

Asymptotic iteration method for eigenvalue problems

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Received 8 August 2003

Published 12 November 2003

Online at stacks.iop.org/JPhysA/36/11807

Abstract

An asymptotic iteration method for solving second-order homogeneous linear differential equations of the form $y'' = \lambda_0(x)y' + s_0(x)y$ is introduced, where $\lambda_0(x) \neq 0$ and $s_0(x)$ are C_∞ functions. Applications to Schrödinger-type problems, including some with highly singular potentials, are presented.

PACS number: 03.65.Ge

1. Introduction

Second-order homogeneous linear differential equations arise naturally in many fields in mathematical physics. There are many techniques available in the literature that can be used to solve these types of differential equation with boundary conditions. The main task of the present work is to introduce a new technique, which we call the asymptotic iteration method, to solve second-order homogeneous linear differential equations of the form

$$y'' = \lambda_0(x)y' + s_0(x)y \quad (1.1)$$

where $\lambda_0(x)$ and $s_0(x)$ are defined in some interval, not necessarily bounded, and $\lambda_0(x)$ and $s_0(x)$ have sufficiently many continuous derivatives.

2. The asymptotic iteration method

Consider the homogenous linear second-order differential equation

$$y'' = \lambda_0(x)y' + s_0(x)y \quad (2.1)$$

where $\lambda_0(x)$ and $s_0(x)$ are functions in $C_\infty(a, b)$. In order to find a general solution to this equation we rely on the symmetric structure of the right-hand side of (2.1). Indeed, if we differentiate (2.1) with respect to x , we find that

$$y''' = \lambda_1(x)y' + s_1(x)y \quad (2.2)$$

where

$$\lambda_1 = \lambda'_0 + s_0 + \lambda_0^2 \quad \text{and} \quad s_1 = s'_0 + s_0\lambda_0.$$

If we write the second derivative of equation (2.1), we get

$$y'''' = \lambda_2(x)y' + s_2(x)y \quad (2.3)$$

where

$$\lambda_2 = \lambda'_1 + s_1 + \lambda_0\lambda_1 \quad \text{and} \quad s_2 = s'_1 + s_0\lambda_1.$$

Thus, for $(n + 1)$ th and $(n + 2)$ th derivatives, $n = 1, 2, \dots$, we have

$$y^{(n+1)} = \lambda_{n-1}(x)y' + s_{n-1}(x)y \quad (2.4)$$

and

$$y^{(n+2)} = \lambda_n(x)y' + s_n(x)y \quad (2.5)$$

respectively, where

$$\lambda_n = \lambda'_{n-1} + s_{n-1} + \lambda_0\lambda_{n-1} \quad \text{and} \quad s_n = s'_{n-1} + s_0\lambda_{n-1}. \quad (2.6)$$

From the ratio of the $(n + 2)$ th and $(n + 1)$ th derivatives, we have

$$\frac{d}{dx} \ln(y^{(n+1)}) = \frac{y^{(n+2)}}{y^{(n+1)}} = \frac{\lambda_n \left(y' + \frac{s_n}{\lambda_n} y \right)}{\lambda_{n-1} \left(y' + \frac{s_{n-1}}{\lambda_{n-1}} y \right)}. \quad (2.7)$$

We now introduce the ‘asymptotic’ aspect of the method. If we have, for sufficiently large n ,

$$\frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} := \alpha \quad (2.8)$$

then (2.7) reduces to

$$\frac{d}{dx} \ln(y^{(n+1)}) = \frac{\lambda_n}{\lambda_{n-1}} \quad (2.9)$$

which yields

$$y^{(n+1)}(x) = C_1 \exp \left(\int^x \frac{\lambda_n(t)}{\lambda_{n-1}(t)} dt \right) = C_1 \lambda_{n-1} \exp \left(\int^x (\alpha + \lambda_0) dt \right) \quad (2.10)$$

where C_1 is the integration constant, and the right-hand equation follows from (2.6) and the definition of α . Substituting (2.10) into (2.4) we obtain the first-order differential equation

$$y' + \alpha y = C_1 \exp \left(\int^x (\alpha + \lambda_0) dt \right) \quad (2.11)$$

which, in turn, yields the general solution to (1.1) as

$$y(x) = \exp \left(- \int^x \alpha dt \right) \left[C_2 + C_1 \int^x \exp \left(\int^t (\lambda_0(\tau) + 2\alpha(\tau)) d\tau \right) dt \right]. \quad (2.12)$$

