(x_0 + kh)$ with $x_0 = -L$. Here, τ_i is the truncation error for ψ'' at x_i :

$$\tau_i = \frac{h^8}{10!} \frac{1}{5040} \sum_{k=0}^9 (k-i)^{10} a_k^{(i)} \psi^{(10)}(\xi_{k-i}) = O(h^8), \quad i = 1, 2, 3, \quad (17)$$

where ξ_{k-i} is a point between x_i and x_k with $i \neq k$. We refer to the differentiation formulas (16) as the ten-point difference formulas in mostly the forward direction.

Similarly, at the first three interior points on the right, namely x_{N-1} , x_{N-2} and x_{N-3} , the second-order derivative ψ'' is approximated by the ten-point difference formulas in mostly the backward direction:

$$\psi''(x_{N-i}) = \frac{1}{5040h^2} \sum_{k=0}^9 a_k^{(i)} \psi_{N-k} - \tau_{N-i}, \quad i = 1, 2, 3, \quad (18)$$

which are obtained from (2) and (7) for the cases $(n_1, n_2) = (-8, 1), (-7, 2), (-6, 3)$, respectively, with $(s, p) = (2, 8)$, where $\psi_{N-k} = \psi(x_N - kh)$ with $x_N = L$, and τ_{N-i} is given by:

$$\tau_{N-i} = \frac{h^8}{10!} \frac{1}{5040} \sum_{k=0}^9 (i-k)^{10} a_k^{(i)} \psi^{(10)}(\xi_{i-k}) = O(h^8). \quad (19)$$

Here, ξ_{i-k} lies between x_{N-i} and x_{N-k} , where $i \neq k$, and $a_k^{(i)}$ are listed in table 1. For consistency, the ten-point difference formulas (16) and (18) are maintained at the same order of accuracy as the nine-point central difference formula (10).

If we replace the second-order derivative in the discretized version of (12):

$$-\psi''(x_i) + V(x_i)\psi(x_i) = E\psi(x_i), \quad i = 1, 2, \dots, N-1, \quad (20)$$

by the ten-point difference formulas (16) and (18) for the mesh points $\{x_1, x_2, x_3\}$ and $\{x_{N-3}, x_{N-2}, x_{N-1}\}$, respectively, and the central difference formula (10) for the rest of the mesh points, and then multiply both sides of (20) by $-5040h^2$, we obtain after dropping all truncation errors a system of $N-1$ linear equations:

$$\begin{aligned}
& \sum_{k=0}^9 a_k^{(i)} \psi_k + U(x_i) \psi_i = \varepsilon \psi_i, \quad i = 1, 2, 3, \\
& \sum_{k=-4}^4 b_k \psi_{i+k} + U(x_i) \psi_i = \varepsilon \psi_i, \quad i = 4, 5, \dots, N-4, \\
& \sum_{k=0}^9 a_k^{(N-i)} \psi_{N-k} + U(x_i) \psi_i = \varepsilon \psi_i, \quad i = N-3, N-2, N-1,
\end{aligned} \tag{21}$$

where $b_0 = -14350$, $b_{\pm 1} = 8064$, $b_{\pm 2} = -1008$, $b_{\pm 3} = 128$, $b_{\pm 4} = -9$, $\varepsilon = -5040h^2E$ and $U(x_i) = -5040h^2V(x_i)$.

Now we can rewrite these equations as a single matrix eigenvalue equation:

$$\mathbf{A}\Psi = \varepsilon\Psi, \tag{22}$$

where Ψ is the column vector of the unknowns $\Psi = (\psi_1, \psi_2, \dots, \psi_{N-1})^T$, and \mathbf{A} is the $(N-1) \times (N-1)$ coefficient matrix which can be partitioned into the form:

$$\mathbf{A} = (\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3)^T. \tag{23}$$

Here the superscript T denotes the transpose of a row vector, and

$$\mathbf{A}_1 = \begin{pmatrix} d_1 & a_2^{(1)} & a_3^{(1)} & a_4^{(1)} & a_5^{(1)} & a_6^{(1)} & a_7^{(1)} & a_8^{(1)} & a_9^{(1)} & 0 & \dots & 0 \\ a_1^{(2)} & d_2 & a_3^{(2)} & a_4^{(2)} & a_5^{(2)} & a_6^{(2)} & a_7^{(2)} & a_8^{(2)} & a_9^{(2)} & 0 & \dots & 0 \\ a_1^{(3)} & a_2^{(3)} & d_3 & a_4^{(3)} & a_5^{(3)} & a_6^{(3)} & a_7^{(3)} & a_8^{(3)} & a_9^{(3)} & 0 & \dots & 0 \end{pmatrix}, \tag{24}$$

$$\mathbf{A}_2 = \begin{pmatrix} b_3 & b_2 & b_1 & d_4 & b_1 & b_2 & b_3 & b_4 & 0 & 0 & 0 & \dots & 0 \\ b_4 & b_3 & b_2 & b_1 & d_5 & b_1 & b_2 & b_3 & b_4 & 0 & 0 & \dots & 0 \\ 0 & b_4 & b_3 & b_2 & b_1 & d_6 & b_1 & b_2 & b_3 & b_4 & 0 & \dots & 0 \\ 0 & 0 & b_4 & b_3 & b_2 & b_1 & d_7 & b_1 & b_2 & b_3 & b_4 & \ddots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \dots & 0 & b_4 & b_3 & b_2 & b_1 & d_{N-5} & b_1 & b_2 & b_3 & b_4 \\ 0 & 0 & \dots & 0 & 0 & b_4 & b_3 & b_2 & b_1 & d_{N-4} & b_1 & b_2 & b_3 \end{pmatrix}, \tag{25}$$

$$\mathbf{A}_3 = \begin{pmatrix} 0 & \dots & 0 & a_9^{(3)} & a_8^{(3)} & a_7^{(3)} & a_6^{(3)} & a_5^{(3)} & a_4^{(3)} & d_{N-3} & a_2^{(3)} & a_1^{(3)} \\ 0 & \dots & 0 & a_9^{(2)} & a_8^{(2)} & a_7^{(2)} & a_6^{(2)} & a_5^{(2)} & a_4^{(2)} & a_3^{(2)} & d_{N-2} & a_1^{(2)} \\ 0 & \dots & 0 & a_9^{(1)} & a_8^{(1)} & a_7^{(1)} & a_6^{(1)} & a_5^{(1)} & a_4^{(1)} & a_3^{(1)} & a_2^{(1)} & d_{N-1} \end{pmatrix}, \tag{26}$$

where d_i stands for the diagonal elements of \mathbf{A} , and it is given by

$$d_i = \begin{cases} a_i^{(i)} + U(x_i), & i = 1, 2, 3, \\ b_0 + U(x_i), & i = 4, 5, \dots, N-4, \\ a_{N-i}^{(N-i)} + U(x_i), & i = N-3, N-2, N-1. \end{cases} \tag{27}$$

For a sufficiently large N , \mathbf{A} is a sparse matrix because only $(9N-11)$ of the $(N-1)^2$ elements of the matrix are nonzero. It must be emphasized that the Dirichlet boundary conditions $\psi(\pm L) = 0$ have been employed in the matrix equation (22) by taking $\psi_0 = \psi_N = 0$. Now, the calculation of the energy spectra and eigenfunctions is reduced to the computation of the eigenvalues and eigenvectors of \mathbf{A} .

