An Analytic Iterative Approach to Solving the Time-Independent Schrödinger Equation

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ABSTRACT: In this article, we introduce a simple analytic method for obtaining approximate solutions of the Schrödinger equation for a wide range of potentials in one- and two-dimensions. We define an operator, called the iteration operator, which will be used to solve for the lowest order state(s) of a system. The method is simple in that it does not require the computation of any integrals in order to obtain a solution. We use this method on several potentials which are well understood or even exactly solvable in order to demonstrate the strengths and weaknesses of this method. © 2008 Wiley Periodicals, Inc. Int J Quantum Chem 109: 982–998, 2009

Key words: iteration operator; Schrödinger equation; analytic approximation

1. Introduction

New approximate solutions to quantum problems are always welcome. Every method has its strengths and limitations, and so they tend to be applied to different kinds of systems.

Variational methods work well for calculating the upper bound for the energy of the system. While the resulting approximate energy is accurate to second order, the corresponding wave function is only approximate to first order. A more accurate approximation of the wave function is desired because it is critical for solving for other physical properties of the system (i.e. angular momentum). Perturbative methods are capable of finding highly accurate energies and wave functions, but they are applicable only when the potential changes little from a problem that has known solutions. Other well-known methods have a myriad of other restrictions.

Modern research into actual quantum systems, for the most part, uses numerical methods to build up approximations of the solution to the Schrödinger equation. There are several problems with numerical approximations. First, a numerical approximation usually computes the value of the solution at a finite number of points. This allows for the possible loss of important information. Second,

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the coding of boundary conditions must be carefully done in order for the solution to be meaningful. Third, numerical methods tend not to handle singularities well.

The purpose of this work is to demonstrate a proof of concept concerning a technique for solving for particular solutions of the Schrödinger equation which takes advantage of the computational efficiency of computers but yields a wave function that is actually an analytic function (of position in this work). The only assumption used in the derivation of the method of approximation described hereafter is that the potential to which it is being applied is real and finite over all space. It is able to give an accurate particular solution to the Schrödinger equation with any given potential. It is also applicable to a system with any number of degrees of freedom. In this article, we have restricted the application to up to 2 degrees of freedom. It is equally successful at computing the ground state wave function, or lowest order state of a given symmetry of the problem, as it is at computing the corresponding eigenvalue.

Our method is based on the idea of applying a first-order iteration operator (IO) to a suitable initial function given in analytic form. Throughout every step in the iteration we produce a (truncated) analytic approximation, monitoring its accuracy with the approximate corresponding energy.

In Section 2 we describe the ideas and algorithms used in this article. Section 3 is concerned with the trivial example of a harmonic oscillator starting with an approximate initial function. In Section 4 we solve the problem of an anharmonic quartic oscillator and compare our results with other methods. A modified Pöschl–Teller (MPT) potential is dealt with in Section 5, followed by a two-dimensional example in Section 6.

2. Theory

The crux of the IO method consists in applying it directly to an initial (trial) wave function, ψ, to obtain an analytic approximation to the ground state wave function. As the iteration progresses, many terms are generated because of the derivatives in the kinetic portion of the Hamiltonian, $\hat{H}$, and because of the multiplication of ψ by the potential portion of $\hat{H}$. To counteract the growing number of terms the result of each iteration (excluding the possible exponential in the initial function) is first turned into a polynomial expanded around the minimum of the potential and is then truncated to a desired order of accuracy.

2.1. THE ITERATION OPERATOR

The derivation of the IO [1] resembles the development of the techniques used in Monte Carlo simulations. Suppose that a time-independent Hamiltonian, $\hat{H}$, describes some quantum system. The time development of the wave function $\psi_n(\vec{x},t)$ can be written, in units of $\hbar = 1$, as

$$\psi_n(\vec{x},t) = \exp[-i\hat{H}t]\phi_n(\vec{x}) \qquad (1)$$

for each eigenfunction ϕ_n.

Making the substitution $\tau = i\,t$ we can follow the τ-evolution of an arbitrary initial function $\psi(x)$ and expand it in the basis $\{\phi_n\}$

$$\exp[-\hat{H}\tau]\psi(\vec{x}) = \exp[-\hat{H}\tau]\sum_{n=0}^{\infty} a_n\phi_n(\vec{x})$$

$$= a_o\exp[-E_o\tau]\phi_o(\vec{x}) + \sum_{n=0}^{\infty} a_n\exp[-E_n\tau]\phi_n(\vec{x}), \qquad (2)$$

where a_n is the set of expansion coefficients of the initial wave function ψ with respect to the basis ϕ_n. For large $\tau \to \infty$, the dominant term is the first one, because $E_o < E_n$ for $n \geq 1$. This way we can extract information about the ground state of the system starting with an arbitrary function $\phi(x)$ with the appropriate boundary conditions [2].

The more general form of the above derivation involves the use of some energy E, often assumed to be the ground state energy E_o, being subtracted off of the Hamiltonian in the exponential $\exp[-(\hat{H} - E)\tau]\psi(\vec{x})$. The use of this more general form may be needed when the ground state energy is negative; in such a case we merely have to set $E \leq E_o$. We will dispense with using this more general form for the remainder of this section but it will be used again in Section 5.

We approximate the imaginary-time evolution operator

$$\exp[-\hat{H}\tau] = \lim_{m\to\infty}\left(1 - \frac{\tau}{m}\hat{H}\right)^m \approx (1 - \alpha\hat{H})^p, \qquad (3)$$

where instead of taking the limit as $m \to \infty$ we set m to some large number p, and we defined the constant

$$\alpha = \frac{\tau}{p}. \tag{4}$$

By fixing α we can force $\tau \to \infty$ as $p \to \infty$. (While theoretically α can be as small as we wish, it has been found that α must remain within an order of magnitude of 0.001 in order for the present method to consistently work.) Thus we obtain the IO,

$$\hat{I}_p = [1 - \alpha\hat{H}]^p. \tag{5}$$

Our algorithm consists of the following steps:

1. Choose an approximate initial (trial) function ψ (usually some exponential function).
2. Apply I, p-times to ψ to generate the set of new functions $\{I_1\psi, I_2\psi, \ldots, I_p\psi\}$.
3. For each step, expand and truncate the additional multiplicative terms as a polynomial of given degree.
4. Stop the iteration when the local energy $\hat{H}\psi/\psi$ becomes constant within a given accuracy.

The resultant approximate eigenfunction typically has the form of a polynomial times an exponential.

2.2. INITIAL FUNCTIONS

The choice of an initial function is a critical part of this procedure. The problem is that the derivation of the IO assumes that the initial function is within the space spanned by the eigenfunctions of the Hamiltonian. There are a few necessary criteria which the initial functions must satisfy: first, the initial function must satisfy all boundary conditions of the system. Second, the initial function and all of its derivatives must go to zero faster than the potential blows up at any point. These criteria will be proved below.

Theorem 1. The resultant approximation of the wave function will, in general, use the initial function ψ and all of its derivatives up to $\nabla^{2p-2}\psi$ for $p \geq 2$, where p is the number of iterations.

Proof. We will prove this by induction. Let ψ be the initial function. After the second iteration the resultant wave function is of the form

$$\psi_{\vec{x}} = \frac{1}{4m^2}\nabla^4\psi - (2 - 2V)\frac{1}{2m}\nabla^2\psi - (\nabla V)\frac{1}{m}\nabla\psi + \left(1 - 2V - \frac{1}{2m}\nabla^2 V + V^2\right)\psi,$$

where we have used the usual form of the Hamiltonian $\hat{H} = 1/2m\nabla^2 + V$.