Consequently, we have proved the following theorem:

Theorem. Given λ_0 and s_0 in $C_\infty(a, b)$, then the differential equation

$$y'' = \lambda_0(x)y' + s_0(x)y$$

has a general solution (2.12) if for some $n > 0$

$$\frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} \equiv \alpha \quad (2.13)$$

where

$$\lambda_k = \lambda'_{k-1} + s_{k-1} + \lambda_0 \lambda_{k-1} \quad \text{and} \quad s_k = s'_{k-1} + s_0 \lambda_{k-1} \quad (2.14)$$

for $k = 1, 2, \dots, n$.

3. Some illustrative examples

3.1. Differential equations with constant coefficients

If $s_0(x)$ and $\lambda_0(x)$ are constant functions, for example, $\lambda_0 = 4$ and $s_0 = -3$, then, for the differential equation $y'' = 4y' - 3y$, the computation of λ_n and s_n by means of equation (2.14) implies

$$\lambda_n = \frac{1}{2}(3^{n+2} - 1) \quad \text{and} \quad s_n = -\frac{3}{2}(3^{n+1} - 1).$$

Condition (2.13) implies $\lim_{n \rightarrow \infty} \frac{s_n}{\lambda_n} = -1$ which yields from (2.12) the general solution $y(x) = C_2 e^x + C_1 e^{3x}$, as expected by the application of elementary methods. Generally speaking, if we consider the differential equation (1.1) with $\lambda_0(x)$ and $s_0(x)$ constants, we have from (2.14)

$$\lambda_n = s_{n-1} + \lambda_0 \lambda_{n-1} \quad \text{and} \quad s_n = s_0 \lambda_{n-1}.$$

Consequently, the ratio s_n/λ_n becomes

$$\frac{s_n}{\lambda_n} = \frac{s_0 \lambda_{n-1}}{s_{n-1} + \lambda_0 \lambda_{n-1}} = \frac{s_0}{s_{n-1}/\lambda_{n-1} + \lambda_0}$$

which yields, by means of (2.13), that

$$\frac{s_n}{\lambda_n} = \frac{s_0}{s_n/\lambda_n + \lambda_0}$$

therefore

$$\left(\frac{s_n}{\lambda_n}\right)^2 + \lambda_0 \frac{s_n}{\lambda_n} - s_0 = 0. \quad (3.1)$$

This is a quadratic equation that can be used to find the ratio s_n/λ_n in terms of λ_0 and s_0 . Therefore, the expected solutions for the differential equation (1.1) with constant coefficients follow directly by means of (2.12).

3.2. Hermite's differential equation

Many differential equations which are important in applications, such as the equations of Hermite, Laguerre and Bessel, can be solved using the method discussed in section 2. As an illustration we discuss here the exact solution of Hermite's equation by means of the iteration method; other differential equations can be solved similarly. Hermite's differential equation takes the form

$$f'' = 2xf' - 2kf \quad -\infty < x < \infty. \quad (3.2)$$

Here we have $\lambda_0 = 2x$ and $s_0 = -2k$. Using (2.14), we can easily show that

$$\delta = \lambda_{n+1} s_n - s_{n+1} \lambda_n = 2^{n+2} \prod_{i=0}^{n+1} (k - i) \quad n = 0, 1, 2, \dots \quad (3.3)$$

Therefore, for the condition $\delta = 0$ to hold, we must have k a non-negative integer, usually

known as the order of the Hermite equation. Consequently, for each k , the ratio s_n/λ_n yields

$$\begin{aligned} k=0 & \quad \frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} = \dots = 0 \Rightarrow f_0(x) = 1 \\ k=1 & \quad \frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} = \dots = -\frac{1}{x} \Rightarrow f_1(x) = x \\ k=2 & \quad \frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} = \dots = -\frac{4x}{2x^2-1} \Rightarrow f_2(x) = 2x^2 - 1 \\ k=3 & \quad \frac{s_3}{\lambda_3} = \frac{s_4}{\lambda_4} = \dots = -\frac{6x^2-3}{2x^3-3x} \Rightarrow f_3(x) = 2x^3 - 3x \\ k=4 & \quad \frac{s_4}{\lambda_4} = \frac{s_5}{\lambda_5} = \dots = \frac{24x-16x^3}{3-12x^2+4x^4} \Rightarrow f_4(x) = 3 - 12x^2 + 4x^4 \end{aligned}$$