To normalize the eigenfunctions $\psi(x)$ in (12), we exploit the linearity of the Schrödinger equation to write the normalized solutions $\bar{\psi}(x)$ in terms of $\psi(x)$ as $\bar{\psi}(x) = c\psi(x)$, where c is a constant, and then impose the normalization condition:

$$\langle \bar{\psi} | \bar{\psi} \rangle = \int_{-L}^L |c\psi(x)|^2 dx = 1, \quad (28)$$

to find the value of c . By using the standard definition of the Riemann sum [22] for definite integrals, we can rewrite (28) in the discretized form:

$$\lim_{h \rightarrow 0} |c|^2 \sum_{i=1}^{N-1} |\psi(x_i)|^2 h = \lim_{h \rightarrow 0} (|c|^2 \|\Psi\|^2 h) = 1, \quad (29)$$

where $\|\Psi\|$ denotes the norm of the vector $\Psi = (\psi_1, \psi_2, \dots, \psi_{N-1})^T$; i.e.

$$\|\Psi\| = \sqrt{\Psi^\dagger \Psi} = \left(\sum_{i=1}^{N-1} |\psi(x_i)|^2 \right)^{1/2} \quad (30)$$

where Ψ^\dagger is the complex conjugate transpose of Ψ . Now, to satisfy (29) we may take for c the positive value $c = 1/\|\Psi\| \sqrt{h}$. This allows us to express the discretized normalized solutions of (12) or (20) as:

$$\bar{\Psi} = \frac{\Psi}{\|\Psi\| \sqrt{h}} = \frac{1}{\|\Psi\| \sqrt{h}} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \end{pmatrix}. \quad (31)$$

Having formulated the problem in terms of an algebraic matrix eigenvalue equation (22), the solution method reduces to the diagonalization of the real square matrix \mathbf{A} in (23) by any numerical algorithm. In principle, the eigenvalues of \mathbf{A} can be obtained by solving the characteristic equation:

$$\det(\mathbf{A} - \varepsilon \mathbf{I}) = 0, \quad (32)$$

which is a polynomial equation of degree $N - 1$ in ε , where \mathbf{I} is the unit matrix. By determining the roots of the characteristic polynomial, i.e. the eigenvalues $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_{N-1}$, we can then find the corresponding eigenvectors by solving the matrix equation $\mathbf{A}\Psi_n = \varepsilon_n \Psi_n$ for $n = 1, 2, \dots, N - 1$. However, this method is not practical at all for large matrices. We therefore turn our attention to an alternative method that is more efficient and practical in the computation of eigenvalues and eigenvectors of a large matrix.

Since only the first few smallest eigenvalues are generally sought, including the ground state energy, it is more appropriate to use the so-called IRA method [17]. This is an efficient numerical method to apply on a large sparse matrix for computing a few of its smallest or largest eigenvalues together with the corresponding eigenvectors. The IRA algorithm was first proposed by Sorensen [17], and implemented later in a software package known formally as ARPACK [23], which stands for Arnoldi Package. The ARPACK software has been used on a wide range of applications. MATLAB has adopted ARPACK for the computation of a selected subset of the eigenvalues and eigenvectors of a large (sparse) matrix. The MATLAB function `eigs` is a command that uses this package [24]. In other words, the ARPACK is accessible in MATLAB via the `eigs` command. In our present computation, we employ the sparse matrix eigensolver in MATLAB, namely `eigs`, to solve (22) for the lowest four eigenvalues and eigenvectors. The eigenvectors computed via this MATLAB command are all normalized to 1, satisfying herein the equation $\|\Psi\| = 1$.

4. Richardson's extrapolation of the energy spectrum

In this section, we show how Richardson's extrapolation [2] can be used to improve the accuracy of the energy eigenvalues obtained from FDM. We begin first by investigating the error term of the energy eigenvalue approximation, showing how it is directly related to the truncation error of $\psi''(x)$.

The truncation error of the second-order derivative $\psi''(x_i)$ in the discretized Schrödinger equation (20) has a direct impact on the accuracy of the energy eigenvalues. This can be clearly seen through the energy expression:

$$E = - \sum_{i=1}^{N-1} \psi(x_i) \psi''(x_i) + \sum_{i=1}^{N-1} V(x_i) \psi^2(x_i), \quad (33)$$

which can be derived from (20) by first multiplying both sides of the equation by $\psi(x_i)$, then summing over i , from 1 to $N - 1$, and finally using the normalization condition:

$$\|\Psi\|^2 = \sum_{i=1}^{N-1} \psi^2(x_i) = 1. \quad (34)$$

Now, by substituting the finite-difference formulas (10), (16) and (18) for $\psi''(x_i)$ in (33) at the relevant mesh points x_i , we realize that the error in E in terms of the step size h is proportional to h^8 , just the same as the truncation error of $\psi''(x_i)$. Hence, we may express the energy eigenvalues given by (33) in the form:

$$E = E_0(h) + O(h^8), \quad (35)$$

where $E_0(h)$ is the approximated value for E , defined in (21) in terms of ε as:

$$E_0(h) = -\frac{1}{5040h^2} \varepsilon. \quad (36)$$

Here, the h -dependent eigenvalue ε is to be computed numerically from the sparse matrix \mathbf{A} in (22) by the IRA method using the `eigs` command in MATLAB.

To obtain much higher accuracy for E , one naturally considers a remarkable reduction in the step size h . But this, however, results in a loss of indispensable significant figures due to the increase of the round-off errors in the floating point arithmetic operations. The Richardson's extrapolation method can be used instead to improve the accuracy to a higher degree, using a sufficient value of h that is not too small to avoid the risk of large round-off errors.

To illustrate the method of Richardson's extrapolation, we begin by expressing the error term in (35) in even powers of h to have E in the form:

$$E = E_0(h) + K_0 h^8 + O(h^{10}), \quad (37)$$

where K_0 is a constant independent of h . This follows from the fact that the approximation of $\psi''(x_i)$ in (33) by the central difference scheme at all mesh points, with the exception of the points next to $\pm L$, can be expressed via Tylor expansion as a series in even powers of h [25, 26]. Our objective now is to eliminate the dominant error term $K_0 h^8$ so that the leading error in E becomes proportional to h^{10} instead. This can be achieved by first replacing h in (37) by $h/2$ to obtain a new approximation $E_0(h/2)$ to E that satisfies:

$$E = E_0\left(\frac{h}{2}\right) + K_0 \frac{h^8}{256} + O\left(\frac{h^{10}}{1024}\right). \quad (38)$$

Then, multiplying (38) by 256 and subtracting it from (37) allows us to eliminate $K_0 h^8$ and rewrite E in a more accurate expression as:

$$E = \bar{E}_1(h) + O(h^{10}), \quad (39)$$

where $\bar{E}_1(h)$ assumes the form:

$$\bar{E}_1(h) = \frac{256 E_0(h/2) - E_0(h)}{255}, \quad (40)$$

which represents the first-order Richardson's extrapolation to E .

Again, if we express the error term in (39) in even powers of h as $K_1 h^{10} + O(h^{12})$, with K_1 as a constant, we can repeat the same process as used above in eliminating the dominant error term to generate the second-order Richardson's extrapolation to E , namely:

$$E = \bar{E}_2(h) + O(h^{12}), \quad (41)$$

with $\bar{E}_2(h)$ given by:

$$\bar{E}_2(h) = \frac{1024 \bar{E}_1(h/2) - \bar{E}_1(h)}{1023}, \quad (42)$$

or equivalently:

$$\bar{E}_2(h) = E_0(h/4) + \frac{1279 E_0(h/4) - 1280 E_0(h/2) + E_0(h)}{260865}. \quad (43)$$

The important point here is that we have reduced the dominant error $K_0 h^8$ in the original approximation (37) for E and increased the order of accuracy to h^{12} , which is the main idea behind Richardson's extrapolation technique.

The extrapolation process above can be repeated over and over again to obtain presumably more accurate approximations for E . However, since the extrapolation to higher-order corrections involves more computations and successive reductions in the step size h that practically increase the round-off errors, we consider only the second-order extrapolation formula (43) in our calculations with h being fixed at 0.04. This choice allows us to obtain results for E that are exact to eleven digits after the decimal point for a wide range of the coupling parameter λ .

In what follows, we use the notation $E_n^{(2m)}(\lambda)$ and $\bar{E}_n^{(2m)}(\lambda)$ to denote, for fixed h and L , the energy eigenvalues $E_0(h)$ in (36) and its extrapolated counterpart $\bar{E}_2(h)$ in (43), respectively. Here, $m = 2, 3, 4$ corresponds to the quartic, sextic and octic anharmonic oscillator, respectively, and n stands for the quantum numbers $\{0, 1, 2, \dots\}$, signifying the energy levels.

5. Results and discussion

To test the accuracy of our approach, we apply it first to the well-known problem of quantum mechanics, namely the SHO. Then, we turn our attention to the familiar problem of the quartic, sextic and octic anharmonic oscillators, evaluating and reporting their energy eigenvalues to eleven decimal places for different values of the coupling constant λ , as well as displaying their behaviours as a function of λ .

