ITERATION METHODS FOR APPROXIMATING THE LOWEST ORDER ENERGY EIGENSTATE OF A GIVEN SYMMETRY FOR ONE- AND TWO-DIMENSIONAL SYSTEMS

by

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ABSTRACT

ITERATION METHODS FOR APPROXIMATING THE LOWEST ORDER ENERGY EIGENSTATE OF A GIVEN SYMMETRY FOR ONE- AND TWO-DIMENSIONAL SYSTEMS

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Master of Science

Using the idea that a quantum mechanical system drops to its ground state as its temperature goes to absolute zero several operators are devised to enable the approximation of the lowest order energy eigenstate of a given symmetry; as well as an approximation to the energy eigenvalue of the same order.

ACKNOWLEDGMENTS

First and foremost, thanks be to Him from whom all blessings flow.

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Chapter 1

Introduction

1.1 The Need for Approximation Methods

Quantum mechanics text books focus on a few problems, and variations thereof, that are easily solved or approximated by analytic methods. These examples are a good representation of techniques that are used to solve simple problems that can be abstracted to appear like actual quantum mechanical systems. The problem is that solving the Schrödinger equation for anything but systems with simple potentials proves to be difficult at best. Some of the approximation methods developed require the integration of functions that contain the potential (i.e. variational method, perturbation method), thus making approximation a difficult task as well. We also find that some of the methods are only valid in certain limiting cases; for example, the WKB method assumes that the potential varies slowly as a function of position.

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 only computes the value of the solution at a finite number of points. This allows for the possible loss of important information. Second, 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.

A method by which an analytic approximation to the solution can be found, with relative ease, is desirable. We are developing such a method.

1.2 Lay Man's Motivation to the Iteration Operator

Given a function ψ which describes a state of a system we can decompose ψ into a sum of eigenfunctions $|\varphi_n\rangle$ of some operator, say the Hamiltonian, for that system

$$|\psi\rangle = \sum_{n=0}^{\infty} a_n|\varphi_n\rangle. \tag{1.1}$$

Suppose we define the following operator

$$\hat{I}_p = (1 - \epsilon(\hat{H} - E_0))^p, \tag{1.2}$$

where $\hat{H}$ is the Hamiltonian of the system and $\epsilon \ll 1$. Then we find

$$\hat{I}_1|\psi\rangle = \sum_{n=0}^{\infty} a_n|\varphi_n\rangle - \epsilon(\hat{H} - E_0)\sum_{n=0}^{\infty} a_n|\varphi_n\rangle = \sum_{n=0}^{\infty} a_n(1 - \epsilon(E_n - E_0))|\varphi_n\rangle, \tag{1.3}$$

which subtracts off a little of each eigenstate, other than the ground state, from the initial function. Not only does it subtract off a little of each eigenstate but it subtracts off a different amount of each eigenstate correlating to the energy of that eigenstate. So the lower order eigenstates have less of themselves subtracted off than the higher order eigenstates. If this is done a large number $p \gg 1$ of times then all that is left is the ground state (or state of lowest order of some given symmetry) plus a little of the lower order states. The result is an approximation to the ground state wave function multiplied by the factor a_0

$$\hat{I}_p|\psi\rangle \approx a_0|\varphi_0\rangle. \tag{1.4}$$

1.3 Rigorous Derivation of the First Order Iteration Operator

We start with the Schrödinger Equation and modify it by subtracting off some value E_o from the Hamiltonian; doing this will shift the energy levels without changing the form of the solution,

$$i\frac{\partial\psi(x,t)}{\partial t} = (\hat{H} - E_o)\psi(x,t). \tag{1.5}$$

Any solution $\psi(x,t)$ of Equation 1.5 can be expanded in the basis of eigenfunctions of $\hat{H}$

$$\psi(x,t) = \sum_n a_n\phi_n(x,t) \tag{1.6}$$

Then the time development of the eigenfunctions can be written in terms of the modified Hamiltonian

$$\phi_n(x,t) = e^{-i(\hat{H}-E_o)t}\phi_n(x) \tag{1.7}$$

If we make the substitution $i\,t = \tau$ in Equation 1.7 then we find

$$\psi_n(x,\tau) = e^{-(\hat{H}-E_o)\tau}\phi_n(x) = a_o e^{-(E_o-E_o)\tau}\phi_o(x) + \sum_{n=1}^{\infty} a_n e^{-(E_n-E_o)\tau}\phi_n(x). \tag{1.8}$$

from which we see that the only term that does not go to zero as $\tau \to \infty$ is the one that contains the ground state eigenfunction.

Suppose we now form a first order expansion of the imaginary-time evolution operator

$$e^{-(\hat{H}-E_o)\tau} = \lim_{m\to\infty}(1 - \frac{\tau}{m}(\hat{H}-E_o))^m \approx (1 - \frac{\tau}{p}(\hat{H}-E_o))^p, \tag{1.9}$$

where instead of taking the limit as $m \to \infty$ we set m to some large natural number p.

In practice we can further simplify the operator by defining a constant

$$\alpha = \frac{\tau}{p}, \tag{1.10}$$

which will allow for the computation times to be shorter. By setting α to some arbitrary value we can force $\tau \to \infty$ as $p \to \infty$. Since we cannot pick p to be infinity and still have an algorithm that runs in a finite amount of time, we must settle with setting p equal to some large number and obtaining the Iteration Operator,

$$\hat{I}_p = (1 - \alpha(\hat{H} - E_o))^p. \tag{1.11}$$

In practice we do not need the ground state energy before approximating the solution. We will see that we can actually set E_o to any of a range of values and still obtain a good approximation; thus we will write the first order Iteration Operator as

$$\hat{I}_p = (1 - \alpha(\hat{H} - E))^p. \tag{1.12}$$

1.4 Second Order Iteration Operator

We can redefine the Iteration Operator by expanding the diffusion operator to second order,

$$e^{-\tau(\hat{H}-E_o)} = \lim_{n\to\infty}(1 - \frac{\tau(\hat{H}-E_o)}{n} + \frac{\tau^2(\hat{H}-E_o)^2}{n^2})^n. \tag{1.13}$$

Following the procedure outlined for the first order Iteration Operator we obtain the second order Iteration Operator from Equation 1.13,

$$\hat{I}_p := (1 - \alpha(\hat{H}-E) + \alpha^2(\hat{H}-E)^2)^p. \tag{1.14}$$

1.5 Other Configurations of the Iteration Operator

The first and second order Iteration Operators both come from a straightforward expansion of the diffusion operator. Hicken and Berrondo [1], developed a radically different form of the Iteration Operator,

$$\hat{I}_p := e^{-\varepsilon V/2}[2/3 + 1/2(e^{\sqrt{3\varepsilon}\nabla} + e^{-\sqrt{3\varepsilon}\nabla})]e^{-\varepsilon V/2}. \tag{1.15}$$

While they used it with success in performing numerical calculations, we found it to be too burdensome[1] in analytic calculations and thus will not discuss it much in this work.

Another form of the Iteration Operator was attempted which involved the use of Fourier integrals. For example, in the one-dimensional case:

$$\hat{I}_p\psi(x) := \frac{1}{2\pi}\, e^{-aV(x)/2}\int_{-\infty}^{\infty} e^{-ak^2/2}\int_{-\infty}^{\infty} e^{-aV(x)/2}\,\psi(x)\,e^{ikx}\,dx\,e^{-ikx}\,dk, \tag{1.16}$$

where it should be noted that the $\partial/\partial x$ in position space becomes k in momentum space. This method uses a extremely large amount of computing power[2], and was thus forsaken.

---

[1] The problem comes from the fact that the displacement operator $exp(\sqrt{3\varepsilon}\nabla)$ translates x by $\sqrt{3\varepsilon}$ resulting in $f(x) \to f(x+\sqrt{3\varepsilon})$. I tried running several cases of this method for the quartic potential well and found that after only a few iterations the result became horribly complicated.