and so on. Clearly, the expressions for the exact solutions $f_k(x)$ generate the well-known Hermite polynomials. We can easily verify that the general form of $f_k(x)$, $k = 0, 1, 2, \dots$, is given in terms of the confluent hypergeometric functions [2] by

$$f_{2k}(x) = (-1)^k 2^k \left(\frac{1}{2}\right)_k {}_1F_1\left(-k; \frac{1}{2}; x^2\right) \quad (3.4)$$

and

$$f_{2k+1}(x) = (-1)^k 2^k \left(\frac{3}{2}\right)_k x {}_1F_1\left(-k; \frac{3}{2}; x^2\right) \quad (3.5)$$

where the Pochhammer symbol $(a)_k$ is defined by $(a)_0 = 1$ and $(a)_k = a(a+1)(a+2)\dots(a+k-1)$ for $k = 1, 2, 3, \dots$, and may be expressed in terms of the Gamma function by $(a)_k = \Gamma(a+k)/\Gamma(a)$, when a is not a negative integer $-m$, and, in these exceptional cases, $(-m)_k = 0$ if $k > m$ and otherwise $(-m)_k = (-1)^k m!/(m-k)!$.

3.3. Harmonic oscillator potential in one dimension

Although the iteration method discussed in section 2 can be applied to any second-order homogeneous linear differential equations of the form (1.1) with $\lambda_0 \neq 0$, we shall concentrate in the rest of the paper on the eigenvalue problems of Schrödinger type. We shall show that equation (2.12) with conditions (2.13) and (2.14) gives a complete solution for many important Schrödinger-type problems. Through a concrete example we explore the exact solutions of Schrödinger's equation for the harmonic oscillator potentials, namely

$$\left(-\frac{d^2}{dx^2} + x^2\right)\psi = E\psi \quad (3.6)$$

where $\psi \in L_2(-\infty, \infty)$. In the limit of large x , the asymptotic solutions of (3.6) can be taken as any power of x times a decreasing Gaussian. With this in mind we write the 'unnormalized' wavefunctions as

$$\psi(x) = \exp\left(-\frac{x^2}{2}\right) f(x) \quad (3.7)$$

where the functions $f(x)$ are to be found by means of the iteration procedure. Substituting (3.7) into (3.6), one obtains

$$\frac{d^2 f}{dx^2} = 2x \frac{df}{dx} + (1-E)f \quad (3.8)$$

which, by comparison with (3.2), yields the exact eigenvalues

$$E_n = 2n + 1 \quad n = 0, 1, 2, \dots$$

and the functions $f_n(x)$, $n = 0, 1, 2, \dots$, are the Hermite polynomials obtained above. Therefore, using (3.4) and (3.5), the unnormalized wavefunctions of the Schrödinger

equation (3.6) are

$$\psi_n(x) = (-1)^n 2^n \left(\frac{1}{2}\right)_n \exp\left(-\frac{x^2}{2}\right) {}_1F_1\left(-n; \frac{1}{2}; x^2\right) \quad (3.9)$$

for $n = 0, 2, 4, \dots$ and

$$\psi_n(x) = (-1)^n 2^n \left(\frac{3}{2}\right)_n x \exp\left(-\frac{x^2}{2}\right) {}_1F_1\left(-n; \frac{3}{2}; x^2\right) \quad (3.10)$$

for $n = 1, 3, \dots$. The normalization constant of $\psi(x)$ can be computed by means of $\|\psi\| = 1$, as we shall shortly show.