The knowledge of the exact normalized eigenfunctions and eigenvalues of the Schrödinger equation (12) for the special case $\lambda = 0$, which corresponds to the SHO, namely:

$$\phi_n(x) = \frac{1}{\sqrt{n!2^n\pi^{1/2}}} \left(x - \frac{d}{dx}\right)^n \exp\left(-\frac{1}{2}x^2\right), \quad (44)$$

$$\kappa_n = 2n + 1, \quad n = 0, 1, 2, \dots, \quad (45)$$

provides an excellent preliminary check up on our numerical computations. Moreover, it helps us decide on the proper value of L which defines the interval $[-L, L]$ beyond which $\phi_n(x)$ is negligibly small. Direct evaluation of (44) for $|x| \geq 8$ shows that $|\phi_n(x)| < 5.5 \times 10^{-12}$ for $n = 0, 1, 2, 3$. Hence, the choice of $L = 8$ is adequate enough to simulate the unbounded oscillator problem ($L \rightarrow \infty$) for the first four energy eigenstates.

On the left side of figure 1, we show the graphs of the lowest four normalized eigenvectors Ψ_n of the SHO, computed numerically from the matrix eigenvalue equation (22) by the IRA algorithm in MATLAB using a step size of length $h = 0.04$ and $L = 8$. On the right side of the figure, we show the absolute errors in our numerical finite-difference solutions, defined by the difference [27] $\triangle \Psi_n = \Psi_n - \phi_n$. As shown in figure 1, the maximum values of the absolute errors in the normalized eigenvectors are less than 10^{-12} and 10^{-11} for $n = \{0, 1\}$ and $\{2, 3\}$ respectively. Moreover, we present in tables 2 and 3 the numerical results for the lowest four energy eigenvalues obtained from the FDM, namely $E_n^{(2m)}(\lambda)$, and the corresponding Richardson's extrapolation $\bar{E}_n^{(2m)}(\lambda)$ for the SHO ($\lambda = 0$), using various values of L and h . By comparison, we find that the extrapolated energy eigenvalues converge more rapidly to the exact results κ_n of the SHO than those obtained solely from the FDM. However, we can see that the accuracy of both $E_n^{(2m)}$ and $\bar{E}_n^{(2m)}$ for a fixed L grows remarkably by gradually decreasing h .

Henceforth, all further calculations will be performed with L being fixed at 8 and $h = 0.04$. This choice is found to be suitable enough to yield very accurate eigenvalues for the three types of the anharmonic oscillators ($m = 2, 3, 4$) over a very wide range of λ . For example, the extrapolated eigenvalues $\bar{E}_n^{(2m)}(\lambda)$ for $n = 0, 1, 2, 3$ and $m = 2, 3, 4$ are shown to be correct and precise to eleven digits after the decimal point for all values $\lambda \in [0, 1000]$. In addition, we wish to point out that by this choice of L and h , the square matrix \mathbf{A} in (23), which makes the basis of our numerical analysis for the determination of the eigenvalues, becomes of the order 399×399 with only 3589 nonzero elements distributed on the main diagonal and the diagonals around it. The size of this sparse matrix turns out to be sufficient enough for the computation of the lowest four eigenvalues and eigenvectors simultaneously in fractions of a second with minimum round-off errors by using MATLAB on a PC with the third generation Intel core i7-3770 (3.40 GHz) processor, and 64 bit operating system.

Tables 4, 5 and 6 summarizes our results for the lowest four energy eigenvalues of the quartic, sextic and octic anharmonic oscillators that are computed for various values of the coupling constant λ by the FDM, denoted by $E_n^{(2m)}(\lambda)$, and the corresponding Richardson's extrapolation, denoted by $\bar{E}_n^{(2m)}(\lambda)$, using the step size $h = 0.04$ and $L = 8$. The computed eigenvalues in these tables are all rounded off to eleven figures after the decimal point.

In order to confirm the accuracy of our results for the three types of the anharmonic oscillators, we appeal to the non-perturbative technique of Banerjee [10, 11], known as the scaled Hill determinant method, for comparisons. This method that produces very accurate energy eigenvalues for the anharmonic oscillators stems from the assumption that the eigenfunctions for $m = 2, 3, 4$ are all expressible in terms of the expansion:

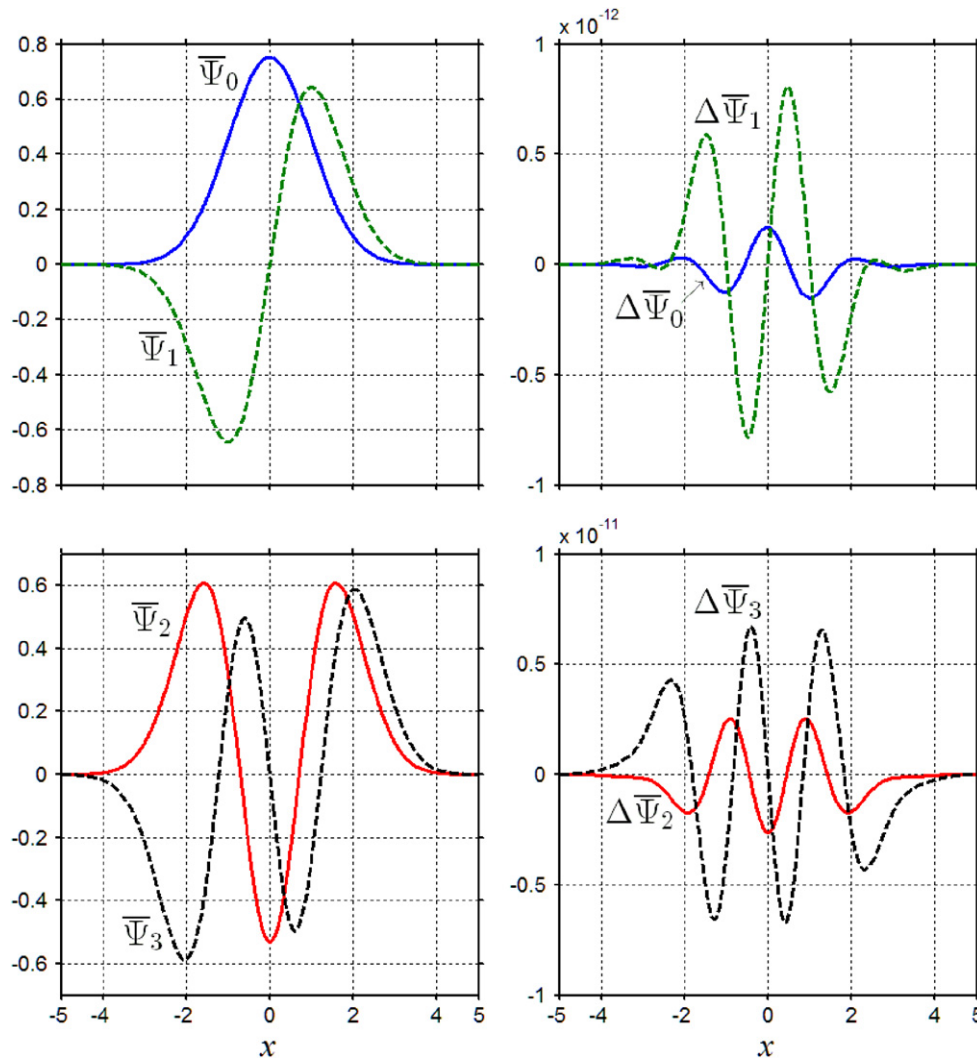


Figure 1. The linear harmonic oscillator eigenfunctions of the ground-state energy level (blue solid line), first excited energy level (green dashed line), second excited energy level (red solid line) and third excited energy level (black dashed line), all depicted on the left side. On the right are shown the corresponding absolute errors of the eigenfunctions.

$$\psi_n^{(2m)}(x, \lambda) = e^{-\alpha_m x^2} \sum_{k=0}^{\infty} a_k^{(2m)} x^k, \quad n = 0, 1, 2, \dots, \quad (46)$$

where $a_k^{(2m)}$ stands for the expansion coefficients, and α_m is a scaling parameter depending on both n and λ in such a way that can be approximated empirically as:

$$\alpha_m(n, \lambda) = \frac{1}{2} + B_m n^{(m-1)/(m+1)} \lambda^{1/(m+1)}. \quad (47)$$

Here, $B_2 \in (1.2, 1.4)$, $B_3 \in (1.5, 2)$ and $B_4 \in (2.5, 3)$. The substitution of (46) into the Schrödinger equation (12) yields a 4-term recurrence relation in the expansion coefficients:

Table 2. Comparison of the energy eigenvalues $E_n^{(2m)}$, obtained numerically from the FDM, to their corresponding Richardson's extrapolated counterparts $\bar{E}_n^{(2m)}$ for various values of L and h , given that $\lambda = 0$ and $n = 0, 1$.