Assume next that the theorem is true for n iterations.

$$\psi_{\vec{x}} = (-1)^n\frac{1}{2^n m^n}\nabla^{2n}\psi + c_1\nabla^{2n-2}\psi + c_2\nabla^{2n-3}\psi + \ldots + c_3\psi$$

Finding the $n + 1$ iteration

$$\begin{aligned}\psi_{\vec{x}} = {} & (-1)^{n+1}\frac{1}{2^{n+1}m^{n+1}}\nabla^{2n+2}\psi \\ & - \frac{1}{2m}[(\nabla^2 c_1)\nabla^{2n-2}\psi + 2(\nabla c_1)\nabla^{2n-1}\psi \\ & + c_1\nabla^{2n}\psi] \\ & - \frac{1}{2m}[(\nabla^2 c_2)\nabla^{2n-3}\psi + 2(\nabla c_2)\nabla^{2n-2}\psi \\ & + c_2\nabla^{2n-1}\psi] \\ & + \ldots \\ & - \frac{1}{2m}[(\nabla^2 c_3)\psi + 2(\nabla c_3)\nabla\psi + c_3\nabla^2\psi] \\ & + V(-1)^n\frac{1}{2^n m^n}\nabla^{2n}\psi + Vc_1\nabla^{2n-2}\psi \\ & + Vc_2\nabla^{2n-3}\psi + \ldots + Vc_3\psi,\end{aligned}$$

where the c's are functions of V.

After some algebra we see that the $n + 1$ iteration has the form

$$\psi_r = (-1)^n\frac{1}{2^{n+1}m^{n+1}}\nabla^{2n+2}\psi + d_1\nabla^{2n-1}\psi + d_2\nabla^{2n-2}\psi + \ldots + d_3\psi,$$

where the d's are functions of V. □

Theorem 2. If the initial function is not an eigenstate of the system then the initial function and all of its derivatives must go to zero faster than the corresponding potential blows up at a point.

Proof. Let V be a potential that diverges at a point, or set of points, $\vec{x} = \vec{a}_i$. Let ψ be an initial function. Suppose that ψ or one of its derivatives $\psi^{(q)}$ fails to converge to zero faster than the potential blows up at one of the points, $\vec{x} = \vec{a}_j \in \{\vec{a}_i\}$. Then,

$$[V\psi^{(m)}]_{\vec{x}=\vec{a}_j} = \infty \tag{6}$$

where $\psi^{(m)}$ is the mth derivative of ψ. Every iteration of the wave function that contains $\psi^{(m)}$ fails to be analytic causing the approximation to fail.□

Because the initial function, and its derivatives, must be finite throughout all space, it is reasonable to assume an initial function with an exponential function in it. Any symmetries of the system should be considered when choosing the initial function. This method projects the initial function into the subspace of energy eigenfunctions that has the same symmetry as the initial function.

2.3. FINDING STATES OTHER THAN THE GROUND STATE

Our derivation of the IO involved taking some initial function ψ, which was, in general, a linear combination of all of the energy eigenstates of the system, and projecting out the ground state. Suppose now that the ground state is lowest order state of some symmetry of the system (i.e., the potential is even about the origin) then the first excited state would be the lowest order state that is odd. To find the first excited state we must provide an initial function that is odd.

2.4. TESTING THE RESULT

We will compute the local energy [3, 4] associated with the state in question via

$$E(\vec{x}) = \frac{\hat{H}\psi}{\psi}. \tag{7}$$

A local energy that is constant over the classically allowed region is a necessary condition for the resultant wave function to be a good approximation of the eigenfunction, but we will show that it is not sufficient. Equation (7) seems to be the best method for testing a solution and we will show how this can be used to confidently obtain a solution.

3. Simple Harmonic Oscillator

The simple harmonic oscillator, referred to hereafter as SHO, is a natural choice for working through the process of how to actually perform the iteration approximation, as well as for discovering the limitations of the procedure. The SHO potential is continuous and finite over all space, can be centered around any point in space, and can be abstracted to n-dimensions. The solutions to the SHO are simple and can be found analytically. We will use the SHO to explore the functionality of the IO method of approximation.

Using Eq. (5) the IO for the SHO is given by

$$\hat{I}_p = \left(1 + \frac{\alpha}{2}\frac{d^2}{dx^2} - \frac{\alpha}{2}x^2\right)^p. \tag{8}$$

In solving for the ground state energy eigenvalue and eigenfunction, a range of iteration coefficient values, from $\alpha = 0.00002$ to $\alpha = 0.07$, were used. We will see that the ability of the iteration method to solve for the correct eigenvalues and eigenfunctions will depend on the particular combination of values for α and the initial function.

3.1. GUASSIAN INITIAL FUNCTION

We use asymptotic analysis to obtain an initial function for use in the IO method. Unfortunately, for our purposes, the asymptotic solution happens to be the unnormalized ground state eigenfunction. We will thus use Gaussians of the form

$$\psi(x) = \exp[-\eta x^2], \tag{9}$$

where $\eta = \{0.2, 0.4, 0.6, 0.8, 1.0, 2.0\}$, as initial functions. Recall that the exact solution corresponds to $\eta = 0.5$.

3.2. APPROXIMATIONS WITH POLYNOMIALS OF INCREASING ORDER IN x

Figure 1 shows the results of using the IO method to compute the wave function and energy of the ground state for the SHO, for a particular choice of α and η. The top and middle graphs are self-explanatory, and the bottom graph was produced by dividing our approximate wave function by the ground state eigenfunction. Notice that the wave functions appear to be Gaussian. As was stated in Section 2.4, the correct approximation is

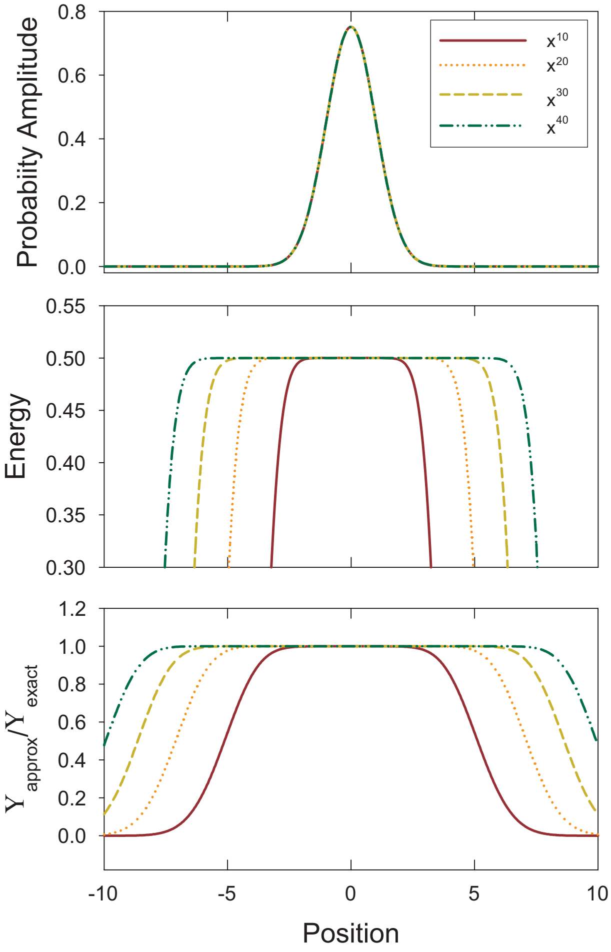

FIGURE 1. Example of how the region of constant energy increases with order in x, for the cases where $\alpha = 0.005$ and $\eta = \sqrt{2}/2$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

said to be found if the energy is constant over a range in position. We also see that the area over which the energy is found to be constant is related to the magnitude of the order in x to which the approximation is taken to.

If we divide the approximate wave function by the eigenfunction, and graph with respect to position, the area over which the approximation essentially equals the eigenfunction expands with increasing order in x. Note also that both the region of constant energy and the region where $\psi_{\text{approx}}/\psi_{\text{exact}}$ equals 1 are, for all orders of x computed, at least a couple times larger than the area enclosed by the classical turning points. This ensures that the approximation is meaningful. Table I lists the probability of finding the particle within the area enclosed by each approximation.

3.3. APPROXIMATIONS WITH DIFFERENT GAUSSIAN INITIAL FUNCTIONS

Not surprisingly, the closer an initial function is to the eigenfunction the better the resultant approximation, as can be seen in Figure 2. Notice that the result for $\eta = 0.2$ obtains the correct energy but the wave function has "wings." The bottom graph suggests, and computation shows, that if we were to ignore the wings and normalize over the range $x = (-3, 3)$ then the Gaussian between the wings is a very good approximation of the eigenfunction.