[2] I ran several cases for the Fourier integral formulation of the Iteration Operator in Maple® 7 on a PC with a 1.3 MHz CPU, 258 MB RAM, and running Windows® 2000; in each case I finally stopped Maple® after it had ran for three days and found that it had only completed around eight iterations.

1.6 The Value of E in the Iteration Operator

For simplicity in the remainder of this section we will assume a system where all eigenvalues are positive.

Until now we have set the value of E in the Iteration Operator to be zero, and have found that this works perfectly well in obtaining good approximations to the eigensolutions. The reason for this is that as we set E to some value we have the following trichotomy:

$$\lim_{\tau\to\infty} e^{-(E_n-E)\tau} = \begin{cases} \infty, & \text{if } (E_n - E) < 0; \\ 1, & \text{if } (E_n - E) = 0; \\ 0, & \text{if } (E_n - E) > 0. \end{cases} \tag{1.17}$$

As we have stated earlier, if $E = E_0$ then as $\tau \to \infty$ we are left with only the ground state eigenfunction. But what if we set $E < E_0$? Setting $E < E_0$ causes $e^{-(E_n-E)\tau} \to 0$ as $\tau \to \infty$; but in our approximation we do not actually get to the point where τ is infinite. We find then that all of the terms are dropping to zero but not at the same rate. The higher order terms fall off faster than the lower order terms; thus the ground state falls off the slowest. If we only take τ to some large but finite number then we are left with the ground state plus smaller amounts of the lower order states. If we set $E_0 < E < E_1$ then as $\tau \to \infty$ the ground state becomes exponentially large, while all of the other terms go to zero. As before, since we will not actually take τ to infinity we will end up with the ground state times some large constant which can be normalized. Or if $E_N < E_{N+1}$ then all of the states $n \leq N$ blow up the lowest order states the fastest, and all of the states $N+1 \leq n$ will fall to zero. Again, we are taking the limit as τ goes to some large but finite value; thus, the ground state grows large the quickest followed in turn by each of the states of order less than N. A simple example might be illustrative.

The 1-dimensional simple harmonic oscillator has eigenfunctions of the form

$$\phi_n(x) := A_n\, H_n(x)\, e^{-\frac{1}{2}x^2}, \tag{1.18}$$

with natural units, where A_n is the normalization constant and $H_n(x)$ is the n^{th} order Hermite polynomial. The corresponding energies are given by

$$E_n = n + \frac{1}{2}. \tag{1.19}$$

Suppose now that we want to take the superposition of all of the eigenfunctions and evolve them in imaginary-time according to

$$\phi_n(x,\tau) = e^{-(\hat{H}-E)\tau}\phi_n(x) = e^{-(E_n-E)\tau}\phi_n(x), \tag{1.20}$$

from $\tau = 0$ to $\tau = 10^5$and we set $E = 2.5$. We find

$$\psi(x, 10^5) = \sum_{n=0}^{\infty} e^{-(E_n-2.5)10^5} a_n\, H_n(x)\, e^{-\frac{1}{2}x^2}, \tag{1.21}$$

where a_n is the summation constant that allows for normalization. Let's look at the first several terms of this summation

$$\begin{aligned} \psi(x, 10^5) =& 7.877 * 10^{86858}\, a_0\, H_0(x)\, e^{-\frac{1}{2}x^2} + 2.807 * 10^{43429}\, a_1\, H_1(x)\, e^{-\frac{1}{2}x^2} \\ &+ a_2\, H_2(x)\, e^{-\frac{1}{2}x^2} + 3.562949565 * 10^{-43430}\, a_3\, H_3(x)\, e^{-\frac{1}{2}x^2} \\ &+ \dots \end{aligned} \tag{1.22}$$

1.7 Finding States Other Than The Ground State

Our derivation of the first order Iteration Operator involved taking some wave function ψ which was in general a linear combination of all of the energy eigenstates of the system. Suppose now that we do not want to find the ground state but the lowest order state of some symmetry. In order to do this we must find an initial function that is orthogonal to the ground state wave function and within the space of functions which belong to that symmetry. For example, if we have a symmetric potential then each of the eigenfunctions of the system is either even or odd. Thus, in order to find the lowest order odd eigenstate we must provide an initial function that is odd.

1.8 Boundary Conditions

When analytically solving (partial) differential equations one first acquires the general solution and then applies boundary conditions to obtain the particular solution. In numerical methods one must deal with boundary conditions as an integral part of the difference equations. With the Iteration Operator method, as with variational methods, one must start with a trial function that satisfies the boundary conditions. Not only must the trial function satisfy the boundary conditions but it must ensure the boundary conditions for each of the iterations. An example will be given in Section 2.4 of what happens when a trial function does not satisfy these conditions. Asymptotic analysis provides a method for choosing a trial function that will satisfy the appropriate boundary conditions.

1.9 Energy Approximation

The method by which we decide if we have a close approximation to the energy eigenfunction being sought is by looking at the "energy" of the system E,

$$E(x) = \frac{\hat{H}\psi(x)}{\psi(x)}, \tag{1.23}$$

where $\psi(x)$ is the resultant wave function.

If Equation 1.23 gives a constant value for the energy over some region of space then we can be relatively sure that we have found the eigenfunction of the system and the eigenvalue is equal to the constant energy. The preceding statement must be qualified by saying that the value obtained for the energy can be found to be stable without being close to the right value by not taking enough terms in the expansion of the wave function, as will be seen in Sections 3.2.

1.10 Implementation On The Computer

Each iteration of the iteration operator adds terms to the resultant wave function. The addition of terms thus forces us to truncate the resultant wave function after each iteration. The truncation is accomplished by dividing out the exponential portion of the initial function and then truncating the remaining polynomial. The result of this is multiplied by the exponential portion of the initial function.

It must also be noted that we want to run the approximation for enough iterations that we will be sure that the solution calculated has settled down to a particular solution. Thus, as we will see for the Simple Harmonic Oscillator, because the form of the solution stops changing significantly after several thousand iterations we will run the simulations for ten thousand iterations to be sure that we have given each case time to settle down.

Examples of the implementation in both Mathematica® and Maple® are given in Appendix A.

1.11 Classification of The Approximation.

In studying the behavior of the Iteration Operator we ran a large number of cases for each system, where each case had certain differences in the values of the parameters used in the Iteration Operator method (i.e. the value of α, the number of iterations, the form of the initial function). With running large numbers of cases for each system comes the problem of having a quick and easy method of classifying results. We need a system that allows us to see any trends in how the Iteration Approximation method succeeds or fails to give a correct approximation to the ground state wave function and energy. A quick and dirty method of classification is as follows:

1. If a case gives a constant energy over an area of position space within and around the classically allowed region then we will say that it "passes" and assign a "2" to it.
2. If a case gives an almost constant energy within and around the classically allowed region of space then we will say that it is "close" and assigned it a "1."
3. If a case does neither of the first two possibilities then we will say that it "fails" and assign it a "0."

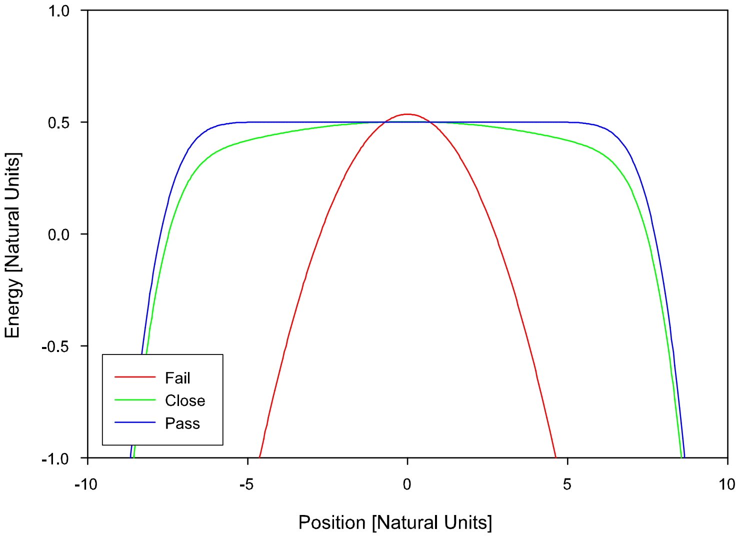


Figure 1.1: Examples of Pass, Close, Fail.