L	h	$E_0^{(2m)}(\lambda = 0)$	$\bar{E}_0^{(2m)}(\lambda = 0)$	$E_1^{(2m)}(\lambda = 0)$	$\bar{E}_1^{(2m)}(\lambda = 0)$
5	0.40	0.999 994 959 062	1.000 000 000 324	2.999 946 845 090	3.000 000 014 908
	0.25	0.999 999 869 992	1.000 000 000 235	2.999 998 655 731	3.000 000 010 988
	0.20	0.999 999 978 267	1.000 000 000 213	2.999 999 797 028	3.000 000 010 035
	0.10	1.000 000 000 236	1.000 000 000 179	3.000 000 014 047	3.000 000 008 501
6	0.40	0.999 994 949 010	1.000 000 000 000	2.999 946 365 867	2.999 999 999 995
	0.25	0.999 999 867 620	1.000 000 000 000	2.999 998 564 189	3.000 000 000 000
	0.20	0.999 999 977 165	1.000 000 000 000	2.999 999 751 078	3.000 000 000 000
	0.10	0.999 999 999 907	1.000 000 000 000	2.999 999 998 984	3.000 000 000 000
7	0.40	0.999 994 948 965	1.000 000 000 000	2.999 946 365 047	2.999 999 999 995
	0.25	0.999 999 867 620	1.000 000 000 000	2.999 998 564 180	3.000 000 000 000
	0.20	0.999 999 977 165	1.000 000 000 000	2.999 999 751 075	3.000 000 000 000
	0.10	0.999 999 999 907	1.000 000 000 000	2.999 999 998 984	3.000 000 000 000
8	0.40	0.999 994 948 965	1.000 000 000 000	2.999 946 365 047	2.999 999 999 995
	0.25	0.999 999 867 620	1.000 000 000 000	2.999 998 564 180	3.000 000 000 000
	0.20	0.999 999 977 165	1.000 000 000 000	2.999 999 751 075	3.000 000 000 000
	0.10	0.999 999 999 907	1.000 000 000 000	2.999 999 998 984	3.000 000 000 000

Table 3. Comparison of the energy eigenvalues $E_n^{(2m)}$, obtained numerically from the FDM, to their corresponding Richardson's extrapolated counterparts $\bar{E}_n^{(2m)}$ for various values of L and h , given that $\lambda = 0$ and $n = 2, 3$.

L	h	$E_2^{(2m)}(\lambda = 0)$	$\bar{E}_2^{(2m)}(\lambda = 0)$	$E_3^{(2m)}(\lambda = 0)$	$\bar{E}_3^{(2m)}(\lambda = 0)$
5	0.40	4.999 728 962 871	5.000 000 326 942	6.999 151 287 370	7.000 004 547 776
	0.25	4.999 993 865 894	5.000 000 245 886	6.999 991 041 977	7.000 003 492 537
	0.20	4.999 999 548 899	5.000 000 225 803	7.000 006 445 985	7.000 003 225 772
	0.10	5.000 000 324 178	5.000 000 193 099	7.000 004 560 299	7.000 002 785 662
6	0.40	4.999 714 491 023	4.999 999 999 978	6.998 967 116 764	7.000 000 000 174
	0.25	4.999 992 167 426	5.000 000 000 012	6.999 970 885 278	7.000 000 000 258
	0.20	4.999 998 634 139	5.000 000 000 011	6.999 994 889 970	7.000 000 000 232
	0.10	4.999 999 994 398	5.000 000 000 009	6.999 999 979 162	7.000 000 000 191
7	0.40	4.999 714 493 354	4.999 999 999 960	6.998 967 236 625	6.999 999 999 799
	0.25	4.999 992 167 196	5.000 000 000 000	6.999 970 881 292	6.999 999 999 999
	0.20	4.999 998 634 057	5.000 000 000 000	6.999 994 888 389	7.000 000 000 000
	0.10	4.999 999 994 380	5.000 000 000 000	6.999 999 978 781	7.000 000 000 000
8	0.40	4.999 714 493 341	4.999 999 999 960	6.998 967 236 427	6.999 999 999 799
	0.25	4.999 992 167 196	5.000 000 000 000	6.999 970 881 292	6.999 999 999 999
	0.20	4.999 998 634 057	5.000 000 000 000	6.999 994 888 389	7.000 000 000 000
	0.10	4.999 999 994 380	5.000 000 000 000	6.999 999 978 781	7.000 000 000 000

Table 4. The lowest four energy eigenvalues of the quartic anharmonic oscillator, computed for several values of λ by the FDM, denoted by $E_n^{(4)}(\lambda)$, and the corresponding Richardson's extrapolation, denoted by $\bar{E}_n^{(4)}(\lambda)$, using the step size $h = 0.04$ and $L = 8$. The underlined digits indicate the inaccuracy of the computed result of $E_n^{(4)}(\lambda)$ as compared to its counterpart $\bar{E}_n^{(4)}(\lambda)$.

λ	n	$E_n^{(4)}(\lambda)$	$\bar{E}_n^{(4)}(\lambda)$	λ	n	$E_n^{(4)}(\lambda)$	$\bar{E}_n^{(4)}(\lambda)$
0.1	0	1.065 285 509 54	1.065 285 509 54	100	0	4.999 417 543 <u>95</u>	4.999 417 545 14
	1	3.306 872 013 15	3.306 872 013 15		1	17.830 192 <u>700 13</u>	17.830 192 715 95
	2	5.747 959 268 <u>82</u>	5.747 959 268 83		2	34.873 984 <u>121 92</u>	34.873 984 261 99
	3	8.352 677 825 <u>74</u>	8.352 677 825 79		3	54.385 290 <u>757 57</u>	54.385 291 571 60
0.2	0	1.118 292 654 37	1.118 292 654 37	200	0	6.262 768 326 <u>13</u>	6.262 768 329 88
	1	3.539 005 287 90	3.539 005 287 90		1	22.374 508 <u>452 35</u>	22.374 508 502 02
	2	6.277 248 616 <u>98</u>	6.277 248 617 00		2	43.813 795 <u>859 15</u>	43.813 796 298 02
	3	9.257 765 617 <u>70</u>	9.257 765 617 78		3	68.365 045 <u>675 91</u>	68.365 048 224 36
0.3	0	1.164 047 157 35	1.164 047 157 35	300	0	7.152 377 <u>567 96</u>	7.152 377 575 29
	1	3.732 484 274 27	3.732 484 274 27		1	25.570 753 <u>988 62</u>	25.570 754 085 65
	2	6.705 719 378 <u>29</u>	6.705 719 378 31		2	50.096 678 <u>125 03</u>	50.096 678 981 55
	3	9.975 312 795 <u>00</u>	9.975 312 795 12		3	78.186 322 <u>220 44</u>	78.186 327 190 79
0.6	0	1.275 983 566 34	1.275 983 566 34	400	0	7.861 862 <u>666 47</u>	7.861 862 678 28
	1	4.189 283 971 <u>38</u>	4.189 283 971 39		1	28.118 453 <u>387 74</u>	28.118 453 543 77
	2	7.689 565 294 <u>94</u>	7.689 565 295 00		2	55.102 867 <u>956 89</u>	55.102 869 333 50
	3	11.593 147 265 <u>15</u>	11.593 147 265 43		3	86.010 533 <u>624 60</u>	86.010 541 608 52
1	0	1.392 351 641 53	1.392 351 641 53	500	0	8.461 642 <u>612 00</u>	8.461 642 629 08
	1	4.648 812 704 <u>20</u>	4.648 812 704 21		1	30.271 505 <u>030 30</u>	30.271 505 255 84
	2	8.655 049 957 <u>66</u>	8.655 049 957 76		2	59.332 642 <u>740 48</u>	59.332 644 729 53
	3	13.156 803 897 <u>49</u>	13.156 803 898 05		3	92.620 584 <u>924 13</u>	92.620 596 454 25

Table 4. (Continued.)