3.4. FIRST EXCITED STATE OF THE SHO

The IO is a method to approximate the lowest order state of any given symmetry, not just the ground state. Thus far we have focused on finding the ground state wave function which is the lowest order state that is even about $x = 0$. We can also find the first excited state which is the lowest order odd state. A suitable initial function for the first excited state is

$$\psi(x) = x^{\kappa}\exp[-\eta x^2], \tag{10}$$

where κ is any odd number. Cases which have been investigated include {1, 3, 5, 7, 9, 21, 23, 25}, and most of these have produced satisfactory results; of course, Eq. (10) also allows for even trial functions; suitable results have been found for the ground state energy eigenfunction and energy eigenvalue for $\kappa = \{2, 4, 6, 8, 20, 22, 24\}$ (see Fig. 3 and Table II).

TABLE I
Probability of finding SHO particle within a given area.

Order	Range	Eigenfunction probability	Approx. probability
10	[−2, 2]	99.5322265018953	99.535204873
20	[−4, 4]	99.9999984582742	99.999998529
30	[−6, 6]	$99.9_{12}97848$	100.00000004
40	[−7, 7]	$99.9_{18}96$	100.00000007

Note that the subscripts "12" and "18" are in replacement of the respective number of 9s in a row within the probabilities given.

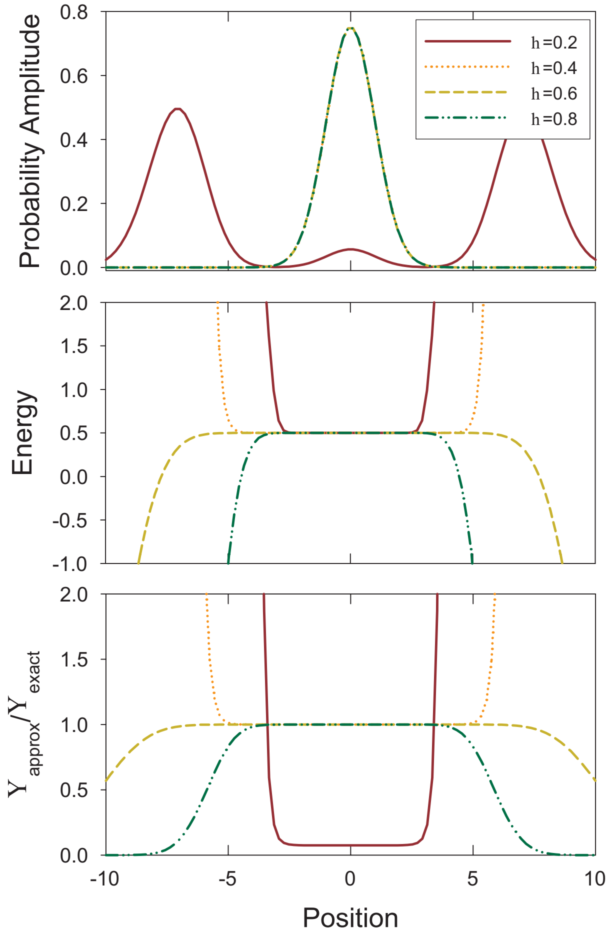

FIGURE 2. Example resultant functions for the Gaussian initial functions with $\eta = \{0.2,0.4,0.6, 0.8\}$, an iteration coefficient $\alpha = 0.001$, and keeping up through 20 orders in x. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

3.5. QUALITY OF APPROXIMATION

In any interesting system we will have a harder time finding out whether the solution that we have found actually approximates the energy eigenfunction and energy eigenvalue. If the same form of solution is found, with the same value for the energy, for a battery of cases, then we can be confident that the solution we seek is reasonably approximated by any one of these cases.

In analyzing the area over which the approximation is accurate we have used the ground state solution, but we will not be able to do this with a system in which there is no known closed form solution. It is then of interest to know that for this system we find that the area over which the energy is constant corresponds to the area over which the solution is accurate (see Fig. 4).

3.6. TRENDS

In performing the large number of cases we have identified trends as to the conditions under which the IO method will work. We have found that the likelihood of the method converging to a solution depends inversely on the order in x to which the approximation was truncated and, as might be expected, proportionally with the closeness of the trial function to the actual eigenfunction. This can be seen in Figure 5.

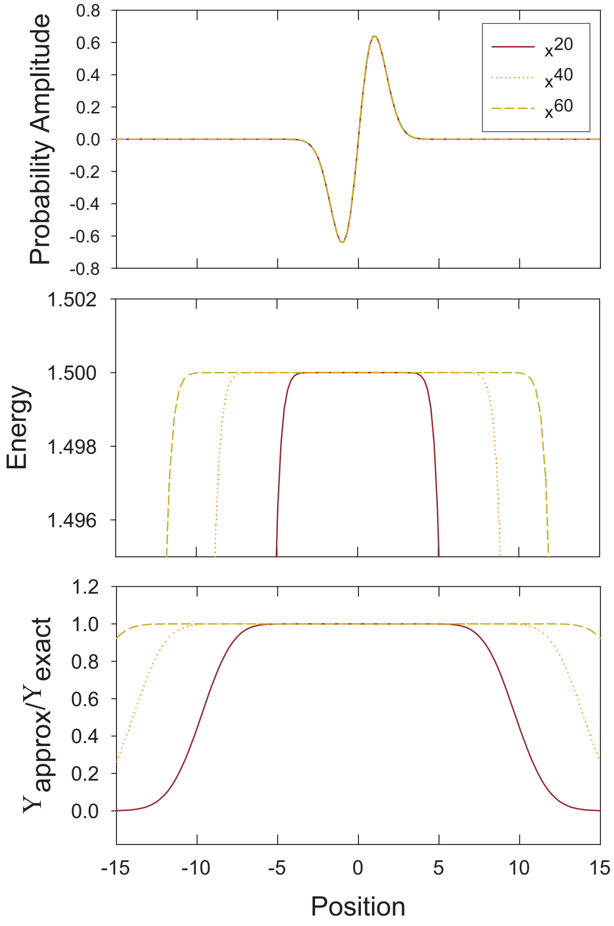

FIGURE 3. Results found for the first excited state of the SHO, using an iteration coefficient of $\alpha = 0.001$, the initial function $x^3 \exp[-0.4x^2]$, and keeping polynomials up to order x^p, where $p = \{20, 40, 60\}$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

TABLE II
Results for SHO with the trial function $\psi(x) = x_{\kappa}\exp[-0.6x^2]$.

κ	Energy	κ	Energy
0	0.5000000005	1	1.500000003
2	0.4999999966	3	1.500000000
4	0.4999999932	5	1.499999996
6	0.4999999900	7	1.499999992
8	0.4999999856	9	1.499999988
20	0.4999999646	21	1.499999973
22	0.4999999649	23	NR
24	NR	25	NR

NR, no result.

We also see what appears to be a lower bound on the iteration coefficient for which this method will work reliably. It was thought that the lower bound on the iteration coefficient might be an artifact of how many significant figures we keep. Maple®'s default setting is 10 significant figures. We ran a set of cases where the number of significant figures was increased to 50. We found that this produced no change in the bounding values of the iteration coefficient. We thus conclude that the iteration coefficient has a lower bound, at least for the method currently under consideration, but can give no mathematical reason for it.