Examples of each of these cases is given for the Simple Harmonic Oscillator in Figure 1.1. The numbers are assigned so that one can look at the results in the form of graphs as well as tables.

Chapter 2

The 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, can be found analytically, and the boundary conditions are a natural result of the potential. We will use the SHO to explore the functionality of the Iteration Operator method of approximation.

2.1 Guassian Trial Function

We would like to use asymptotic analysis to give us a trial function for use in the Iteration Operator method. Unfortunately, the asymptotic solution happens to be the unnormalized ground state eigenfunction. Since using the ground state eigenfunction would do us little good in discovering the intricacies of this method, we will use as initial functions Gaussians of the form

$$\psi(x) = e^{-\eta x^2}, \tag{2.1}$$

where $\eta = \{0.2, 0.4, 0.6, 0.8, 1.0, 2.0\}$. Using Gaussians of this form seems to be a reasonable way of probing the use of the iteration method because the asymptotic solution is going to have the basic form of the eigenfunction though maybe not in the right proportions.

2.1.1 First Order Iteration Operator

Using Equation 1.12 with $E = 0$ the first order Iteration Operator of the SHO is given by

$$\hat{I}_p := (1 + \frac{\alpha}{2}\frac{d^2}{dx^2} - \frac{\alpha}{2}x^2)^p. \tag{2.2}$$

In solving for the ground state energy eigenvalue and eigenfunction a range of iteration coefficient values, from $\alpha = 0.00002$ to $\alpha = 0.07$, are 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 η.

As was stated in the last chapter, the correct approximation is said to be found if the energy is constant over a range in position. From Figure 2.1 we see that the area over which the energy is found to be constant, for a particular choice of α and η, is directly dependent on the magnitude of the order in x to which the approximation is taken to. It is also seen if we divide the approximate wave function by the eigenfunction, and graph that with respect to position, that the area over which the approximation essentially equals the eigenfunction expands with increasing order in x; see Figure 2.2. Note also that both the region of constant energy and the region where $\psi_{approximate}/\psi_{eigenfunction}$ equals one are, for all orders of x computed, at least a couple times larger than the area enclosed by the classical turning points. This is encouraging; while we would like the approximation to be accurate for all of space, and thus be *the solution*, this ensures us that the approximation is meaningful. Table 2.1 lists the probability of finding the particle within the area enclosed by each approximation.

Order	Endpoints	Eigenfunction Prob.	Approximation Prob.
10	$x = \pm\ 2$	99.5322265018953	99.5352048735378
20	$x = \pm\ 4$	99.9999984582742	99.9999985294360
30	$x = \pm\ 6$	99.999999999999997848	100.00000004956711271
40	$x = \pm\ 7$	99.9999999999999999999958	100.00000007339472218

Table 2.1: Probability of finding SHO particle within a given area.

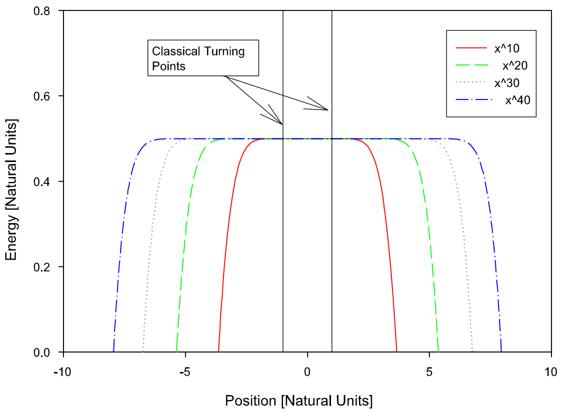


Figure 2.1: Example of how the region of constant energy increases with order in x. For the cases where $\alpha = 0.005$ and $\eta = \sqrt{2}/2$.

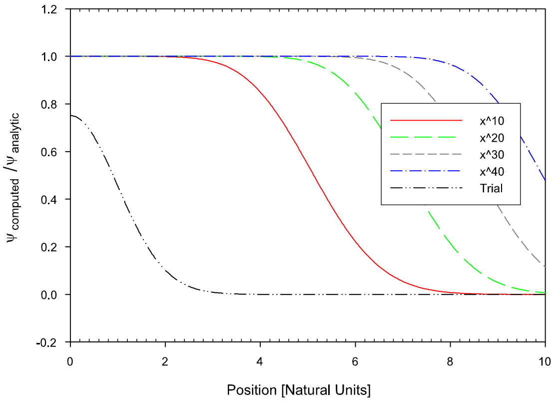


Figure 2.2: Example of how the region of close fit increases with order in x. For the cases where $\alpha = 0.005$ and $\eta = \sqrt{2}/2$.

The Iteration Operator is a method to approximate the lowest order state of a given symmetry, not just the ground state. The solutions to the Schrödinger equation with a symmetric potential, centered at the origin, always have a definite parity. Thus far we have focused on finding the ground state wave function which is the eigenfunction of the lowest order that is even about $x = 0$. We can also find the first excited state which is the lowest order state that is odd. A suitable trial function for the first excited state is

$$\psi(x) = x^{\kappa} e^{-\eta x^2}, \tag{2.3}$$

where κ is any odd number. Cases which have been investigated include $\kappa = 1, 3, 5, 7, 9, 21, 23, 25$ and most of these have produced satisfactory results, see Table A.1.

It should be noted that Equation 2.3 also allows for even trial functions; suitable results have been found for the ground state energy eigenfunction and energy eigenvalue for $\kappa = 2, 4, 6, 8, 20, 22$.

2.2 An Incorrect Approximation

In taking a closer look at the solutions to the SHO we notice that there is a class of initial conditions for the Iteration Operator and its initial function that results in the failure to obtain a "good" approximation to the ground state eigenfunction. In all cases where the constant $\eta = 0.2$ in the initial function, the resultant function gives the appropriate energy and is a Gaussian with the appropriate width but has a wing on each side, as can be seen in Figure 2.3.

This sort of approximation is obviously incorrect, but we can argue that while the approximation is not what we desire, it will work when we cannot find anything better. Since the approximation gives the correct energy then we know the classical turning point and we can say that the wave function should be falling to zero outside of the classically allowed region and thus these wings should be discarded. We can then normalize the approximation over the range of the classically allowed region. Again this sort of "normalization" isn't mathematically kosher, but it is better than

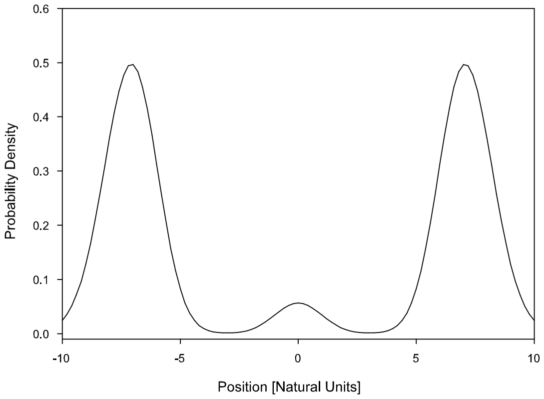


Figure 2.3: Example resultant function for when the the trial function had $\eta = 0.2$, for the case where $\alpha = 0.002$.

nothing. We are thus left with an approximation that will work as long as we do not stray far from the classically allowed region.

2.3 The Offset SHO

Offsetting the minimum of the potential, so that it is centered at some point $x = a$, does not change the form of the solutions of the Schrödinger equation in any way other than centering them around $x = a$. It is thus expected that the Iteration Operator method will give the proper approximations to the offset SHO potential.

We choose to center the SHO potential at the point $x = 2$. It is thus reasonable to center the initial wave function around $x = 2$,

$$\psi(x) = e^{-\eta(x-2)^2}. \tag{2.4}$$

It also necessary to expand the series around $x = 2$.

Doing all of this leads to results similar to what was found with the SHO centered around $x = 0$, as expected.