λ	n	$E_n^{(4)}(\lambda)$	$\bar{E}_n^{(4)}(\lambda)$	λ	n	$E_n^{(4)}(\lambda)$	$\bar{E}_n^{(4)}(\lambda)$
2	0	1.607 541 302 47	1.607 541 302 47	600	0	8.986 305 <u>354 06</u>	8.986 305 377 15
	1	5.475 784 <u>535 99</u>	5.475 784 536 02		1	32.154 484 <u>725 76</u>	32.154 485 030 51
	2	10.358 583 <u>375 01</u>	10.358 583 375 28		2	63.031 <u>288 679 45</u>	63.031 291 366 16
	3	15.884 807 <u>967 24</u>	15.884 807 968 78		3	98.400 <u>203 941 14</u>	98.400 219 508 49
4	0	1.903 136 945 <u>45</u>	1.903 136 945 46	700	0	9.455 720 <u>922 25</u>	9.455 720 952 03
	1	6.585 735 642 <u>78</u>	6.585 735 642 87		1	33.838 <u>909 645 34</u>	33.838 910 038 37
	2	12.607 761 134 <u>12</u>	12.607 761 134 89		2	66.339 <u>555 993 09</u>	66.339 559 457 25
	3	19.454 646 <u>340 94</u>	19.454 646 345 41		3	103.569 <u>533 241 77</u>	103.569 553 305 76
10	0	2.449 174 072 <u>09</u>	2.449 174 072 12	800	0	9.882 484 <u>285 46</u>	9.882 484 322 60
	1	8.599 003 454 <u>44</u>	8.599 003 454 81		1	35.370 090 <u>099 76</u>	35.370 090 589 67
	2	16.635 921 <u>489 13</u>	16.635 921 492 41		2	69.346 <u>588 800 65</u>	69.346 593 117 75
	3	25.806 276 <u>196 01</u>	25.806 276 215 06		3	108.267 <u>978 290 04</u>	108.268 003 284 85
30	0	3.410 168 532 <u>48</u>	3.410 168 532 64	900	0	10.275 141 <u>378 72</u>	10.275 141 423 83
	1	12.094 733 866 <u>83</u>	12.094 733 869 01		1	36.778 <u>758 657 68</u>	36.778 759 252 66
	2	23.565 623 <u>112 37</u>	23.565 623 131 81		2	72.112 <u>835 668 92</u>	72.112 840 910 88
	3	36.682 747 <u>123 02</u>	36.682 747 236 01		3	112.590 <u>058 646 12</u>	112.590 088 985 19
50	0	4.003 992 767 <u>90</u>	4.003 992 768 28	1000	0	10.639 788 <u>657 64</u>	10.639 788 711 33
	1	14.241 706 990 <u>86</u>	14.241 706 995 91		1	38.086 832 <u>751 48</u>	38.086 833 459 38
	2	27.803 962 <u>818 96</u>	27.803 962 863 80		2	74.681 <u>397 964 42</u>	74.681 404 200 16
	3	43.321 550 <u>213 71</u>	43.321 550 474 41		3	116.603 <u>162 858 08</u>	116.603 198 937 29

Table 5. The lowest four energy eigenvalues of the sextic anharmonic oscillator, computed for several values of λ by the FDM, denoted by $E_n^{(6)}(\lambda)$, and the corresponding Richardson's extrapolation, denoted by $\bar{E}_n^{(6)}(\lambda)$, using the step size $h = 0.04$ and $L = 8$. The underlined digits indicate the inaccuracy of the computed result of $E_n^{(6)}(\lambda)$ as compared to its counterpart $\bar{E}_n^{(6)}(\lambda)$.

λ	n	$E_n^{(6)}(\lambda)$	$\bar{E}_n^{(6)}(\lambda)$	λ	n	$E_n^{(6)}(\lambda)$	$\bar{E}_n^{(6)}(\lambda)$
0.1	0	1.109 087 078 47	1.109 087 078 47	100	0	3.716 974 727 <u>61</u>	3.716 974 729 21
	1	3.596 036 921 22	3.596 036 921 22		1	13.946 206 <u>608 35</u>	13.946 206 622 90
	2	6.644 391 708 <u>63</u>	6.644 391 708 66		2	28.977 293 <u>708 95</u>	28.977 293 817 63
	3	10.237 873 721 <u>25</u>	10.237 873 721 42		3	47.564 983 <u>922 49</u>	47.564 984 581 58
0.2	0	1.173 889 345 13	1.173 889 345 13	200	0	4.386 681 632 29	4.386 681 636 11
	1	3.900 835 570 <u>25</u>	3.900 835 570 26		1	16.506 275 <u>672 78</u>	16.506 275 707 33
	2	7.381 647 216 <u>29</u>	7.381 647 216 35		2	34.360 578 <u>708 99</u>	34.360 578 965 83
	3	11.547 467 607 <u>01</u>	11.547 467 607 38		3	56.447 707 <u>756 87</u>	56.447 709 311 34
0.3	0	1.223 687 130 82	1.223 687 130 82	300	0	4.838 160 521 <u>91</u>	4.838 160 528 27
	1	4.125 479 108 <u>00</u>	4.125 479 108 01		1	18.228 580 <u>086 56</u>	18.228 580 143 82
	2	7.909 026 083 <u>17</u>	7.909 026 083 26		2	37.977 461 <u>366 02</u>	37.977 461 790 65
	3	12.467 755 953 <u>66</u>	12.467 755 954 24		3	62.412 319 <u>857 05</u>	62.412 322 424 62
0.6	0	1.332 895 943 37	1.332 895 943 37	400	0	5.188 358 845 <u>31</u>	5.188 358 854 44
	1	4.600 549 616 <u>09</u>	4.600 549 616 11		1	19.563 129 <u>920 04</u>	19.563 130 001 91
	2	8.996 752 679 <u>76</u>	8.996 752 679 96		2	40.778 190 <u>021 81</u>	40.778 190 628 34
	3	14.339 566 236 <u>32</u>	14.339 566 237 61		3	67.029 667 <u>071 84</u>	67.029 670 737 13
1	0	1.435 624 619 00	1.435 624 619 00	500	0	5.478 379 078 <u>40</u>	5.478 379 090 46
	1	5.033 395 937 <u>68</u>	5.033 395 937 72		1	20.667 621 <u>291 06</u>	20.667 621 399 09
	2	9.966 621 999 <u>35</u>	9.966 621 999 72		2	43.095 134 <u>751 43</u>	43.095 135 551 10
	3	15.989 440 785 <u>49</u>	15.989 440 787 83		3	70.848 733 <u>154 78</u>	70.848 737 985 14

Table 5. (Continued.)

λ	n	$E_n^{(6)}(\lambda)$	$\bar{E}_n^{(6)}(\lambda)$	λ	n	$E_n^{(6)}(\lambda)$	$\bar{E}_n^{(6)}(\lambda)$
2	0	1.609 931 952 <u>01</u>	1.609 931 952 02	600	0	5.727 956 280 <u>61</u>	5.727 956 295 75
	1	5.749 347 752 <u>51</u>	5.749 347 752 62		1	21.617 648 <u>053 75</u>	21.617 648 189 22
	2	11.543 934 571 <u>02</u>	11.543 934 571 88		2	45.087 457 <u>299 98</u>	45.087 458 302 20
	3	18.649 694 <u>585 64</u>	18.649 694 591 01		3	74.132 290 <u>037 55</u>	74.132 296 089 50
4	0	1.830 437 343 <u>73</u>	1.830 437 343 75	700	0	5.948 233 085 <u>79</u>	5.948 233 104 13
	1	6.635 112 629 <u>64</u>	6.635 112 629 90		1	22.455 844 <u>833 34</u>	22.455 844 997 35
	2	13.467 064 865 <u>64</u>	13.467 064 867 65		2	46.844 861 <u>978 52</u>	46.844 863 191 47
	3	21.870 071 <u>981 35</u>	21.870 071 993 82		3	77.028 392 <u>131 59</u>	77.028 399 454 10
10	0	2.205 723 269 <u>51</u>	2.205 723 269 60	800	0	6.146 173 <u>576 52</u>	6.146 173 598 17
	1	8.114 843 118 <u>02</u>	8.114 843 118 82		1	23.208 836 <u>630 33</u>	23.208 836 823 86
	2	16.641 218 <u>102 01</u>	16.641 218 108 25		2	48.423 <u>339 815 52</u>	48.423 341 246 43
	3	27.155 085 <u>566 28</u>	27.155 085 604 63		3	79.629 430 <u>329 26</u>	79.629 438 965 73
30	0	2.809 381 130 <u>69</u>	2.809 381 131 03	900	0	6.326 447 <u>026 60</u>	6.326 447 051 67
	1	10.458 825 012 <u>39</u>	10.458 825 015 61		1	23.894 463 <u>789 73</u>	23.894 464 013 68
	2	21.619 812 <u>727 86</u>	21.619 812 752 24		2	49.860 393 <u>212 02</u>	49.860 394 867 41
	3	35.406 964 <u>445 53</u>	35.406 964 594 18		3	81.997 276 <u>614 51</u>	81.997 286 604 04
50	0	3.159 021 200 <u>40</u>	3.159 021 201 06	1000	0	6.492 350 103 <u>75</u>	6.492 350 132 33
	1	11.805 779 996 <u>65</u>	11.805 780 002 76		1	24.525 315 <u>831 75</u>	24.525 316 086 92
	2	24.466 245 <u>872 19</u>	24.466 245 918 16		2	51.182 478 <u>220 49</u>	51.182 480 106 31
	3	40.114 068 <u>356 91</u>	40.114 068 636 44		3	84.175 <u>572 397 35</u>	84.175 583 775 59