3.4. Gol'dman and Krivchenkov potential

The Gol'dman and Krivchenkov Hamiltonian is the generalization of the harmonic-oscillator Hamiltonian in three dimensions; namely

$$\left(-\frac{d^2}{dr^2} + r^2 + \frac{\gamma(\gamma+1)}{r^2}\right) \psi = E\psi \quad (3.11)$$

where $\psi \in L_2(0, \infty)$ and satisfies the condition $\psi(0) = 0$ known as the Dirichlet boundary condition. The generalization lies in the parameter γ ranging over $[0, \infty)$ instead of the angular momentum quantum number $l = 0, 1, 2, \dots$. For large r , the exact solutions of (3.11) are asymptotically equivalent to the exact solutions of the harmonic-oscillator problem with eigenfunctions vanishing at the origin. Therefore, we may assume that the unnormalized wavefunction ψ takes the form

$$\psi(r) = r^{\gamma+1} \exp\left(-\frac{r^2}{2}\right) f(r) \quad (3.12)$$

where, again, $f(r)$ is to be determined through the iteration procedure discussed in section 2. Substituting (3.12) into (3.11), we obtain

$$\frac{d^2 f}{dr^2} = 2\left(r - \frac{\gamma+1}{r}\right) \frac{df}{dr} + (2\gamma+3-E)f \quad (3.13)$$

where $\lambda_0(r) = 2(r - (\gamma+1)/r)$ and $s_0(r) = 2\gamma+3-E$. By means of equation (2.14) we may compute $\lambda_n(r)$ and $s_n(r)$. That result, combined with condition (2.13), yields

$$E_0 = 3 + 2\gamma \quad E_1 = 7 + 2\gamma \quad E_2 = 11 + 2\gamma \quad \dots$$

respectively, that means

$$E_n = 4n + 2\gamma + 3 \quad \text{for } n = 0, 1, 2, \dots \quad (3.14)$$

Furthermore, with the use of $f(r) = \exp(-\int s_n/\lambda_n dr)$, equation (2.13), after some straightforward computations, yields

$$f_n(r) = \sum_{k=0}^n (-1)^k 2^{n-2k} \frac{\Gamma(n+1)\Gamma(2\gamma+2n+2)\Gamma(\gamma+n-k+1)}{\Gamma(k+1)\Gamma(n-k+1)\Gamma(n+\gamma+1)\Gamma(2n+2\gamma-2k+2)} r^{2n-2k}. \quad (3.15)$$

In order to show that (3.15) together with (3.12) yields the exact wavefunctions for the Gol'dman and Krivchenkov Hamiltonian, we may proceed as follows. Using the Pochhammer identity $(a)_{-k} = \Gamma(a-k)/\Gamma(a)$, we can write (3.15) as

$$f_n(r) = 2^n r^{2n} \sum_{k=0}^n (-1)^k \frac{(\gamma+n+1)_{-k}}{k!(n+1)_{-k}(2n+2\gamma+2)_{-2k}} \left(\frac{1}{2r}\right)^{2k}$$

Since $(a)_{-k} = (-1)^k / (1-a)_k$ we have

$$f_n(r) = 2^n r^{2n} \sum_{k=0}^n \frac{(-n)_k (-n - \gamma - \frac{1}{2})_k}{k!} \left(\frac{1}{r^2}\right)^k \quad (3.16)$$

in which we have used Gauss's duplication formula

$$(a)_{2n} = 2^{2n} \left(\frac{a}{2}\right)_n \left(\frac{a+1}{2}\right)_n.$$

The finite sum in (3.16) is the series representation of the hypergeometric function ${}_2F_0$. Therefore

$$\begin{aligned} f_n(r) &= 2^n r^{2n} {}_2F_0\left(-n, -n - \gamma - \frac{1}{2}; -; -\frac{1}{r^2}\right) \\ &= (-1)^n 2^n! L_n^{\gamma+\frac{1}{2}}(r^2) \\ &= (-1)^n 2^n (\gamma + \frac{3}{2})_n {}_1F_1\left(-n; \gamma + \frac{3}{2}; r^2\right). \end{aligned}$$

Consequently, the unnormalized wavefunctions take the form

$$\psi(r) = (-1)^n 2^n (\gamma + \frac{3}{2})_n r^{\gamma+1} \exp\left(-\frac{r^2}{2}\right) {}_1F_1\left(-n; \gamma + \frac{3}{2}; r^2\right)$$

for $n = 0, 1, 2, \dots$. The normalization constant for $\psi(r)$ can be found using $\|\psi\| = 1$ which leads to the exact wavefunctions of the Gol'dman and Krivchenkov potential, namely

$$\psi(r) = (-1)^n \sqrt{\frac{2(\gamma + \frac{3}{2})_n}{n! \Gamma(\gamma + \frac{3}{2})}} r^{\gamma+1} \exp\left(-\frac{r^2}{2}\right) {}_1F_1\left(-n; \gamma + \frac{3}{2}; r^2\right). \quad (3.17)$$