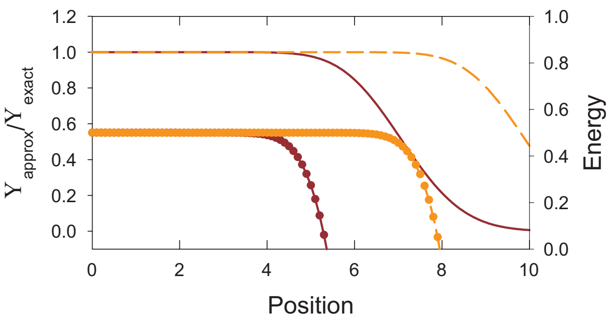

FIGURE 4. Example of how the region of close-fit corresponds to the region of constant energy for the case where $\alpha = 0.005$, $\eta = \sqrt{2}/2$. Top: Truncation after 20 orders in *x*. Bottom: Truncation after 40 orders in *x*. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

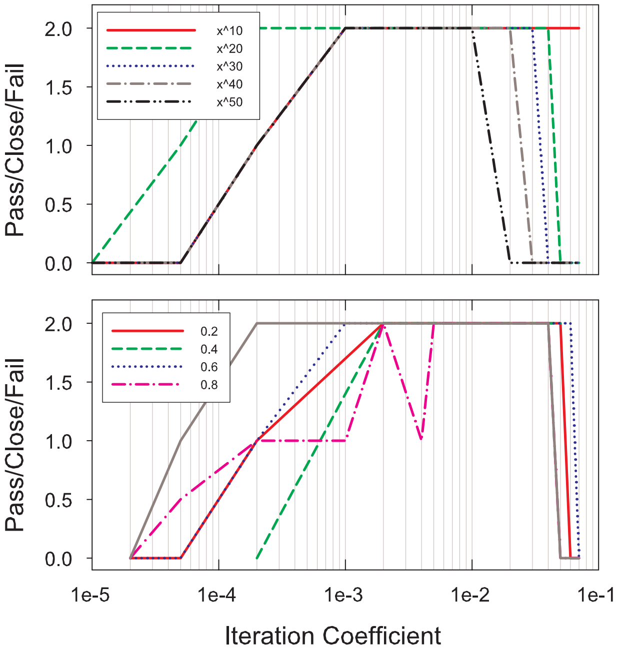

FIGURE 5. Graphical display of when the first-order iteration operator gives the proper result for the cases where $\eta = \sqrt{2}/2$. Top: Each line represents the order in *x* after which the solution was truncated; $\alpha = 0.005$. Bottom: Each line represents a value of the iteration constant; truncation after 20 orders in *x*. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

4. Anharmonic Oscillator

The potential used in this section is of the form

$$V(x) = \frac{m\omega^2}{2}x^2 + \lambda x^4. \tag{11}$$

We follow the works of others [5–7] and set the following: $\omega = 2$, $m = 0.5$, and $\lambda = \{0.1, 0.2, 0.3, 1, 2, 3\}$.

The leading order approximation [8] of the Schrödinger equation,

$$\psi(x) = \exp\left[\pm\frac{\sqrt{\lambda}}{3}x^3\right], \tag{12}$$

cannot be used because of its inability to satisfy the boundary conditions at $x = \pm\infty$ simultaneously. But suppose if we took the negative exponential in Eq. (12) and expand the x^3 in the following manner

$x^3 \rightarrow (x^2 + \xi)^{\frac{3}{2}}$, where ξ is a parameter chosen to give a good initial function, it results in a wave function of the form

$$\psi(x) = \exp\left[-\frac{\sqrt{\lambda}}{3}(x^2 + \xi)^{\frac{3}{2}}\right]. \tag{13}$$

When we go on to solve for the first excited state we make use of the symmetry of the potential and multiply Eq. (13) by x, changing the even function into an odd function,

$$\psi(x) = x\exp\left[-\frac{\sqrt{\lambda}}{3}(x^2 + \xi)^{\frac{3}{2}}\right]. \tag{14}$$

In practice, we chose values for ξ that were not small, $\xi = \{2, 4, 6, 8\}$, but we were able to find that these values worked in solving the problem.

4.1. PROCEDURE

For the cases of $\lambda = \{0.1, 0.2, 0.3\}$ we were able to find a range of values for ξ that would give a valid approximation. The initial function, Eq. (13), did not work for $\lambda = \{1, 2, 3\}$. Equation (13) was used for values of λ up through $\lambda = 0.5$. The resultant wave function for $\lambda = 0.5$ was then used as the initial function for the case of $\lambda = 0.6$. The result for $\lambda = 0.6$ was then used as the initial function for $\lambda = 0.7$. This step-up process was used incrementally to find approximations for the cases with $\lambda = \{1, 2, 3\}$.

4.2. RESULTS

While several cases (with different values for α and ξ) were run for each of the systems that were looked at, we will focus here only on the case that gave the best approximation for each system. The choice of the best result was based on the region, in position space, over which it gave a nearly constant local energy using Eq. (7). As was stated in Section 3, the region over which the energy is constant (or nearly so) is similar to the area over which the approximation of the wave function equals the eigenfunction. It should also be noted that the energy is constant over a region larger than the classically allowed region; this implies that the wave function is well approximated over the region where the particle is most likely to be found.

Figure 6 shows the approximate wave functions and energies for the ground state, respectively.

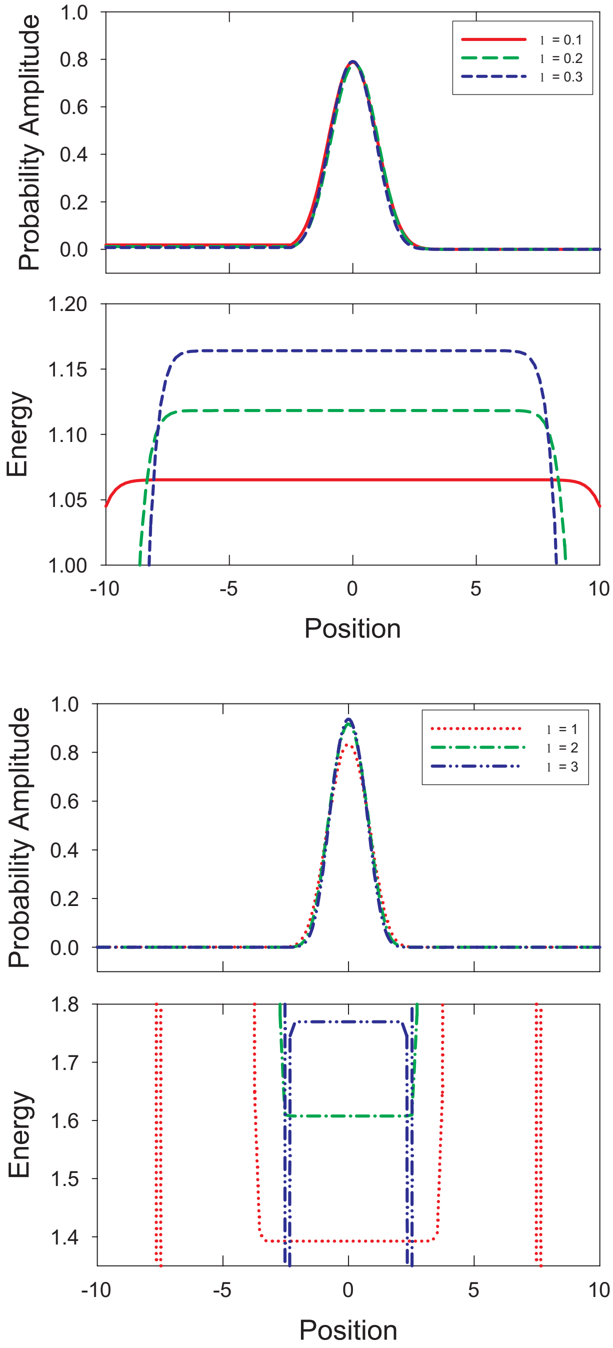

FIGURE 6. Examples of approximation of the ground state wave function and energy for different values of λ for the anharmonic oscillator. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

Table III shows quantitatively that the energy is roughly constant over a range that is around twice the width of the classically allowed region. We feel

TABLE III

Energy approximation, in natural units, for the ground state at several different points.

λ	Energy $_{x\,=\,0}$	Energy $_{x\,=\,1}$	Energy $_{x\,=\,2}$
0.1	1.065285510	1.065285509	1.065285519
0.2	1.118292650	1.118292661	1.118292701
0.3	1.164047149	1.164047166	1.164047175
1	1.392351640	1.392351641	1.392351647
2	1.607541302	1.607541294	1.607541364
3	1.769588840	1.769588857	1.769584287

confident that the best approximation of the energy eigenvalue can be found at the center of the anharmonic potential well, in this case at $x = 0$.

Figure 7 shows the wave functions and the energy approximations of the first excited state. The analysis is the same as in the ground state. Table IV displays the constancy of the energy approximation with what is the most likely best approximation of the energy at $x = 0$.

The second moment for the ground state and first excited state were calculated using

$$\langle x^2 \rangle = \int_{-10}^{10} \psi^*(x)\, x^2 \psi(x)\, dx, \tag{15}$$

where $\psi(x)$ is the solution given by the present method (see Table V).