Table 6. The lowest four energy eigenvalues of the octic anharmonic oscillator, computed for several values of λ by the FDM, denoted by $E_n^{(8)}(\lambda)$, and the corresponding Richardson's extrapolation, denoted by $\bar{E}_n^{(8)}(\lambda)$, using the step size $h = 0.04$ and $L = 8$. The underlined digits indicate the inaccuracy of the computed result of $E_n^{(8)}(\lambda)$ as compared to its counterpart $\bar{E}_n^{(8)}(\lambda)$.

λ	n	$E_n^{(8)}(\lambda)$	$\bar{E}_n^{(8)}(\lambda)$	λ	n	$E_n^{(8)}(\lambda)$	$\bar{E}_n^{(8)}(\lambda)$
0.1	0	1.168 970 453 24	1.168 970 453 25	100	0	3.188 654 343 05	3.188 654 346 49
	1	3.939 721 361 03	3.939 721 361 04		1	12.195 021 909 82	12.195 021 933 63
	2	7.639 948 490 52	7.639 948 490 64		2	26.033 458 190 62	26.033 458 321 25
	3	12.281 167 731 55	12.281 167 732 28		3	43.902 112 648 06	43.902 113 333 20
0.2	0	1.241 027 905 05	1.241 027 905 06	200	0	3.632 500 775 56	3.632 500 782 50
	1	4.275 477 259 90	4.275 477 259 94		1	13.939 391 733 32	13.939 391 781 00
	2	8.453 030 681 16	8.453 030 681 40		2	29.821 379 420 19	29.821 379 680 64
	3	13.737 162 631 49	13.737 162 632 92		3	50.336 225 214 69	50.336 226 577 37
0.3	0	1.292 356 010 11	1.292 356 010 12	300	0	3.923 907 253 28	3.923 907 263 72
	1	4.507 017 156 72	4.507 017 156 77		1	15.081 761 841 09	15.081 761 912 57
	2	9.001 872 388 02	9.001 872 388 39		2	32.298 148 451 86	32.298 148 841 52
	3	14.708 893 774 74	14.708 893 776 87		3	54.540 411 358 92	54.540 413 395 48
0.6	0	1.397 708 762 01	1.397 708 762 03	400	0	4.146 188 546 72	4.146 188 560 64
	1	4.969 310 385 17	4.969 310 385 29		1	15.951 984 683 93	15.951 984 779 14
	2	10.078 268 999 70	10.078 269 000 45		2	34.183 308 623 80	34.183 309 142 19
	3	16.597 433 359 74	16.597 433 363 96		3	57.739 243 389 57	57.739 246 097 40
1	0	1.491 019 895 64	1.491 019 895 66	500	0	4.328 012 362 84	4.328 012 380 25
	1	5.368 778 061 54	5.368 778 061 75		1	16.663 196 499 51	16.663 196 618 38
	2	10.993 737 334 25	10.993 737 335 50		2	35.723 166 977 13	35.723 167 623 87
	3	18.191 100 011 50	18.191 100 018 51		3	60.351 548 733 28	60.351 552 110 33

Table 6. (Continued.)

λ	n	$E_n^{(8)}(\lambda)$	$\bar{E}_n^{(8)}(\lambda)$	λ	n	$E_n^{(8)}(\lambda)$	$\bar{E}_n^{(8)}(\lambda)$
2	0	1.641 370 357 <u>08</u>	1.641 370 357 13	600	0	4.482 952 760 <u>63</u>	4.482 952 781 52
	1	5.999 607 358 <u>81</u>	5.999 607 359 24		1	17.268 869 <u>071 67</u>	17.268 869 214 14
	2	12.421 035 878 <u>86</u>	12.421 035 881 41		2	37.034 004 <u>084 88</u>	37.034 004 859 64
	3	20.660 642 <u>890 90</u>	20.660 642 904 88		3	62.574 958 <u>483 41</u>	62.574 962 527 98
4	0	1.822 179 869 <u>97</u>	1.822 179 870 09	700	0	4.618 593 154 <u>70</u>	4.618 593 179 06
	1	6.744 486 896 <u>57</u>	6.744 486 897 45		1	17.798 837 884 <u>55</u>	17.798 838 050 58
	2	14.086 998 <u>016 35</u>	14.086 998 021 51		2	38.180 650 <u>000 90</u>	38.180 650 903 41
	3	23.527 660 <u>703 61</u>	23.527 660 731 48		3	64.519 621 <u>516 44</u>	64.519 626 227 05
10	0	2.114 544 621 <u>62</u>	2.114 544 621 94	800	0	4.739 632 650 <u>55</u>	4.739 632 678 37
	1	7.929 683 080 <u>06</u>	7.929 683 082 35		1	18.271 573 <u>185 30</u>	18.271 573 374 84
	2	16.711 022 <u>368 98</u>	16.711 022 381 99		2	39.203 215 <u>505 83</u>	39.203 216 535 84
	3	28.022 750 <u>163 50</u>	28.022 750 232 93		3	66.253 670 <u>663 85</u>	66.253 676 039 21
30	0	2.558 941 387 <u>91</u>	2.558 941 388 92	900	0	4.849 199 <u>187 65</u>	4.849 199 218 93
	1	9.705 583 028 <u>47</u>	9.705 583 035 53		1	18.699 360 <u>410 48</u>	18.699 360 623 49
	2	20.607 759 434 <u>62</u>	20.607 759 473 85		2	40.128 367 <u>784 91</u>	40.128 368 942 19
	3	34.671 581 <u>394 57</u>	34.671 581 601 72		3	67.822 394 <u>306 11</u>	67.822 400 345 05
50	0	2.806 065 087 <u>62</u>	2.806 065 089 32	1000	0	4.949 487 405 <u>30</u>	4.949 487 440 03
	1	10.685 249 379 <u>22</u>	10.685 249 391 07		1	19.090 814 <u>030 58</u>	19.090 814 267 02
	2	22.746 620 097 <u>14</u>	22.746 620 162 54		2	40.974 798 <u>573 04</u>	40.974 799 857 39
	3	38.313 050 <u>091 20</u>	38.313 050 435 40		3	69.257 531 <u>131 62</u>	69.257 537 833 10

$$a_{k+2}^{(2m)} + d_{k,k} a_k^{(2m)} + d_{k,k-2} a_{k-2}^{(2m)} + d_{k,k-2m} a_{k-2m}^{(2m)} = 0, \quad (48)$$

where

$$d_{k,k} = -\frac{(4k\alpha_m + 2\alpha_m - E)}{(k+1)(k+2)}, \quad d_{k,k-2} = \frac{4\alpha_m^2 - 1}{(k+1)(k+2)},$$

$$d_{k,k-2m} = -\frac{(-1)^m \lambda}{(k+1)(k+2)}. \quad (49)$$

The even and odd parity solutions in (46) are subjected to the initial conditions $(a_0^{(2m)}, a_1^{(2m)}) = (1, 0)$ and $(a_0^{(2m)}, a_1^{(2m)}) = (0, 1)$ respectively. The recurrence relation (48) yields an infinite set of linear homogenous equations in the unknowns $a_k^{(2m)}$. Consistency of the resulting system of linear homogeneous equations is assured [11] by setting the infinite-dimensional determinant (Hill determinant) $\Delta(E, \lambda)$ of the corresponding $d_{i,j}$ coefficient matrix of the linear system equal to zero. The roots of $\Delta(E, \lambda) = 0$ give the required energy eigenvalues. Having defined $\Delta_{k+2}(E, \lambda)$ as the determinant obtained from $\Delta(E, \lambda)$ by omitting all rows and columns beyond the element $d_{k,k}$, Banerjee [11] derived a 4-term recursion relation similar to (48), connecting the sub-determinants Δ_{k+2} , Δ_k , Δ_{k-2m} as:

$$\Delta_{k+2} - d_{k,k} \Delta_k + d_{k,k-2} \Delta_{k-2} - d_{k,k-2m} \Delta_{k-2m} = 0. \quad (50)$$