The real question in all of this is what happens if we center the trial wave function around a point other than $x = 2$ and expand the resultant wave functions around the same point. In doing this we find that in spite of starting with a Gaussian that is centered around some point, say $x = 1$, we end up with some thing that looks

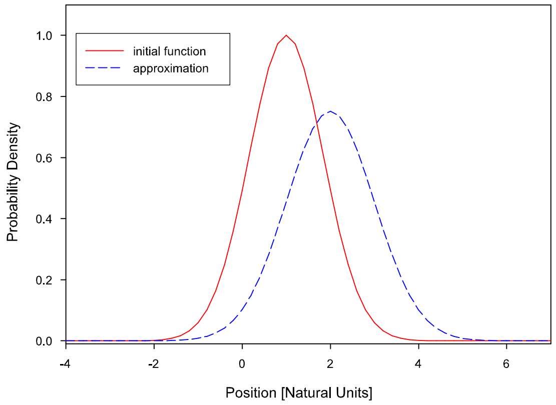


Figure 2.4: Result of starting with a wave function centered around the point $x = 1$ and expanding around the same point, when the potential is centered at $x = 2$.

like a Gaussian centered around $x = 2$; see Figure 2.4. We find, not unexpectedly, that the resultant wave function is not as good as if we started with a Gaussian centered around $x = 2$.

The result that even if we center the initial wave function, and expand the resultant wave functions, around the wrong point we still get a proper approximation is important because of its possible implications for harder systems. Say, for example, we have a system in which the potential is not symmetric around any point; how do we know where to center our trial wave function? We don't, but we can make guesses, and as we have seen here, if we make a guess that is close we will still get an approximation to an eigenfunction.

2.4 The sin(x)/x Initial Function

Suppose now that we try the initial function

$$\psi_0 = \frac{\sin(x)}{x}. \tag{2.5}$$

While such a trial function is finite over all space and falls to zero as $x \rightarrow \infty$, after only one iteration the wave function has a term that diverges as $x \rightarrow \infty$,

$$\psi_1 = .999\frac{\sin(x)}{x} - .001x\sin(x) - \frac{.002\cos(x)}{x^2} + .002\frac{\sin(x)}{x^3}. \tag{2.6}$$

Successive iterations gain terms that diverge even faster. This leads us to the belief that for an initial function to work it, and all of its derivatives, must fall to zero faster then the potential blows up at the boundaries.

2.5 Insights On The Iteration Operator Method

In any interesting system (a system where we don't know the solution from other methods) we will have a harder time finding out if 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 Figure 2.5). We will talk more of this in later chapters.

In performing the large number of cases we have identified trends as to the conditions under which the Iteration Operator 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 2.6.

In Figure 2.6 we 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 increase to 50. We found that this produced no change in the bounding values of the iteration coefficient. We thus conclude that

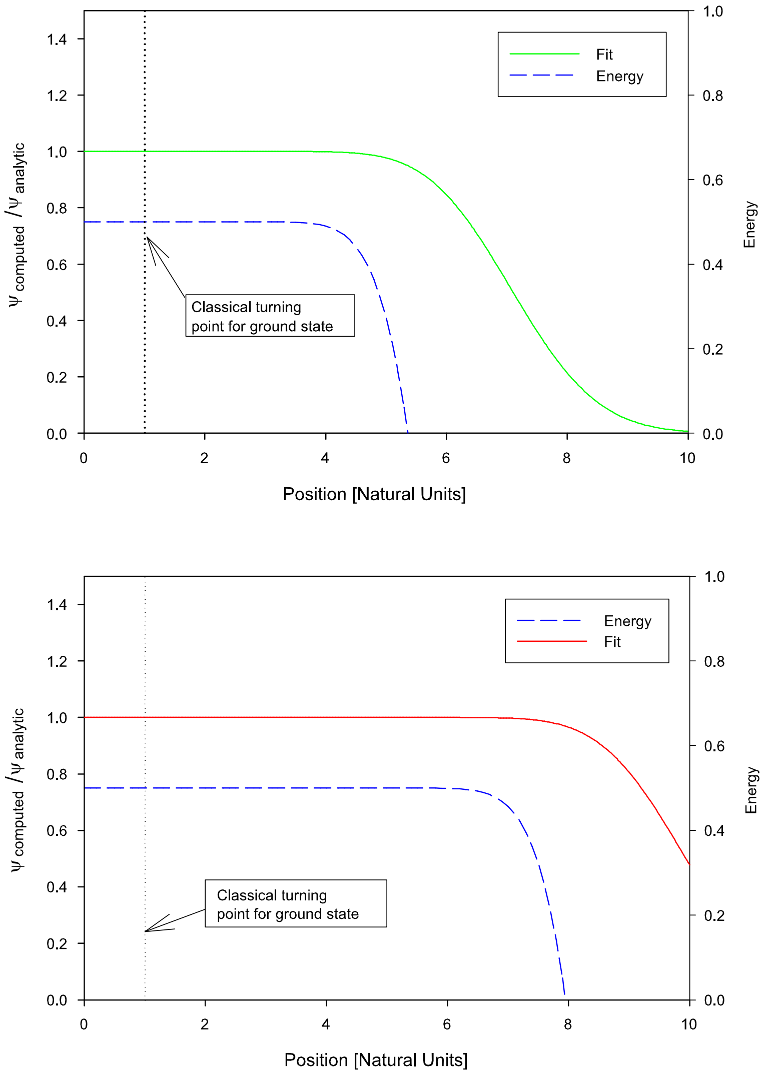
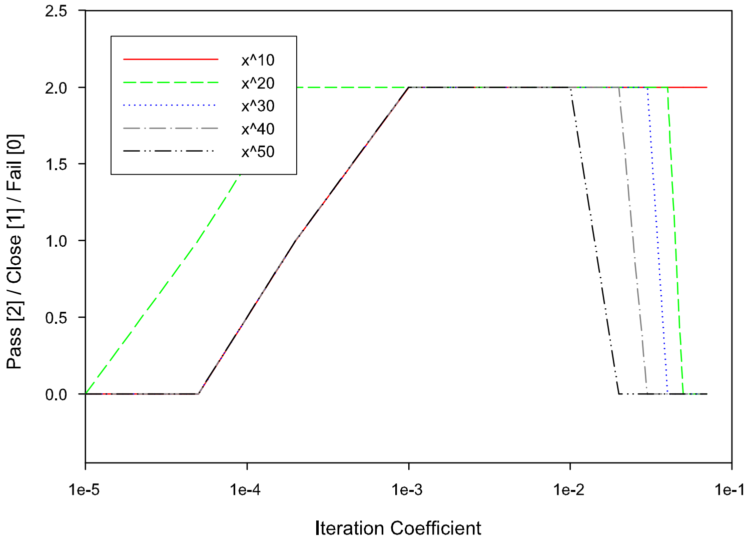


Figure 2.5: Example of how the region of close fit corresponds to the region of constant energy. For the case where $\alpha = 0.005$, $\eta = \sqrt{2}/2$. **TOP** Truncation after 20 orders in x. **BOTTOM** Truncation after 40 orders in x.



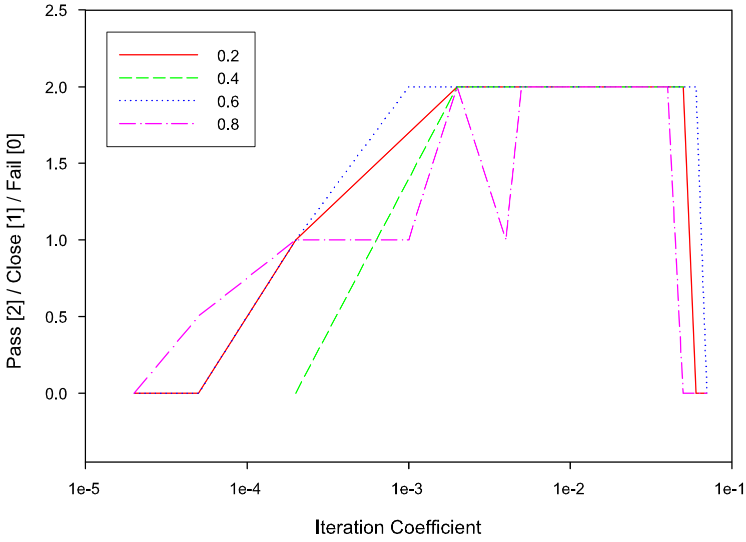


Figure 2.6: Graphical display of when the first order Iteration Operator gives the proper result. For the cases where $\eta = \sqrt{2}/2$. **TOP** Each line represents the order in x after which the solution was truncated; $\alpha = 0.005$. **BOTTOM** Each line represents a value of the iteration constant; truncation after 20 orders in x.

the iteration coefficient has a lower bound, at least for the method currently under consideration, but can give no mathematical reason for it.