4.3. COMPARISON WITH OTHER METHODS

Starting in the late sixties or early seventies after quantum field theorists started to see the importance of anharmonic oscillator-like potentials, a large effort was made in obtaining solutions to the Schrödinger equation of such systems. Bender and Wu [9] showed that perturbation theory failed to converge for any value of λ. The failure of convergence for the anharmonic oscillator was later proved by Simon and Dicke [10].

The perturbative energy levels were first found using Padé approximants by Reid [6]. Numerous other methods, both analytic and numerical, have been used in an effort to establish methods for solving this problem. We will compare our results with the results of Reid, Biswas et al. [7], and the effective operator [5]. It can be seen in Tables VI and VII that the present method is able to give energy eigenvalues which are in excellent agreement with those in other methods, with an explicit analytic form for the approximate wave function.

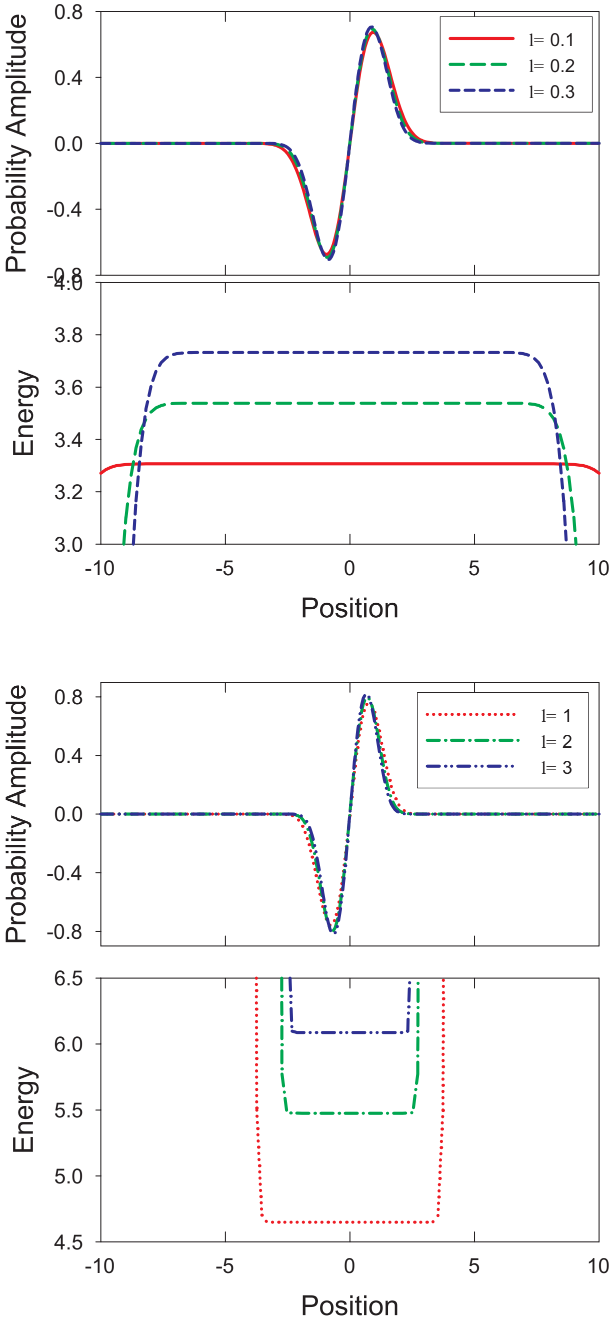

FIGURE 7. Examples of the first excited state wave functions and energy approximations of the anharmonic oscillator. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

TABLE IV

Energy approximation, in natural units, for the first excided state at several different points.

λ	Energy $_{x=0}$	Energy $_{x=1}$	Energy $_{x=2}$
0.1	3.306872014	3.306872004	3.306872008
0.2	3.539005273	3.539005288	3.539005290
0.3	3.732484278	3.732484274	3.732484261
1	4.648812705	4.648812698	4.648812712
2	5.475784528	5.475784532	5.475784586
3	6.086896438	6.086896434	6.086899518

TABLE VI

Comparison of the ground state energies.

λ	E_o	$\langle\hat{H}\rangle$	Effective operator [5]	Biswas et al. [7]
0.1	1.06528551	1.065285509	1.06529	1.06528550954
0.2	1.11829265	1.118292655	1.11831	1.11829265437
0.3	1.16404715	1.164047158	1.16407	1.16404715735
1	1.39235164	1.392351640	1.39238	1.39235164153
2	1.60754130	1.607541303	1.60757	1.60754130247
3	1.76958884	1.769611059	1.76962	1.76958884428

5. Modified Pöschl-Teller

In this section, we will discuss the accuracy of the energies and wave functions of the MPT potential well [11]. We chose to study this potential because its depth is easily varied by adjusting a parameter λ, allowing us to investigate how the accuracy of our results varied by changing the depth of the well. The MPT has the form

$$V(x) = \frac{1}{2m}a^2\frac{\lambda(\lambda-1)}{\cosh^2(ax)} \tag{16}$$

where $\lambda > 1$. Because the Taylor expansion of the potential produces powers of $1/x$ we chose to rewrite the potential as

$$V(x) = \frac{1}{2m}a^2\lambda(\lambda-1)\tanh^2(ax). \tag{17}$$

Using natural units the MPT well takes the form

$$V(x) = \frac{\lambda}{2}(\lambda-1)\tanh^2(x). \tag{18}$$

The potential has an absolute minimum at $x = 0$ (i.e., $V(0) = 0$) and is bounded above by $\lambda/2(\lambda-1)$ which approaches asymptotically as x approaches $\pm\infty$ (see Fig. 8).

The exact energy of the bound states is then given by

$$E_n = \frac{1}{2}(\lambda-1) + n\left(\lambda - 1 - \frac{n}{2}\right). \tag{19}$$

Because the energy of a bound state must be less that $1/2\lambda(\lambda-1)$ we can find how many bound states exist for a given λ. The result is that there are $n < (\lambda - 1)$, where n is an integer. Notice that there is always at least one bound state because we have assumed that $\lambda > 1$. This method is able to compute the ground state and first excited states of this

TABLE V

Second moments for the ground state and first excited state approximations.

λ	Ground	Excited
0.1	0.4690374046	1.263891213
0.2	0.4125253695	1.140746818
0.3	0.3885654659	1.058502237
1	0.3388630869	0.8012563761
2	0.2860134629	0.6628382181
3	0.2536595001	0.5892497696

The moments were calculated using the range $x = [-10, 10]$.

TABLE VII

Comparison of the first excited state energies.

λ	E_o	$\langle\hat{H}\rangle$	Effective operator [5]	Biswas et al. [7]
0.1	3.306872014	3.306872011	NA	3.30687201
0.2	3.539005273	3.539005288	NA	3.53900528
0.3	3.732484278	3.732484272	NA	3.73248427
1	4.648812705	4.648812705	NA	4.64881270
2	5.475784528	5.475784539	NA	5.4757845
3	5.086896438	6.086906450	NA	6.0868964

NA: no results using the effective operator have been reported.

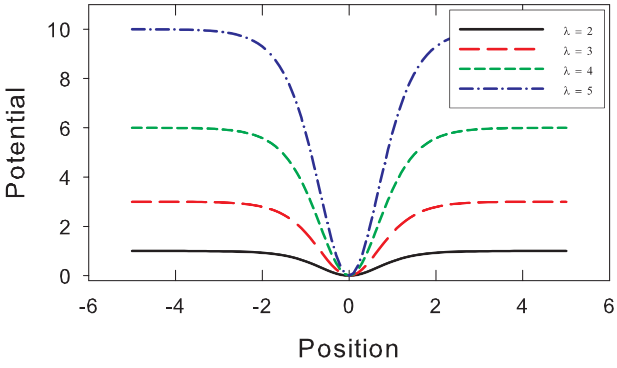

FIGURE 8. Examples of the modified Pöschl-Teller potential for different values of $\lambda = 2, 3, 4, 5$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

system. Their respective energies are given by $E_0 = 1/2(\lambda - 1)$ and $E_1 = 3/2(\lambda - 2)$.