Here, by definition, $\Delta_i = 0$ for any negative subscript value i , whereas Δ_0 and Δ_1 satisfy the conditions $(\Delta_0, \Delta_1) = (1, 0)$ and $(\Delta_0, \Delta_1) = (0, 1)$ for the even and odd parity solutions, respectively. The determinants $\Delta_{2k}(E, \lambda)$ and $\Delta_{2k+1}(E, \lambda)$ are polynomials in E of degree k . In the limit $k \rightarrow \infty$, $\Delta_k(E, \lambda)$ approaches $\Delta(E, \lambda)$. The zeroes of $\Delta_k(E, \lambda)$ were computed by Newton's method to a high degree of accuracy for some values of λ , and they were shown [11] to be stable for large k .

To double check our results and assure accuracy for a wider range of λ , we made use of Banerjee's formula (50) for calculating the eigenvalues by finding the roots of both $\Delta_{2k}(E, \lambda)$ and $\Delta_{2k+1}(E, \lambda)$ for $k = 500$, using the well-known symbolic computation language of MAPLE 17. The resulting eigenvalues in MAPLE turned out to be in full agreement with those obtained in MATLAB from Richardson's extrapolation formula (43) which are listed in tables 4, 5 and 6 for $\lambda \in [0.1, 1000]$. The exact agreement of the extrapolated eigenvalues with those obtained from the scaled Hill determinant method in the three cases of x^{2m} anharmonicity ($m = 2, 3, 4$) for a wide range of λ is a clear sign of the accuracy improvement of the finite-difference eigenvalue approximation by Richardson's extrapolation. Moreover, this suggests that the choice of taking $L = 8$ and $h = 0.04$ in our computations is very appropriate.

Detailed results obtained from different methods [3, 9, 26, 28, 29] have been reported for the energy eigenvalues of the quartic, sextic and octic anharmonic oscillators. Biswas *et al* [9] produced results of 14 decimal places of accuracy but only for the ground state energy of the quartic anharmonic oscillator in the range $\lambda \in [0.1, 100]$. On the other hand, their results for the sextic and octic anharmonic oscillators were much less accurate even for the ground state energies. Vinette and Čížek [28] achieved slightly better accuracy for the ground state energies of the quartic, sextic and octic anharmonic oscillators by using the so-called renormalized inner projection. By comparison, our extrapolated results for the quartic anharmonic oscillator in the ground state agree to the relevant digits with those of Biswas *et al* [9] as well as Vinette and Čížek [28]. However, our extrapolated results for the sextic and octic anharmonic oscillators are superior to theirs in terms of the number of decimal places of accuracy, and agree completely to the listed digits with the numerical results reported by

Witwit [26] for the ground state energy eigenvalues associated with $\lambda \in \{0.1, 1, 10, 50, 100, 500, 1000\}$.

Furthermore, Meißner and Steinborn [3] used an iterative method based on the generalized Bloch equation for computing the energy eigenvalues of the quartic, sextic and octic anharmonic oscillators, giving illustrative results to 9 decimal places for the ground and excited energy levels with $\lambda \in \{0.2, 2, 10, 100, 400, 2000\}$. The results provided for the relevant values of λ and energy levels are found to be very consistent with ours except for some values of the two lowest energy levels of the octic anharmonic oscillator which turned to be less accurate than ours in the last decimal digits. A further comparison with the 15 significant figures of Banerjee's results [11] for the relevantly available values of λ , namely $\lambda \in \{0.1, 1, 10, 100, 1000\}$, shows a full agreement with all the extrapolated results listed in tables 4, 5 and 6. This shows the power of combining the FDM with Richardson's extrapolation for computing numerically the energy eigenvalues of the anharmonic oscillators and similar systems in one dimension.

By investigating the results obtained from the FDM for the eigenvalues $E_n^{(2m)}(\lambda)$ in tables 4, 5 and 6, we note that their accuracy in comparison with the extrapolated results decreases gradually with increasing λ , where the inaccuracy of the results is indicated by the underlined digits. In figure 2, we have plotted for comparison the graphs of the lowest four energy eigenvalues $E_n^{(2m)}(\lambda)$ for the quartic ($m = 2$, black solid line), sextic ($m = 3$, red dashed line) and octic ($m = 4$, blue dotted line) anharmonic oscillators as a function of the coupling parameter λ over the range $0 \leq \lambda \leq 100$. It looks evident from the figure that the behaviour of the energy of the excited states for any fixed m is qualitatively similar to that of the ground state $E_0^{(2m)}(\lambda)$. Moreover, we observe from the graphs in figure 2 that for any fixed quantum number n the energy levels for the three oscillators split apart gradually from their common minimum at $\lambda = 0$ in such a way that leads eventually to $E_n^{(8)}(\lambda) < E_n^{(6)}(\lambda) < E_n^{(4)}(\lambda)$ by appreciably increasing λ .

In figure 3 we illustrate the graphs obtained from the FDM for the first four normalized eigenfunctions $\bar{\Psi}_n^{(2m)}(x, \lambda)$, $n = 0, 1, 2, 3$, of the quartic ($m = 2$, black solid line), sextic ($m = 3$, red dashed line) and octic ($m = 4$, blue dotted line) anharmonic oscillators, corresponding to $\lambda = 1$ (on the left side) and $\lambda = 10$ (on the right side). As shown in figure 3, the eigenfunctions of the three anharmonic oscillators ($m = 2, 3, 4$) are very similar in the qualitative structure (i.e. number of nodes, parity, functional form, etc) for the same quantum number n . This feature holds true for all values of λ . In addition, we illustrate in figure 3 the fact that the size of the spatial domain over which the eigenfunctions have appreciable magnitude decreases gradually with increasing λ . This is because the potentials $x^2 + \lambda x^{2m}$ of the anharmonic oscillators behave in the sense of confinement like a symmetric potential well with two quasi-impenetrable barriers at equal distances from the origin. As λ increases the distance between the two barriers decreases, and hence the relevant domain of the eigenfunctions shrinks.

6. Conclusion

We have shown that higher-order finite-difference eigenvalue approximations when combined with Richardson's extrapolation become capable of producing highly accurate results for the ground and excited energy eigenvalues of the quartic, sextic and octic anharmonic oscillators over a wide range of the coupling parameter λ . The extrapolated eigenvalues reported herein for the small, intermediate and large values of λ are all accurate and correct to eleven decimal