Chapter 3

The Quartic Potential Well

The quartic potential well (hereafter called QPW), like the SHO, is a system whose potential becomes infinite as $x \to \infty$. The x^4 term that is contained in the potential does not allow for a solution in closed form.

We chose to use a QPW of the form

$$V(x) := (x^2 - 3)^2. \tag{3.1}$$

This choice was made due to the fact that approximations to the ground state and first excited state energies were readily accessible [1].

3.1 Choice of The Initial Function

Choosing the correct trial function makes the most difference in if the Iteration Operator method is going to converge to a "good" approximation of the desired state. In the first attempts to obtain an approximation for the ground state of the QPW a set of Gaussians were used, see Equation 2.1. These should be a good place to start because of the way they fulfilled the boundary conditions. Indeed it was our hope that a Gaussian would be a good initial function for any such boundary. Unfortunately we quickly found that the use of a Gaussian initial function gave a approximations that are in physically unreal positions and the associated energies are wildly erratic in the regions where a particle is most likely to be, see Figure 3.1.

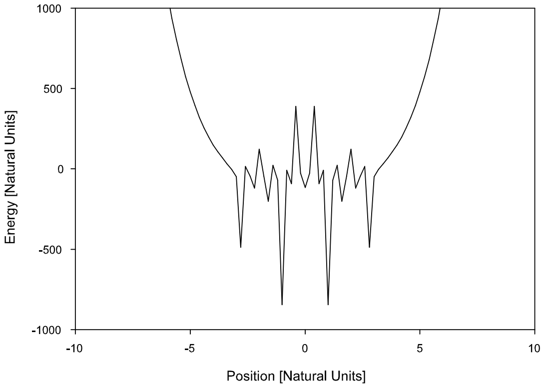


Figure 3.1: Energy computed for the QPW using the initial Gaussian function $e^{-0.4x^2}$ with the iteration coefficient $\alpha = 0.002$.

Since our efforts to obtain an approximation of the QPW using a Gaussian initial function were thwarted, we turned to obtaining an initial function from asymptotics. The zeroth order WKB approximation,

$$\psi(x) = e^{\pm x^3}, \tag{3.2}$$

was considered and then rejected due to it's inability to satisfy the boundary conditions at $x = \pm\infty$ simultaneously. We considered trying to approximate the eigenfunction for the region $x \geq 0$ and then saying that the potential's symmetry under reflection would cause the wave function to be symmetric under reflection also. We chose to find a different initial function that would allow for the both boundary conditions, though it might still be possible to use the argument just outlined to make Equation 3.2 give an approximation to the ground state of the QPW.

3.1.1 Modified WKB Approach

The problem that we encounter with the normal WKB approximation can be overcome, in some sense, if we do not assume that we can drop everything other than the x^4 term in the potential. The details of how this changes the wave function will be worked out in some detail.

The energy eigenvalue equation can be rewritten as

$$\frac{d^2\psi(x)}{dx^2} - 2(x^2-3)^2\psi(x) = -2E\psi(x). \tag{3.3}$$

Following WKB theory we assume that the leading order behavior of the wave function has the form

$$\psi(x) = e^{S(x)}. \tag{3.4}$$

Substituting this form of $\psi(x)$ into Equation 3.3 the energy eigenvalue equation turns into a non-linear second order differential equation for $S(x)$,

$$S''(x) + (S'(x))^2 - 2x^4 + 12x^2 + (2E-18) = 0. \tag{3.5}$$

Here we make a slight departure from WKB theory. Suppose we say that as $x \to \infty$ the x^2 term is large enough in comparison with the x^4 term that we cannot get rid of it in forming an asymptotic solution. Thus, assuming that $S(x) \sim x^n$, where n is positive, Equation 3.5 becomes in the asymptotic regime

$$(S'(x))^2 \sim 2x^4 - 12x^2, \tag{3.6}$$

which implies

$$S(x) \sim \pm\frac{\sqrt{2}}{3}(x^2-6)^{\frac{3}{2}}. \tag{3.7}$$

Due to the boundary conditions we choose the negative solution, resulting in the asymptotic wave function

$$\psi(x) \sim e^{-\frac{\sqrt{2}}{3}(x^2-6)^{\frac{3}{2}}}. \tag{3.8}$$

This wave function ends up being only a mathematical solution, it leads to complex energies in the region $|x| < 3$.

Fortunately, due to a serendipitous mistake when performing the above calculation I ended up with the wave function

$$\psi(x) \sim e^{-\frac{\sqrt{2}}{3}(x^2+6)^{\frac{3}{2}}}. \tag{3.9}$$

The change of the negative sign under the radical consequently gives us a wave function that satisfies the boundary conditions, gives real energies, and when acted upon by the iteration operator gives suitable approximations for the ground state eigenfunction and eigenvalue.

While the form of Equation 3.9 was originally a mistake it can be argued that this form for an asymptotic solution is reasonable. If we start with the WKB approximation as given by Equation 3.2 we can perturb the x^2 by a small amount δ, giving

$$\psi(x) \sim e^{-\frac{\sqrt{2}}{3}(x^2+\delta)^{\frac{3}{2}}}, \tag{3.10}$$

and still have an asymptotic solution. In practice we chose values for δ that weren't strictly small, $\delta = \{2, 4, 6, 8\}$, but we were able to find that these values still worked in solving the problem.

3.2 Results

Using Equation 3.10 we find that good approximations can be obtained for the ground state of the QPW. Figure 3.2 displays the results for a particular case.

As we saw with the SHO, Figure 3.3 shows that the area over which the energy is constant increases with powers in x. We also see a new and interesting feature in Figure 3.3; the energy found changes with the power in x. This is a result of not keeping enough terms in x. We see that the energy drops considerably when going from 10 orders in x to 20 orders in x. The drop in energy from 20 to 30 orders in x is small, with no apparent change when going to higher orders in x. We will see this more dramatically when we look at the an-harmonic oscillator.

Since we choose to pick δ large we must look to see what effect this has on the energy. We expect to find that as we go to larger values for δ that energy approximation will be worse than for smaller values of δ. We see in Figure 3.4 that as we expect the $\delta = 2$ energy approximation is the best. Unfortunately, as we look to $\delta = 4$ we find that it is a worse approximation than $\delta = 6$; we must conclude that our choice of δ does not affect the result in an intelligible way.

Finally, as we saw in the last chapter the range in α for the Iteration Operator method to give a constant energy decreases with increasing powers in x.