We will also calculate the expectation value of the Hamiltonian, $\langle H \rangle$, to approximate the energy. We will use both methods in what follows.

5.1. GENERAL SOLUTION

Before considering how the IO responds to changes in well depth, we will first discuss the method of finding a solution to the MPT and the general properties of the IO observed in finding these solutions.

For the ground state, we chose our initial function to be a Gaussian of the form

$$\psi = \exp\left[-\frac{1}{2}\sqrt{\omega}x^2\right]$$

where ω is the coefficient of the x^2 term in the Taylor expansion of the potential well around $x = 0$. Thus,

$$\omega = \frac{1}{2}\lambda(\lambda - 1).$$

However, after some trial runs we found that this was not the best initial function. We found that, in general, the ideal initial function is a Gaussian of the form

$$\psi = \exp[-\varrho\sqrt{\omega}x^2] \tag{20}$$

where ϱ is a parameter that varies with well depth and number of terms kept in the polynomial approximation.

For the first excited state, we desire an odd initial function and so we choose $x\exp[-\varrho\sqrt{\omega}x^2]$, where again ϱ varies with well depth and the number of terms in the polynomial.

When determining which result is the best approximation to the actual solution, there are several factors to consider. First, we consider how closely the local $E(0)$ and $\langle H \rangle$ approximate the actual energy. Second, we consider the size of the region in which our approximation is valid. This region is estimated by the region over which the energy is constant. Because solutions to the MPT well are known, we can compare directly the approximate wave function with the exact solution. In particular, we will compare the ratio of the approximate solution to that of the exact solution. In the region where this ratio is ~1, the approximated solution is valid.

Consider the specific well depth given by $\lambda = 3$. This has a ground state energy of $E_0 = 1$. In this case, when retaining a polynomial of degree x^{44}, we found that the best solution was obtained by $p = 2.1 \pm 0.05$ (see Table VIII). We observe that for values of ϱ less than this the wave function has anomalies. Specifically, it has "bumps" on the wings of the decaying exponential (see Fig. 9). Because this behavior is not physical, we know that this result is not valid. It turns out that this is a general result; the best value of ϱ is the smallest value for which the wave function is well behaved.

As we compare the values of the energy (both $E(0)$ and $\langle H \rangle$) we find that for values of ϱ greater

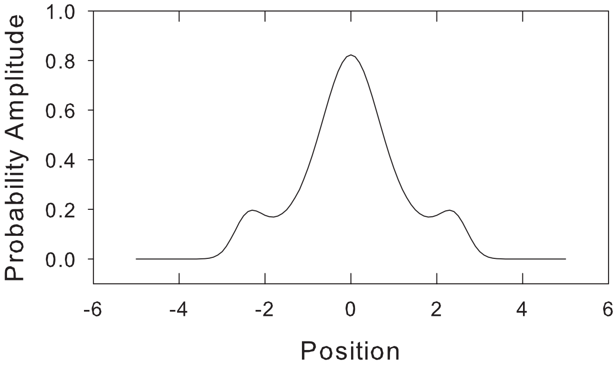

FIGURE 9. Example of an approximate wave function that is incorrect, when $\lambda = 3$, $\varrho = 1.9$, with the truncation at x^{44}. The bumps on either side of the maximum are unphysical.

TABLE VIII
Results for ground state energy using $\psi = \exp[-\varrho\sqrt{\omega}x^2]$, $\lambda = 3$ (exact energy = 1.0).

x^f	ϱ	Energy $E(0)$	% Error	$\langle H \rangle$	% Error	Comments
44	1.9	0.971089	−2.8911	1.132384	13.2384	Bumps
44	2.0	0.994280	−0.5720	1.004474	00.4474	Small bumps
44	2.1	1.000102	0.0102	1.000415	00.0415	
44	2.2	1.001876	0.1876	1.000927	00.0927	
44	2.3	1.002747	0.2748	1.001354	00.1354	
48	2.0	0.953635	−4.6364	1.383053	38.3054	Bumps
48	2.1	0.990169	−0.9831	1.015881	01.5888	Small bumps
48	2.2	0.998958	−0.1042	1.000463	00.0463	
48	2.3	1.001301	0.1301	1.000691	00.0691	
48	2.4	1.002212	0.2212	1.001110	00.1110	
52	2.1	0.925836	−7.4164	1.948836	94.8836	Bumps
52	2.2	0.983606	−1.6394	1.052664	05.2664	Small bumps
52	2.3	0.997363	−0.2637	1.001380	00.1380	Small bumps
52	2.4	1.000711	0.0711	1.000487	00.0487	
52	2.5	1.001775	0.1775	1.000910	00.0910	
56	2.3	0.972942	−2.7058	1.164430	16.4430	Bumps
56	2.4	0.994946	−0.5054		%	Small bumps
56	2.5	1.000011	0.0011	1.000350	00.0350	
56	2.6	1.001385	0.1385	1.000733	00.0733	
56	2.7	1.001981	0.1981	1.001039	00.1039	

than the ideal, both approximations are greater than the exact energy. As ϱ decreases, the approximated energies also decrease. As ϱ decreases below its ideal value, the $E(0)$ approximation decreases much more rapidly and is less than the exact energy, indicating that we have crossed the ideal value. This is not true for $\langle H \rangle$ because it is always above the exact energy, as expected. This result is also general.

As we keep larger polynomials in our approximation we find that the ideal value of ϱ changes. A larger polynomial always requires a larger value of ϱ (see Table VIII). As a general rule, keeping a larger polynomial does not correlate to a more accurate energy approximation. It seems that the key to having a good approximation of the energy is the proper initial function. This sensitivity of the final result on the initial function was not expected.

All of these results are valid for calculations of either the ground state or the first excited state.

As we investigate the range over which the wave function is valid, we find that the wave function with the most accurate energy approximation has the greatest range of validity (see Fig. 10). Thus, our two criteria for evaluating the accuracy of our approximations can both be met simultaneously.

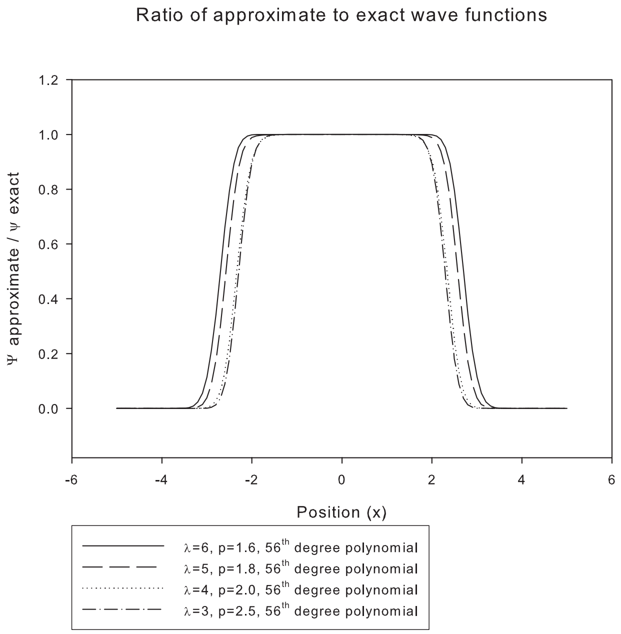

FIGURE 10. Ratios of the approximate wave function to the exact wave function. Observe that the range of validity increases as the accuracy of the approximate energy increases.

5.2. SENSITIVITY TO WELL DEPTH

Now considering various well depths we can see that for a given order polynomial, the ideal value of ϱ decreases as the depth of the well increases (see Table X).

We would like to compare the accuracy of the results obtained for different well depths. To do this, we must define a suitable measure for comparing approximations among different well depths. We have noted that for any well depth, the accuracy of the approximation is dependant on the initial function and not on the size of the polynomial. However, because there was some variation in accuracy as the size of the polynomial is adjusted, we will compare calculations using the same degree polynomial in the approximation.

We will also only compare the best results at each depth to the best results at any other depth. Having noted that the final result depends on a correct choice of initial function, this standard in the comparison deserves further comment. Clearly, finding the best result corresponds to finding the ideal value of ϱ, which, as noted, decreases with the depth of the well. Naturally, we will not require that the same value of ϱ be used at each depth. For each depth we found the ideal value of ϱ within an error of 0.1.