Some remarks are in order:

- (1) The exact odd and even solutions of the harmonic oscillator potential in one dimension can be recovered from (3.17) by setting $\gamma = 0$ and $\gamma = -1$ respectively.
- (2) The exact solutions of the harmonic oscillator potential in three dimensions can be recovered from (3.17) by setting $\gamma = l$, where $l = 0, 1, 2, \dots$ is the angular momentum quantum number.
- (3) The exact solutions of the harmonic oscillator potential in N dimensions can be recovered from (3.17) by setting $\gamma = l + \frac{1}{2}(N - 3)$ where $N \geq 2$.

4. Singular potentials

We discuss in this section the application of the iteration method discussed in section 2 to investigate two important classes of singular potentials. The first class is characterized by the generalized spiked harmonic oscillator potentials which have a singularity at the origin, and the second class is characterized by the quartic anharmonic oscillator potentials where the perturbative term diverges strongly at infinity. Different approaches are usually applied to deal with each of these classes. The asymptotic iteration method, however, can be used to investigate the eigenvalues for both classes of potentials.

4.1. Generalized spiked harmonic oscillator potentials

Since the interesting work of Harrell [7] on the ground-state energy of the singular Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{A}{x^\alpha} \quad x \in [0, \infty) \quad A \geq 0 \quad \alpha > 0 \quad (4.1)$$

known as the spiked harmonic oscillator Hamiltonian, the volume of research in this field has grown rapidly. A variety of techniques has been employed in the study of this interesting family of quantum Hamiltonians [4–14]. We shall investigate here the solutions of the spiked harmonic oscillator Hamiltonian (4.1) in arbitrary dimensions by means of the iteration method. That is to say, we examine the eigenvalues of the Hamiltonian known as the generalized spiked harmonic oscillator Hamiltonian

$$H = -\frac{d^2}{dx^2} + x^2 + \frac{\gamma(\gamma + 1)}{x^2} + \frac{A}{x^\alpha} \quad x \in [0, \infty) \quad A \geq 0 \quad \alpha > 0 \quad (4.2)$$

where $\gamma = l + (N - 3)/2$ for $N \geq 2$. Clearly we may compute the eigenvalues of the spiked harmonic oscillator Hamiltonian (4.1) directly by setting $N = 3$ and $l = 0$ in (4.2).

The wavefunctions (3.12) of the Gol'dman and Krivchenkov Hamiltonian suggest that the exponent in the power of x term of the exact solutions of (4.2) should depend, at least, on the parameters γ and A . Since the exact form of this term is unknown, we write the exact wavefunctions in the simpler form

$$\psi(x) = \exp\left(-\frac{x^2}{2}\right) f(x) \quad (4.3)$$

where the functions $f(x)$ must satisfy the condition $f(0) = 0$ and remain to be determined by the iteration method. Substituting (4.3) into (4.2), we obtain

$$\frac{d^2 f}{dx^2} = 2x \frac{df}{dx} + \left(1 - E + \frac{A}{x^\alpha} + \frac{\gamma(\gamma + 1)}{x^2}\right) f. \quad (4.4)$$

With $\lambda_0(x) = 2x$ and $s_0(x) = 1 - E + A/x^\alpha + \gamma(\gamma + 1)/x^2$, we may compute $\lambda_n(x)$ and $s_n(x)$ using (2.14) and the eigenvalues may be calculated by means of the condition (2.13). For each iteration, the expression $\delta = s_n \lambda_{n-1} - s_{n-1} \lambda_n$ will depend on two variables E and x . The eigenvalues E computed by means of $\delta = 0$ should, however, be independent of the choice of x . Actually, this will be the case for most iteration sequences. The choice of x can be critical to the speed of the convergence to the eigenvalues, as well as for the stability of the process. Although, we do not have at the moment a specific method to determine the best initial value of x , we may suggest the following approaches. For the spiked harmonic oscillator potential $V(x) = x^2 + A/x^\alpha$, one choice of $x = x_0$ could be the value of x_0 that minimizes the potential V , namely $x_0 = (\frac{\alpha A}{2})^{1/(\alpha+2)}$. Another possible choice comes from noting that the ground-state energy of the harmonic oscillator or that of the Gol'dman and Krivchenkov potential can be obtained by setting $s_0 = 0$. We may therefore start our iteration with x_0 obtained from $s_0 = 0$. For example, if $\alpha = 4$, then