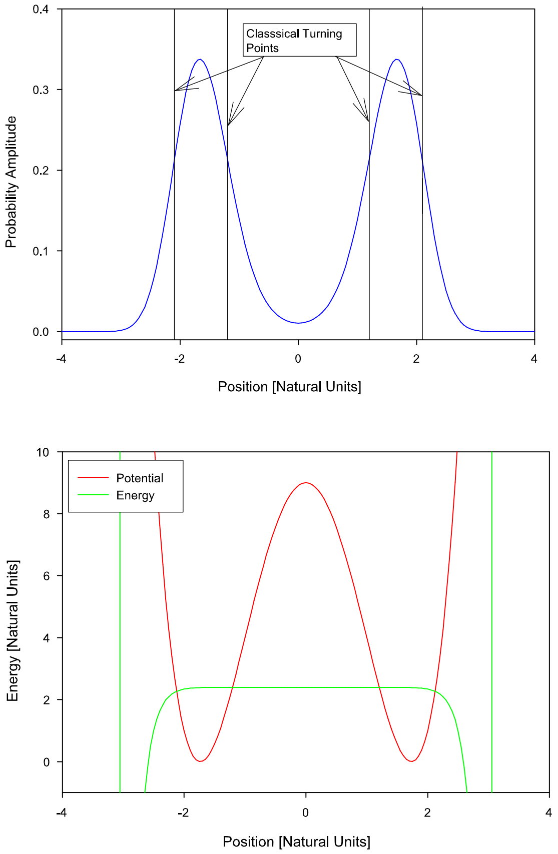


Figure 3.2: **Top:** Resultant wave function for the case using Equation 3.9 with $\alpha = 0.005$ and keeping up through the x^{30} terms. **Bottom:** Energy approximation for the same system.

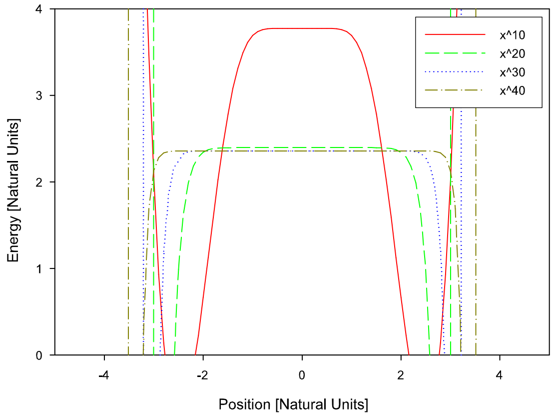


Figure 3.3: Graphical display of when the first order Iteration Operator gives the proper result. For the case where $\alpha = 0.005$, $\eta = \sqrt{2}/2$. Each line represents a value of the iteration constant.

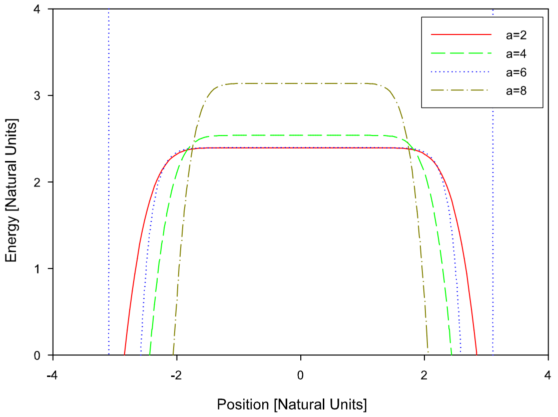


Figure 3.4: Energy eigenvalue approximation for different values of δ.

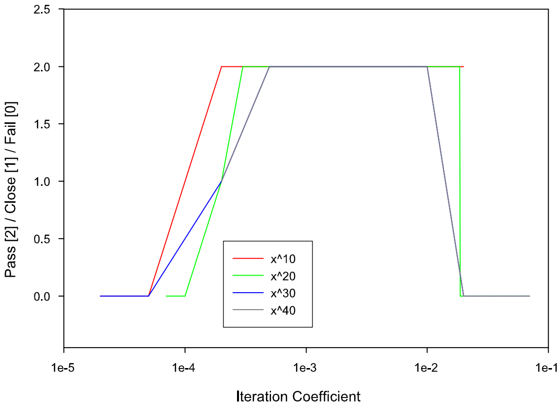


Figure 3.5: Graphical display of when the first order Iteration Operator gives the proper result. For the case where $\alpha = 0.005$, $\eta = \sqrt{2}/2$. Each line represents a value of the iteration constant.

3.3 Conclusions

We have learned that the order in x at which we truncate the series developed by the Iteration Operator method not only affects the region over which the approximation is good but also the value of the energy obtained. Thus, in order to make sure that the energy obtained approximates the actual eigenvalue we must continue to run the Iteration Operator method to higher orders in x until the energy does not change appreciably from a particular order in x to a higher order in x. It also seems reasonable that the change in order in x must be large to accurately judge this.

Chapter 4

The Anharmonic Oscillator

As yet the problems that we have discussed have had even potentials which were symmetric under reflection. We will now look at a problem that is asymmetric: the an-harmonic potential. The next chapter will then deal with a problem that is totally asymmetric.

As with the QPW, the anharmonic potential can have many similar forms. I chose to perform a slight change to the QPW used in Chapter 3. Actually, we will study two different but similar potentials:

$$\begin{aligned} V(x) &:= (x^2-3)^2 + x^3, \qquad (4.1) \\ V(x) &:= (x^2-3)^2 - x^3. \end{aligned}$$

It is expected that the solutions of the energy eigenvalue equations for each of these potentials will have the same energy but be mirror images of each other.

Due to the similarity of the anharmonic oscillator to the QPW, Equation 3.10 is the trial function we will use for the anharmonic oscillator.

4.1 Variational Approach

The variational approach gives us a basis from which to examine the Iteration method's approximation to the energy eigenvalue solution. We would also like to use the Perturbation method but that supposes that the an-harmonic terms would be small compared with the QPW and it is not. We will use a couple different trial functions in the course of this procedure looking for the best approximation, these are:

$$\psi_{trial1}(x) = e^{-a(x^2+b)}, \tag{4.2}$$

$$\psi_{trial2}(x) = e^{-a(x^2+b)^{\frac{3}{2}}}, \tag{4.3}$$

$$\psi_{trial3}(x) = ae^{-\frac{1}{2}(x^2+2)^{\frac{3}{2}}} + be^{-\frac{1}{2}(x^2+4)^{\frac{3}{2}}} + ce^{-\frac{1}{2}(x^2+6)^{\frac{3}{2}}}, \tag{4.4}$$

The first of these trial functions is of course the easiest to find a solution for. In running through the variational method we find that solving for the expectation value of the energy gives us,

$$\langle \hat{H} \rangle = \begin{cases} 12.80000001 + 8.999999998 * b^2 + b^3 + b^4 + 7.499999999 * b, & \text{if } a = 0.1; \\ 0, & \text{otherwise.} \end{cases} \tag{4.5}$$

Equating $\partial_b \langle \hat{H} \rangle$ to zero and solving for b gives, $b = -.4298113206$, which in turn gives the expectation value for the energy, $\langle \hat{H} \rangle = 11.19378070$.

Looking at the next two cases, Equations 4.3 and 4.4, we find that we cannot integrate the square of the functions. Thus, we cannot give a closed form solution at all.

4.2 Other Approximation Methods

Since the WKB method of approximation assumes that the potential changes slowly, we cannot use it to obtain an approximation of the wave function for the QPW. Perturbation theory assumes that the change of the potential from something that we know the solution to is relatively small. The potential that we have chose is not a slight modification of either the SHO or QPW. The wave function cannot be found using the perturbation method.

4.3 Iteration Operator Method Applied to the Anharmonic Oscillator

The here-to-fore known methods of analytically approximating the solutions of the an-harmonic oscillator have failed to obtain a satisfying result. The Iteration

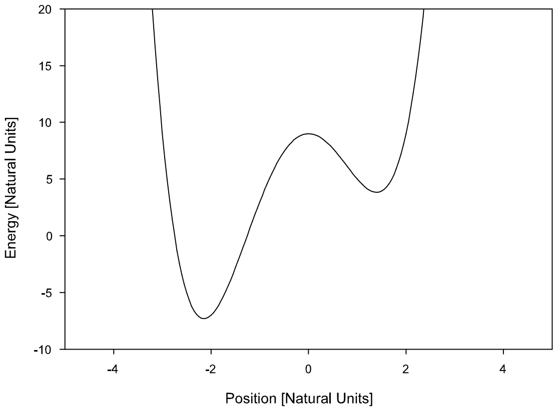


Figure 4.1: Potential energy of the anharmonic oscillator used in this chapter.

Operator method can obtain a result where the other methods have failed because of the fact that we do not have to do any fundamentally hard calculations.