Finally, because a more accurate energy always correlates to a larger range of validity, we will compare the range on which the approximate wave functions are valid for different well depths. This facilitates a simple graphical comparison. By plotting the ratio of the approximate solution to the exact solution, we simply need to compare the range over which the ratios are ~1.

With this criterion established we can easily see that as the depth of the well increases, the accuracy of the approximate wave function increases (see Fig. 10 and Table IX).

As previously mentioned, we found the unexpected result that the accuracy of the resultant wave function had a strong dependence on the initial function, or ϱ value. By comparing the data in Table X, we can see how this dependence varies with well depth. Clearly, for deeper wells, we see that the same change in the value of ϱ results in a smaller change in the final result, particularly for values of ϱ near the ideal. Thus, we conclude that for deeper potential wells, the final result is less dependent on the initial function.

TABLE IX

Results for ground state energy using $\psi = \exp[-\varrho\sqrt{\omega}x^2]$ for various well depths using polynomial degree x^{56} and using the ideal value of ϱ [exact energy = $(\lambda - 1)/2$].

λ	ϱ	Energy $E(0)$	% Error	$\langle H\rangle$	% Error
3	2.5	1.000011	0.0011	1.000350	00.0350
4	2.0	1.500015	0.00099	1.500022	0.00146
5	1.8	2.000023	0.00116	2.000008	0.00039
6	1.6	2.500003	0.00013	2.500003	0.00010

6. Two-Dimensional SHO

Compared with the SHO in one-dimension, the 2D SHO is the most studied two-dimensional problem. We choose to study it here as proof of concept.

The potential for the 2D SHO may be defined as

$$V(x,y) = \frac{1}{2}x^2 + \frac{1}{2}y^2. \tag{21}$$

The ground and first excited state energies are $E = 1$ and $E = 1.5$, respectively. The first excited state is doubly degenerate coming from a mirror symmetry of the potential across the origin.

To solve for the ground state we chose initial functions of the form

$$\psi_{\text{initial}} = \exp[-\beta x^2 - \beta y^2] \tag{22}$$

where β ran from 0.2 to 2.

6.1. RESULTS FOR THE 2D SHO

Figure 11 gives an example of the resultant wave function, the corresponding energy, and a graph of $\psi_{\text{approx}}/\psi_{\text{exact}}$, where $\beta = 0.6$.

Results were also obtained for asymmetric initial functions. For example, the following initial function was used in one instance,

$$\psi_{\text{initial}} = y\exp[-0.6(x^2 + y^2)], \tag{23}$$

which resulted in obtaining the energy $E = 2.000000002$. Other trial functions were used and all of them found the expected energy values (see Table XI).

TABLE X
Results for ground state energy using $\psi = \exp[-\varrho\sqrt{\omega}x^2]$, polynomial degree x^{52} (exact energy = 1.5).

λ	ϱ	Energy $E(0)$	% Error	$\langle H \rangle$	% Error	Comments
4	1.7	1.493155	−0.45635	1.570634	4.70891	Bumps
4	1.8	1.499090	−0.06065	1.500839	0.05593	Small bumps
4	1.9	1.500003	0.00025	1.500023	0.00153	
4	2.0	1.500208	0.01386	1.500074	0.00493	
4	2.1	1.500322	0.02148	1.500118	0.00786	
4	2.2	1.500444	0.02960	1.500168	0.01121	
5	1.5	1.999546	−0.02272	2.001458	0.07288	Small bumps
5	1.6	1.999965	−0.00173	2.000005	0.00024	Small bumps
5	1.7	2.000023	0.00115	2.000007	0.00037	
5	1.8	2.000047	0.00235	2.000016	0.00079	
5	1.9	2.000075	0.00375	2.000020	0.00099	
5	2.0	2.000114	0.00569	2.000032	0.00161	

6.2. THE ADDITION OF AN ASYMMETRIC POTENTIAL

We also included different polynomial functions $\tilde{V}(x,y)$, of order equal to or less than 2, which are added to the 2D SHO potential. A list of the functions $\tilde{V}(x,y)$ and the resultant energies is given in Table XII. The resultant wave functions are stretched and contracted according to the way in which the potential is changed (see Fig. 12).

6.3. OBTAINING BETTER INITIAL FUNCTIONS

An interesting feature of the IO is that as the iteration coefficient increases, to somewhere around $\alpha = 0.005$, the energy draws closer to the ground state eigenvalue. Table XIII gives an example of how the energy decreases as the iteration coefficient increases. It appears that this is a general pattern. Another related feature is that the energy increases as α increases when the Gaussian coefficient $\eta < 1/2$ and the energy decreases as α increases when $\eta > 1/2$.

Knowing that the energy follows this general pattern may be of use in obtaining a better initial function. In the case of the 2D SHO the change of energy acts as a pointer to the actual value of β. If for some system where we do not know the form of the eigenstates we can find a parameter (or set of parameters) that causes the energy to act in this manner, then we can use this to obtain better values for these parameters.

7. Conclusion

We have shown that with the use of the present method we are able to obtain accurate approximations to the ground state and first excited state wave functions and energy eigenvalues. The quality of the result depends most heavily upon the initial function but also depends on the number of terms kept in the expansion and on the iteration coefficient. Assuming a good initial function, the area over which the resultant function shows a high correlation to the eigenfunction is limited by the number of terms kept in the expansion. It appears that with the ability to keep more terms the result can be as accurate as desired.

Appendix: Example Calculations

ONE-DIMENSIONAL CASE

We will perform an example calculation to show how the IO works in practice. The system which we will look at is the SHO. We will use units of $\hbar = m = \omega = 1$ throughout the rest of this work.

The IO has the form

$$\hat{I}_p = \left(1 + \frac{\alpha}{2}\frac{d^2}{dx^2} - \frac{\alpha}{2}x^2\right)^p. \tag{A1}$$

We will assume an initial function of the form

$$\psi(x) = \exp[-0.4x^2]. \tag{A2}$$

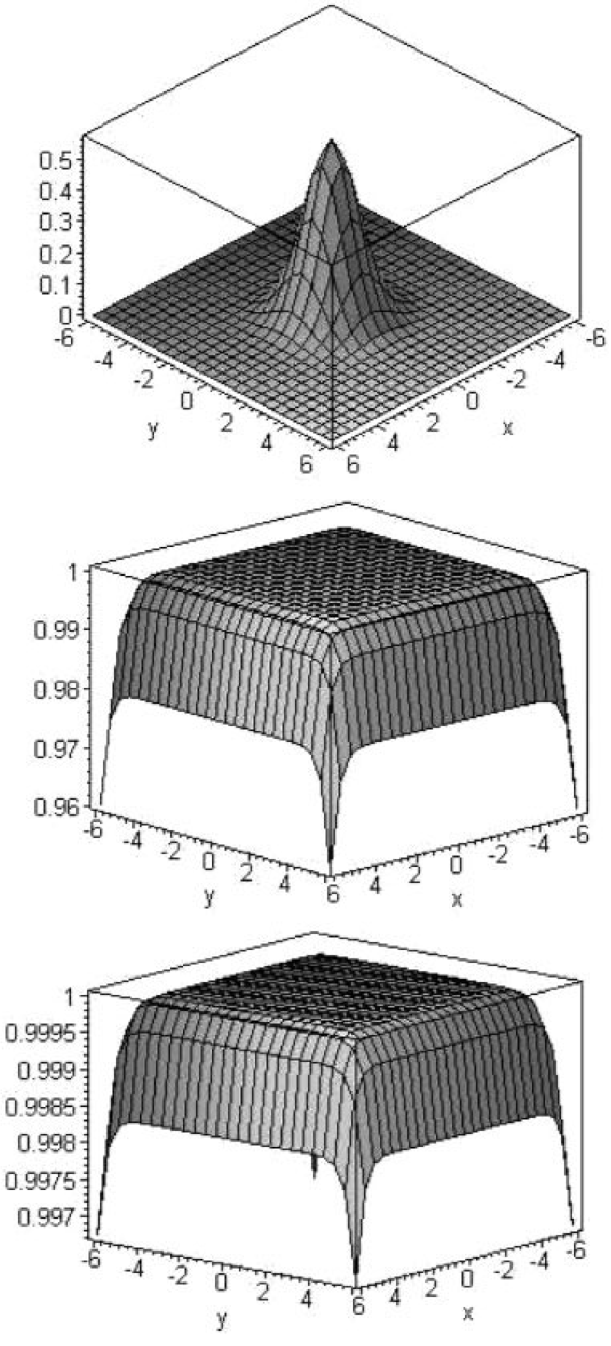

FIGURE 11. Normalized resultant wave function, energy, and fitness for the case where $\psi(x,y) = \exp(-0.6\,(x^2 + y^2))$ and $\alpha = 0.002$.