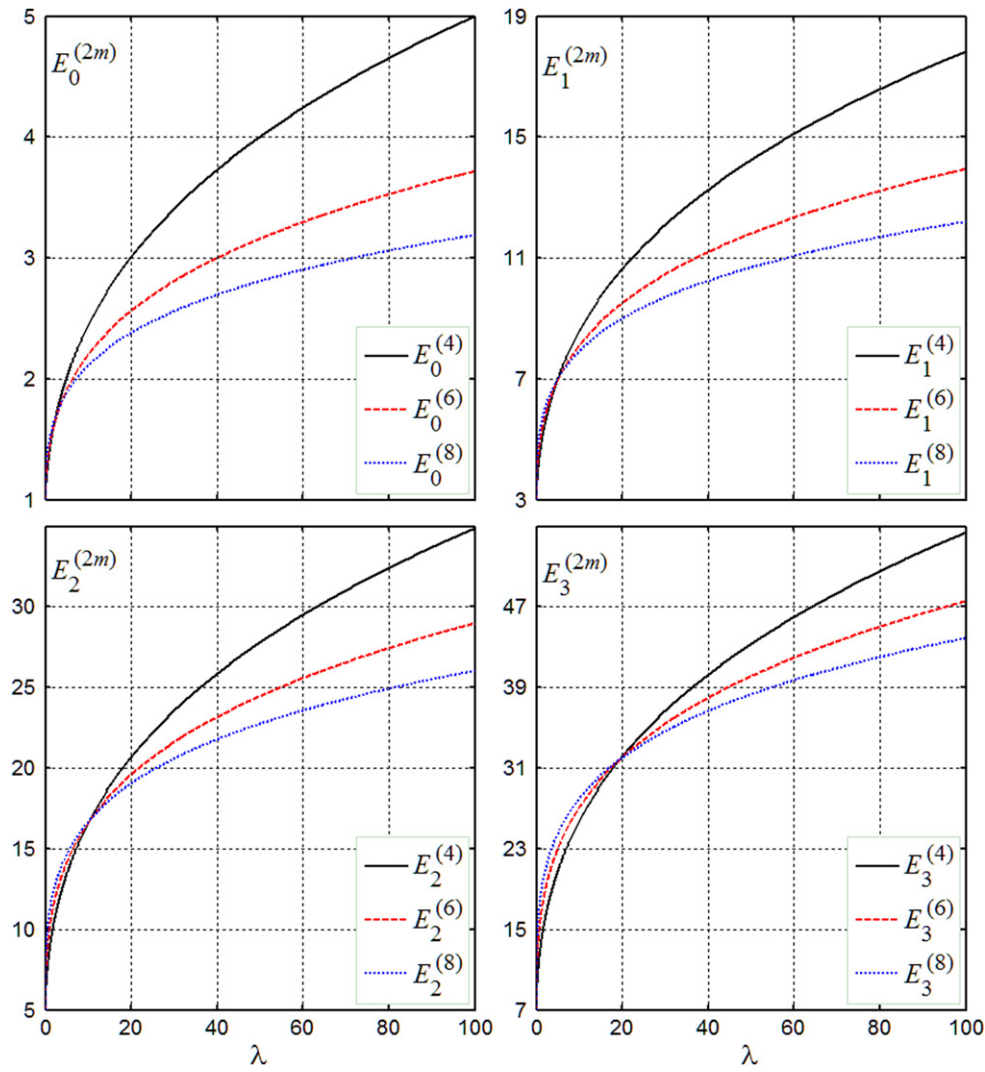


Figure 2. The ground-state and first three excited-state energy eigenvalues of the quartic (black solid line), sextic (red dashed line) and octic (blue dotted line) anharmonic oscillators as a function of the coupling parameter λ , computed by the finite difference method using the step size $h = 0.04$ and $L = 8$.

places. Our results were carefully checked by comparing them with those resulting from different reliable methods such as the scaled Hill determinant approach [11].

Since the exact calculation of the energy eigenvalues of the anharmonic oscillators is still a challenging problem in mathematical physics, we have reported our numerical results to eleven accurate decimal places for the lowest four energy levels in order to offer a reliable reference for comparison to those who seek to test their approximation and computational techniques over a wide range of λ .

By investigating the dependence of the energy eigenvalues of the anharmonic oscillators on the coupling parameter λ using the FDM with the 8th order accuracy, we showed as

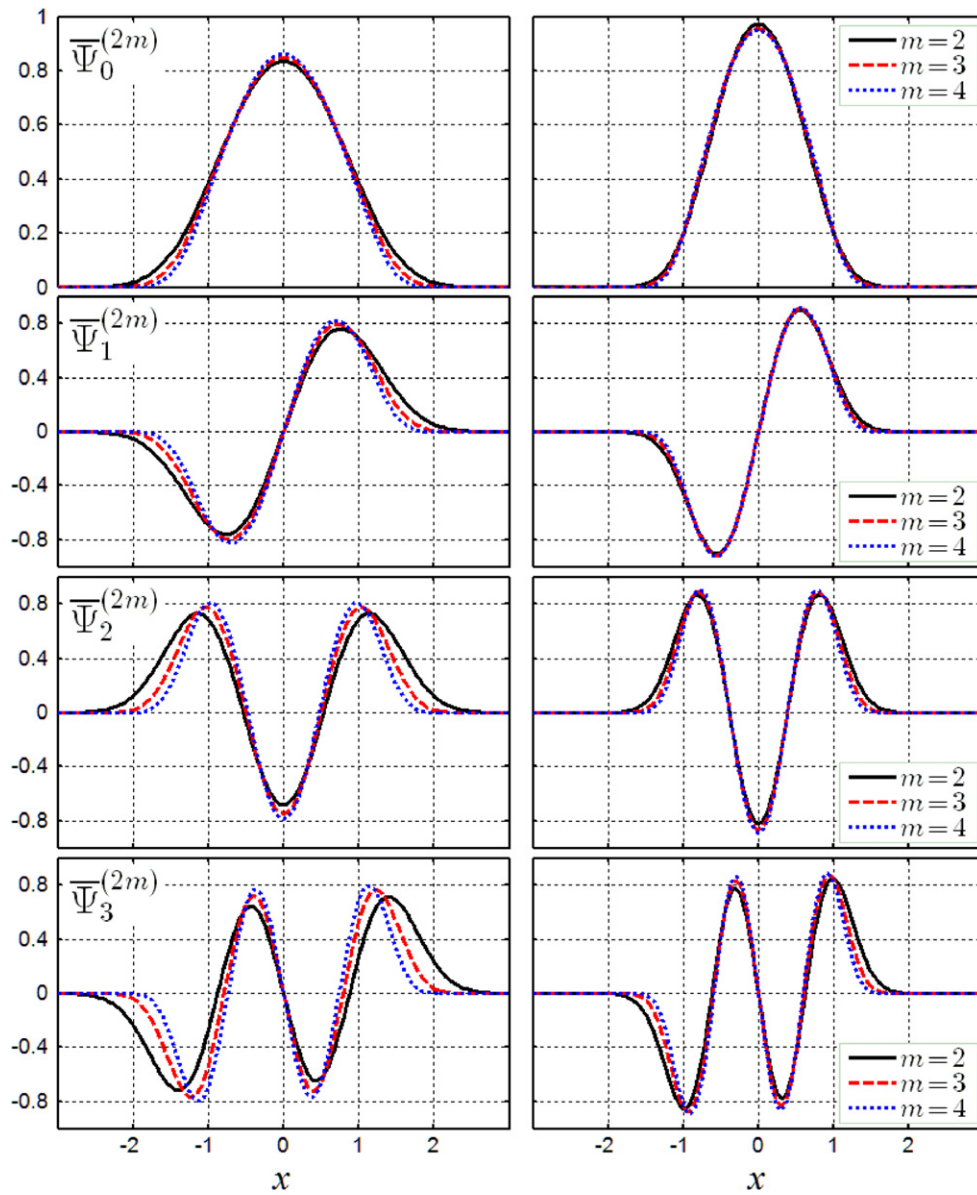


Figure 3. Illustration of the first four normalized eigenfunctions $\bar{\Psi}_n^{(2m)}(x, \lambda)$, $n = 0, 1, 2, 3$, of the quartic (black solid line), sextic (red dashed line) and octic (blue dotted line) anharmonic oscillators for $\lambda = 1$ (on the left side) and $\lambda = 10$ (on the right side). The graphs are computed numerically by the finite difference method using the step size $h = 0.04$ and $L = 8$.

illustrated in figure 2 that the ordering of the eigenvalues beyond a sufficiently large value of λ obeys the inequality: $E_n^{(4)}(\lambda) > E_n^{(6)}(\lambda) > E_n^{(8)}(\lambda)$ for $n = 0, 1, 2, 3$. Moreover, the behaviour of the lowest four energy eigenvalues, namely the set $\{E_0^{(2m)}, E_1^{(2m)}, E_2^{(2m)}, E_3^{(2m)}\}$, for any fixed m is found to be qualitatively very similar. For more illustrations on the higher-

order FDM, we presented in figure 3 the graphs of the relevant energy eigenfunctions of the anharmonic oscillators for $\lambda = 1$ and 10.

We wish to stress that the combination of the FDM and Richardson's extrapolation works very well as a powerful computational tool for calculating energy eigenvalues of general anharmonic oscillators to a high order accuracy, and that our approach can also be used successfully for other kinds of similar confining potentials in one dimensional quantum mechanics. One obvious advantage of the method we described herein is the capability of producing the required number of eigenvalues and eigenvectors together at the same time in fractions of a second with the help of MATLAB.

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