The Iteration Operator for the anharmonic oscillator is

$$\hat{I}_p := [1 + \alpha\frac{1}{2}\frac{d^2}{dx^2} - \alpha(x^4 + x^3 - 6x^2 + 9)]^p. \tag{4.6}$$

As the initial function we will use Equation 3.10, with the same values for δ as in our analysis of the QPW.

Figure 4.3 shows the resultant wave function for different orders in x. We see that the result gives a large probability of being inside the potential minimum near $x = -2$. From a qualitative understanding of quantum mechanics we expect to find that the wave function has some nonzero probability amplitude near $x = 2$. We see that the approximation has a peak in the area around the potential minimum near $x = 2$.

In Figure 4.3 it appears that most of the waves are normalized. This is in part true. Due to the fact that functions containing terms similar to Equation 3.10 cannot be integrated analytically, a numerical integration was used with the integration over the range $-1000 \leq x \leq 1000$. A large range could have been used but this was sufficient to get the general idea of how the normalized wave function appears.

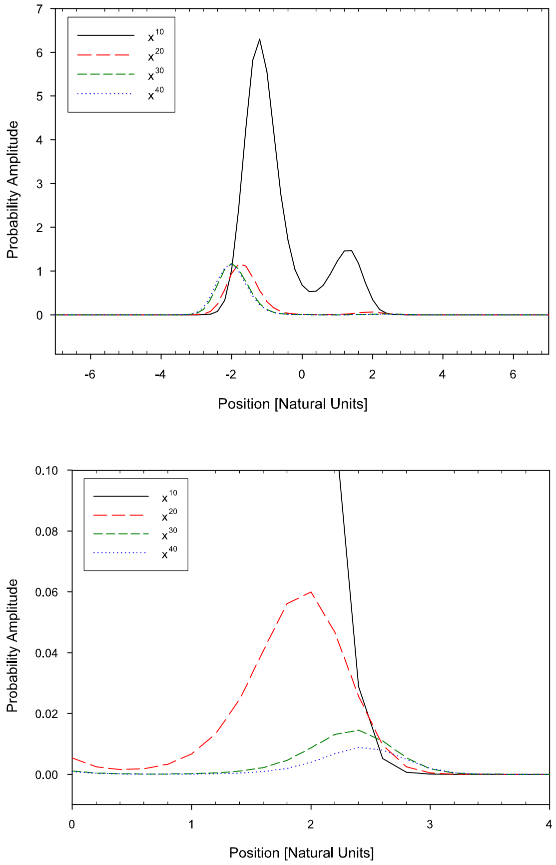


Figure 4.2: Approximation of the anharmonic oscillator ground state.

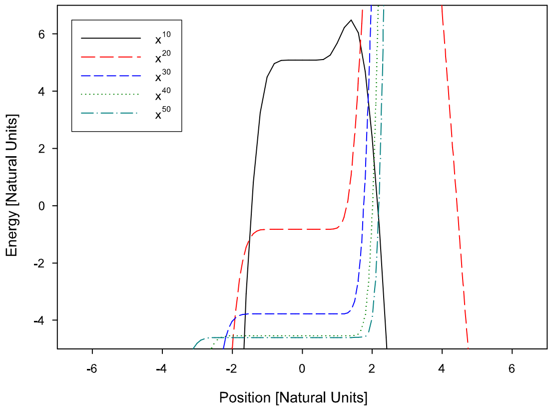


Figure 4.3: Approximations to the ground state energy of the anharmonic oscillator.

As we saw with the QPW the ground state energy computed decreases with increasing orders in x. It appears to begin to hold steady at $E|_{x=0} = -4.6$ after 30 orders in x; see Figure 4.3.

4.4 The Mirror Potential

At the beginning of this chapter we stated that we would see that using one of the potentials in Equation 4.1 would give a wave function with some energy, and that using the other potential would give the same energy but with a mirror image of the other wave function, it is now time to show that this is true. Figures 4.4 and 4.5 show the resultant wave functions and the energies computed for the mirror potentials when the same initial function, iteration coefficient, and truncation scheme is used.

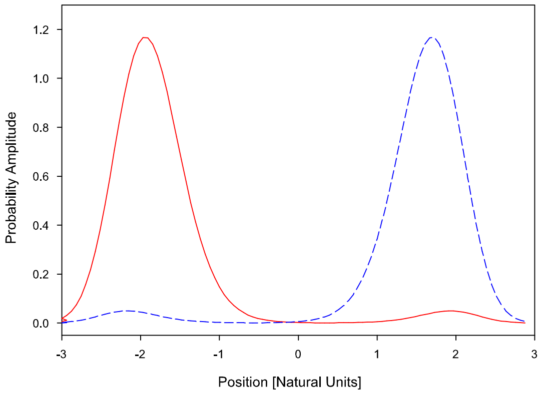


Figure 4.4: Resultant eigenfunction approximations of the two forms of the anharmonic oscillator potential. **Solid Red Line:** For $V(x) = (x^2 - 3)^2 + x^3$. **Dashed Blue Line:** For $V(x) = (x^2 - 3)^2 - x^3$.

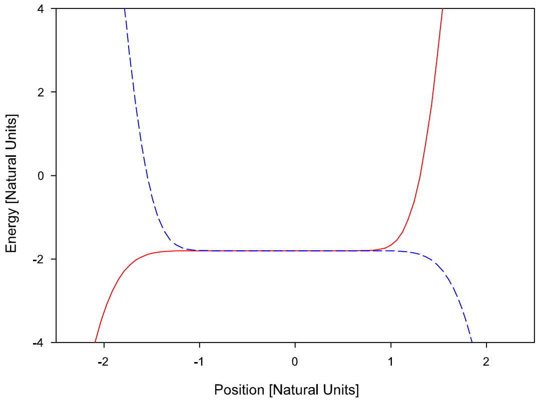


Figure 4.5: Resultant energy approximations of the two forms of the anharmonic oscillator potential. **Solid Red Line:** For $V(x) = (x^2 - 3)^2 + x^3$. **Dashed Blue Line:** For $V(x) = (x^2 - 3)^2 - x^3$.

Chapter 5

The Morse Potential

5.1 Introduction to the Morse Potential

The Morse Potential is an empirical model of the intramolecular forces that cause vibrations between two atoms. The asymmetry of the bond indicates that it is harder to compress the two atoms together than it is to pull them apart. It has been used successively to give useful qualitative results for H_2, Li_2, and other diatomic molecules. As given by Phillip Morse [8] the potential has the form

$$V(r) = De^{-2a(r-r_0)} - 2De^{-a(r-r_0)}, \tag{5.1}$$

where $-D$ is the value of minimum potential energy which lies at $r = r_0$. We will start off with our form of the Morse potential as such

$$V(x) = 4e^{-2\sqrt{2}(x-1)} - 8e^{-\sqrt{2}(x-1)}, \tag{5.2}$$

see Figure 5.1.

We have found the Morse potential to be the most difficult of the systems we have worked with. Due to the difficulty of getting this to work I will outline what was tried in hope that this will help others not fall into our pitfalls.

5.2 Gaussian Initial Function

The first thing that we might try is a Gaussian initial function with the full potential. If we do so we will find that the resultant function gives an energy approximation that changes radically in the region in and around the potential minimum.

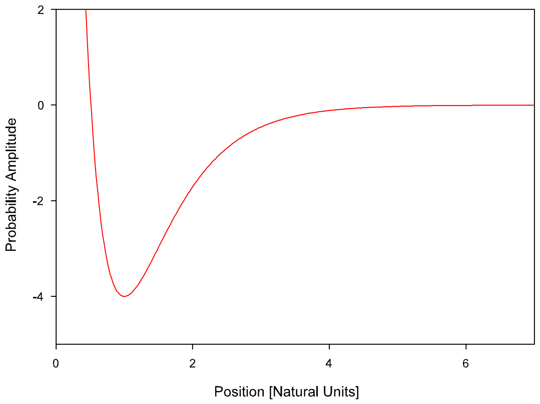


Figure 5.1: Morse potential of the form given in Equation 5.2.