TABLE XI

Results of the iteration operator acting on the initial function $\psi_{\mathrm{initial}} = g(x,y)\exp[-0.6x^2]$, with the iteration coefficient $\alpha = 0.006$.

$g(x, y)$	Energy (natural unit)
x^3y	3.000000004
xy	3.000000007
$-xy$	3.000000002
x	2.000000004
y	2.000000002
x^2y	2.000000003
xy^2	2.000000002
x^2y^2	1.000000000

The IO is implemented on the computer in a loop similar to the following pseudo code:

```
PSI_INITIAL:=exp( − 0.4*Xs2̂)
PSI: = PSI_INITIAL
ALPHA:=0.001
FOR I=1 TO 20
PSI = {
    TRUNCATE_IN_X[
        (
        PSI+ALPHA/2*DIFF(DIFF(PSI,X),X)
        −ALPHA/2*X2̂*PSI
        )/PSI_INITIAL
    ]
  }*PSI_INITIAL
END FOR
```

After the first iteration,

TABLE XII

Results for the potential $V(x,y) = 1/2(x^2 + y^2) + \tilde{V}(x,y)$ with the initial function $\psi(x) = \exp[-0.6(x^2 + y^2)]$ and the iteration coefficient $\alpha = 0.004$.

$\tilde{V}(x,y)$	Energy (natural unit)
$0.2x^2$	1.091607978
$0.2xy$	0.994936153
$0.5x^2$	1.207106781
$2x^2$	1.618016108
x	0.500001014
x^2	1.366025355
$x + y$	0.9999999995
xy	0.9999999995

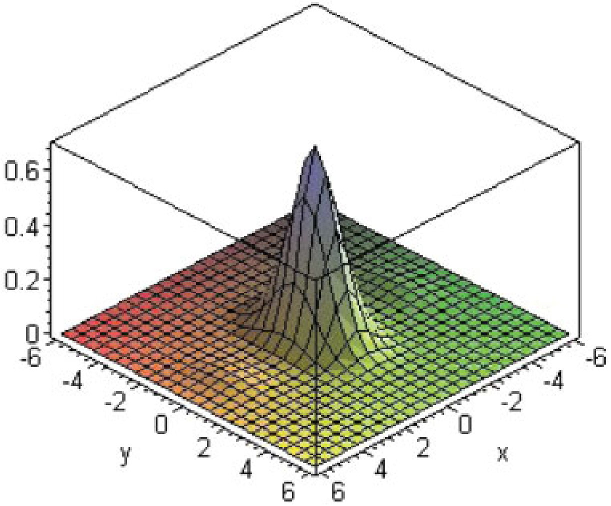

FIGURE 12. Resultant wave function for the added potential $\tilde{V}(x,y) = 2x^2$. [Color figure can be viewed in the online issue, which is available at www.interscience.wiley.com.]

$$\psi(x) = (0.9996 - 0.00018x^2)\exp[-0.4x^2].$$

After the second iteration,

$$\psi(x) = (0.99919998 - 0.000359568x^2 + 3.24 \cdot 10^{-8}x^4)\exp[-0.4x^2]. \quad \text{(A3)}$$

We have decided to keep terms up through order x^2, and thus we divide Eq. (A3) by $\exp[-0.4x^2]$, leaving

$$\frac{\psi(x)}{\exp[-0.4x^2]} = (0.99919998 - 0.000359568x^2 + 3.24 \times 10^{-8}x^4).$$

Then truncating the polynomial,

$$(0.99919998 - 0.000359568x^2 + 3.24 \times 10^{-8}x^4) \rightarrow (0.99919998 - 0.000359568x^2),$$

after which we multiply the exponential back onto the truncated polynomial

$$\psi(x) = (0.99919998 - 0.000359568x^2) \exp[-0.4x^2].$$

After the third iteration the wave function has the form

$$\psi(x) = (0.99879994 - 0.0005387047x^2 + (9.70056 \times 10^{-8}x^4)\exp[-0.4x^2]$$

Again we divide off the exponential, truncate the remaining polynomial, and multiply the exponential back on, leaving the approximate wave function in the form

$$\psi(x) = (0.99879994 - 0.0005387047x^2) \exp[-0.4x^2].$$

This is used in the next iteration, the result of which is used in the next, and so on. After 20 iterations ($p = 20$) the wave function is of the form

$$\psi(x) = (0.9919966979 - 0.003518678753x^2) \exp[-0.4x^2].$$

TWO-DIMENSIONAL CASE

Suppose now that we have a system that has a potential $V(\vec{x})$ that is functionally symmetric, in the sense that if $V(\vec{x})$ has a term such as

$$V(\vec{x}) = \ldots gx^4y^2\ldots, \quad \text{(A4)}$$

then there is also a corresponding term

$$V(\vec{x}) = \ldots gx^2y^4\ldots. \quad \text{(A5)}$$

If we have such a potential then the ground state of the system will also be functionally symmetric.

Because truncations can only be made in one variable at a time, functional symmetry is lost if we

TABLE XIII

The computed energy of the approximation draws closer to the ground state eigenvalue as the iteration coefficient increases with $\beta = 0.6$.

Iteration coefficient	Energy
0.00002	1.129782752
0.00004	1.085169262
0.00006	1.056295463
0.00008	1.037384696
0.0002	1.003330308
0.0004	1.000060612
0.0006	1.000001102
0.0008	1.000000019
0.002	1.000000000

use Eq. (5) and then truncate the result of each iteration first in x and then in y. Thus Eq. (5) needs to be symmetrized, once with truncating in x first and then truncating in y. The second use of Eq. (5) reverses the order truncation. After both are done we add the two results together.

```
PSI_INITIAL:=exp( − 0.4*(X^2 + Y^2))
PSI:=PSI_INITIAL
ALPHA:=0.001
FOR I=1 TO p
PSI={
  TRUNCATE_IN_Y(
    TRUNCATE_IN_X[
      (
      PSI+ALPHA/2*(DIFF(DIFF(PSI,X),X)
      +DIFF(DIFF(PSI,Y),Y))
      V(X,Y)*PSI
      )/PSI_INITIAL
    ]
  )
+
    TRUNCATE_IN_X(
      TRUNCATE_IN_Y[
        (
        PSI+ALPHA/2*(DIFF(DIFF(PSI,X),X)
        +DIFF(DIFF(PSI,Y),Y))
        V(X,Y)*PSI
        )/PSI_INITIAL
      ]
    )
  }*PSI_INITIAL
END FOR
```

As an example of such an operation we will perform the first few iterations of the 2D SHO calculation. We will use the following forms for the IO and initial function:

$$I_p = \left[1 + \frac{\alpha}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{\alpha}{2}(x^2 + y^2)\right]^p, \quad \text{(A6)}$$

$$\psi = \exp[-\beta(x^2 + y^2)]. \quad \text{(A7)}$$

If we set $\alpha = 0.002$ and $\beta = 0.6$, the first two iterations are

$$\psi_1 = (0.9976 + 0.00044x^2 + 0.00044y^2) \exp[-0.6x^2 - 0.6y^2],$$

$$\psi_2 = (0.99520752 + 0.000875776x^2 + 0.000875776y^2 + (3.872 \times 10^{-7})y^2x^2 + (1.936 \times 10^{-7})x^4 + 1.936 \times 10^{-7}y^4)\exp[-0.6x^2 - 0.6y^2].$$

A three-dimensional system would work similarly.

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