$$s_0 = 1 - E + \frac{A}{x^4} + \frac{\gamma(\gamma + 1)}{x^2} = 0$$

implies

$$x_0 = \sqrt{p + \sqrt{p^2 + \frac{A}{E - 1}}} \quad (4.5)$$

where $p = \gamma(\gamma + 1)/2(E - 1)$. The results of our iteration method for the cases of $\alpha = 1.9$ and $\alpha = 2.1$ are reported in table 1 where we compute the eigenvalues E_{nl}^P by means of 12 iterations only. It should be clear that these results could be further improved by increasing the number of iterations. For the case of $\alpha = 4$ we report our results in table 2 wherein we used x_0 to start the iteration procedure, as given by (4.5).

Table 1. A comparison between the exact eigenvalues E_{nl} for dimension $N = 2-10$ of the Hamiltonian (4.2) computed by direct numerical integration of Schrödinger's equation and the eigenvalues E_{nl}^P computed by means of the present work.

| N | $\alpha = 1.9$ | | $\alpha = 2.1$ | |
|-----|----------------|------------|----------------|------------|
| | E_{00} | E_{00}^P | E_{21} | E_{21}^P |
| 2 | 8.485 38 | 8.485 45 | 16.543 63 | 16.543 76 |
| 3 | 8.564 36 | 8.564 42 | 16.904 44 | 16.904 42 |
| 4 | 8.795 44 | 8.795 47 | 17.381 71 | 17.381 45 |
| 5 | 9.163 09 | 9.163 09 | 17.955 44 | 17.955 22 |
| 6 | 9.646 70 | 9.646 68 | 18.607 07 | 18.607 00 |
| 7 | 10.225 04 | 10.225 03 | 19.320 69 | 19.320 73 |
| 8 | 10.879 07 | 10.879 07 | 20.083 41 | 20.083 46 |
| 9 | 11.592 98 | 11.592 98 | 20.885 02 | 20.885 03 |
| 10 | 12.354 18 | 12.354 18 | 21.717 61 | 21.717 59 |

Table 2. A comparison between the exact eigenvalues E_0 for one dimension of the Hamiltonian (4.2) with $\alpha = 4$ computed by direct numerical integration of Schrödinger's equation and the eigenvalues E_0^P computed by means of the present work.

| A | γ | E_0^P | E_0 |
|-------|----------|-------------------|-------------------|
| 0.001 | 3 | 9.000 114 278 33 | 9.000 114 279 12 |
| | 4 | 11.000 063 490 67 | 11.000 063 490 74 |
| | 5 | 13.000 040 403 73 | 13.000 040 403 64 |
| 0.01 | 3 | 9.001 142 196 19 | 9.001 142 199 40 |
| | 4 | 11.000 634 788 92 | 11.000 634 788 89 |
| | 5 | 13.000 404 000 63 | 13.000 404 000 60 |
| 0.1 | 3 | 9.011 363 932 66 | 9.011 364 026 18 |
| | 4 | 11.006 336 099 74 | 11.006 336 099 23 |
| | 5 | 11.004 036 432 57 | 13.004 036 432 52 |
| 1 | 3 | 9.108 660 360 401 | 9.108 658 607 52 |
| | 4 | 11.062 241 826 08 | 11.062 241 719 38 |
| | 5 | 13.040 015 183 18 | 13.040 015 183 06 |

4.2. The quartic anharmonic oscillator potentials

We investigate the Schrödinger equation $H\psi = E(A)\psi$ for the quartic anharmonic oscillators [15–19], where

$$H = -\frac{d^2}{dx^2} + x^2 + Ax^4. \quad (4.6)$$

In order to obtain the energy levels using the iteration method, we write the exact wavefunctions in the form

$$\psi(x) = \exp\left(-\frac{x^2}{2}\right) f(x).$$

Consequently, after substituting in the Schrödinger equation, we obtain

$$\frac{d^2 f}{dx^2} = 2x \frac{df}{dx} + (1 - E + Ax^4) f \quad (4.7)$$

Table 3. A comparison between the eigenvalues E_n , $n = 0, 1, \dots, 5$, for the quartic anharmonic oscillator with $A = 0.1$ computed by direct numerical integration of Schrödinger's equation [19] and the eigenvalues E^P computed by means of the present work.

| n | E^P | E |
|-----|-----------|-----------|
| 0 | 1.065 286 | 1.065 286 |
| 1 | 3.306 871 | 3.306 872 |
| 2 | 5.747 960 | 5.747 959 |
| 3 | 8.352 642 | 8.352 678 |
| 4 | 11.098 35 | 11.098 60 |
| 5 | 13.966 95 | 13.969 93 |

or $\lambda_0(x) = 2x$ and $s_0(x) = 1 - E + Ax^4$. We start the iteration in this case with $x_0 = 0$, the value of x at which the potential takes its minimum value. We report our computational results in table 3.

5. Conclusion

One can find a Taylor polynomial approximation about x_0 for an initial value problem by differentiating the equation itself and back substituting to obtain successive values of $y^{(k)}(x_0)$. This method is perhaps as old as the very notion of a differential equation. In this paper we develop a functional iteration method related to this general idea and specifically tailored for an important base-class of linear equations of the form $L(y) = y'' - \lambda y' - sy = 0$. The iteration is assumed either to terminate by the condition $s_n/\lambda_n = s_{n-1}/\lambda_{n-1} \equiv \alpha$, or this condition is imposed, as an approximation. After looking at some well-known problems which are exactly of this sort, our principal application is to Schrödinger eigen equations. These latter problems are converted to the base-type by first factoring their solutions in the form $\psi(x) = f(x)y(x)$, where $f(x)$ is the large- x asymptotic form, and y satisfies $L(y) = 0$. Some aspects of this approach, such as the iteration termination condition, the construction of asymptotic forms and the choice of x_0 , still await more careful mathematical analysis. However, even in its present rudimentary state, the method offers an interesting approach to some important problems. This is especially so, as it turns out, for problems such as the spiked harmonic oscillator that are known to present some profound analytical and numerical difficulties.

Acknowledgment

Partial financial support of this work under grant nos GP3438 and GP249507 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged by two of us (respectively RLH and NS).

References

- [1] Saad N and Hall R L 2002 *J. Phys. A: Math. Gen.* **35** 4105
- [2] Andrews G E, Askey R and Roy R 1999 *Special Functions* (Cambridge: Cambridge University Press)
- [3] Hall R L, Saad N and von Keviczky A 2001 *J. Phys. A: Math. Gen.* **34** 1169
- [4] Hall R L, Saad N and von Keviczky A 1998 *J. Math. Phys.* **39** 6345
- [5] Hall R L and Saad N 2000 *J. Phys. A: Math. Gen.* **33** 569
- [6] Hall R L and Saad N 2000 *J. Phys. A: Math. Gen.* **33** 5531
- [7] Harrell E M 1977 *Ann. Phys., NY* **105** 379
- [8] Aguilera-Navarro V C, Estévez G A and Guardiola R 1990 *J. Math. Phys.* **31** 99

-
- [9] Aguilera-Navarro V C, Fernández F M, Guardiola R and Ros J 1992 *J. Phys. A: Math. Gen.* **25** 6379
 - [10] Aguilera-Navarro V C, Coelho A L and Ullah Nazakat 1994 *Phys. Rev. A* **49** 1477
 - [11] Znojil M 1991 *Phys. Lett. A* **158** 436
 - [12] Znojil M and Leach P G L 1992 *J. Math. Phys.* **33** 2785
 - [13] Solano-Torres W, Estéves G A, Fernández F M and Groenenboom G C 1992 *J. Phys. A: Math. Gen.* **25** 3427
 - [14] Hall R L, Saad N and von Keviczky A 2002 *J. Math. Phys.* **43** 94
 - [15] Simon B 1970 *Ann. Phys., NY* **58** 79
 - [16] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
 - [17] Bacus B, Meurice Y and Soemadi A 1995 *J. Phys. A: Math. Gen.* **28** L381
 - [18] Hall R L 1985 *Canad. J. Phys.* **63** 311
 - [19] Mostafazadeh A 2001 *J. Math. Phys.* **42** 3372