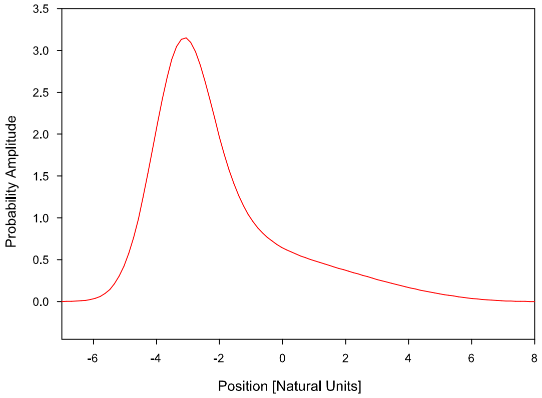


Figure 5.2: Resultant wave function of Gaussian initial function for the Morse potential.

There is a notable exception. If we use the potential

$$V(x) = \frac{1}{2}e^{-0.4x+0.8} - e^{-0.2x+0.4} \tag{5.3}$$

with the initial function $exp[-0.4(x-1)^2]$ and $\alpha = 0.002$ then we find that the energy is constant, $E = -0.5051373606$, over the range where the particle would be bounded. This appears good at the outset but the resultant wave function has a maximum in a region not allowed classically, see Figure 5.2.

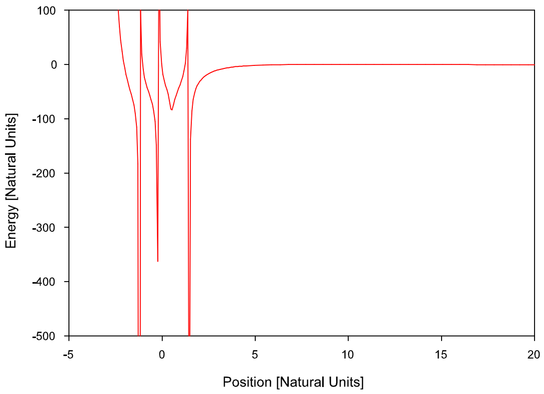


Figure 5.3: Resultant wave function of asymptotic-like initial function for the Morse potential.

5.3 Asymptotic-Like Initial Function

Another function that we might try is an asymptotic-like function

$$\psi_{initial} = xe^{-2x}. \tag{5.4}$$

This gives a solution that has a nearly constant energy at large x, and changes quickly as $x \longrightarrow 0$.

5.4 Change of Variables

After an appropriate change of variables the time-independent Schrödinger equation becomes:

$$y^2 d_y^2 \chi + y d_y \chi - (\frac{\varpi^2}{\varrho^2} - \frac{\gamma}{\varrho} y + \frac{1}{4} y^2)\chi = 0 \tag{5.5}$$

where ϖ contains the energy E.[1] The asymptotic solution of which is

$$\chi = y^{\frac{\varpi}{\varrho}} e^{-\frac{1}{2}y}. \tag{5.6}$$

Equation 5.6 can then be used as the initial function for the Iteration Operator method, where the operator is of the form

$$I_p = \{1 - \alpha[y^2 \partial_y^2 + y\partial_y - (\frac{\varpi^2}{\varrho^2} - \frac{\gamma}{\varrho} y + \frac{1}{4} y^2)]\}^p. \tag{5.7}$$

---

[1] For a full discussion of the change of variables see the excellent text ”Practical Quantum Mechanics” by Flügge. [5]

Once the iteration procedure is complete a change of variables is used to move the resultant wave function back into x-space. The wave function is then used to find the energy using Equations 1.23 and 5.2.

Upon reflection it is obvious that this procedure is doomed to fail because the effective initial function

$$\psi = e^{-0.2*(x-1)\frac{\varpi}{\varrho}} e^{-2e^{-0.2*(x-1)}}. \tag{5.8}$$

does not fall to zero as $x \to \infty$.[2]

5.5 Taylor Expansion of Potential

5.5.1 Introduction

In trying to work with the full Morse potential one runs up on a stumbling block, namely how to limit the number of terms. The problem is two fold. First, from the potential there is a build up of exponential terms. Second, the kinematic portion of the Hamiltonian builds up polynomials through differentiation. One would like a way to limit the number of terms in the polynomials and separately limit the number of exponential terms. It appears that there is no good way to do this.

What is left for us to do is one of two things: either, use the full potential in the iteration operator and then do a Taylor series after each iteration; or make a polynomial approximation of the potential from a Taylor series of the potential. As was already shown the former does not work in this case (at least with the initial functions that were tried) and thus we must use the latter.

5.5.2 SHO Approximation of The Morse Potential

We start off with approximating the Morse potential with a SHO well. If Gaussians such as were used in Chapter 2 are used here we find that the Iteration

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[2] Equation 5.6 was also used in a failed attempt to approximate the solution of 5.5 by the IO method. It should also be noted that the value of the energy E involved in the value of ϖ was set to the value of the ground state energy obtained by Flügge [5].

method does not settle down to a result with a region of constant energy. We find though from calculating the asymptotic solution of the Schrödinger with the potential

$$V(x) = 8(x-1)^2 \tag{5.9}$$

that the ground state solution should be

$$\psi(x) = e^{-2(x-1)^2}. \tag{5.10}$$

If the initial function

$$\psi(x) = e^{-(x-1)^2}, \tag{5.11}$$

is used to test the Iteration Operator method in this case it results in the approximation to the energy $E|_{x=0} = 1.999874$.

5.5.3 QPW Approximation of The Potential

We now turn to the quartic potential well approximation of the Morse potential. At first blush this seems to be a trivial matter because we have already shown that solutions can be found in a similar case. Yet it is not so.

We find that if we use the potential as it is centered around the point $x = 1$

$$V(x) = 8(x-1)^2 - 11.31370850(x-1)^3 + 9.333333333(x-1)^4, \tag{5.12}$$

then the asymptotic solution is

$$\psi := e^{(-1.44002265x^{2}{}^{\frac{3}{2}} + 4.3205x^2 + 4.3205x)^{\frac{3}{2}}}. \tag{5.13}$$

The use of this asymptotic solution does not yield an energy approximation that is constant over a region. Though we do not know why, it appears that having the potential and initial function centered about $x = 1$ prevents the approximation from working.

If we center both around the point $x = 0$ we find that the we are able to obtain a suitable result. As was mentioned in Chapter 3 a truly normalized wave function cannot be obtained due to the inability to analytically integrate the exponential term. Thus the "normalized" wave functions that we obtain are really square integrable over the range $|x| \leq 1000$.

5.5.4 Sixth Order Approximation of The Potential

In trying to obtain a better approximation to the ground state eigenfunction we turn to the following approximation to the Morse potential:

$$V(x) \approx -4+8x^2-11.31370850x^3+9.333333333x^4-5.656854248x^5+2.755555556x^6. \tag{5.14}$$

Whereas before we have been able to use an asymptotic approximation as the initial function to be used with a potential well, the asymptotic solution

$$\psi_{asymptotic} = e^{-0.5868938955x^4} \tag{5.15}$$

fails to work for the potential in Equation 5.14. It is possible to get a satisfactory solution using Equation 3.10.

5.5.5 Higher Order Approximations of The Potential

Higher order approximations of the Morse potential lead to better approximations of the ground state eigenfunction. This can be seen in Figure 5.5, which shows how the approximation to the ground state eigenfunction changes with the approximation to the potential. Higher order approximations of the potential are represented in Figure 5.4 (note that in this graph the approximation is not offset so that its minimum is at $Energy = 0$). We see that as we get to higher order representations of the potential, the wave function falls off slower on the positive-x side, as we expect it should from the shape of the potential.

In Section 2.5 we stated that the area over which the resultant wave function equals the actual wave function corresponds to the area over which the energy is constant. In Figure 5.7 we see that this is roughly true. Thus, we need to back off a little from our stance in Chapter 2 and say that resultant wave function is likely close to the actual wave function over the range in position where the energy is constant.

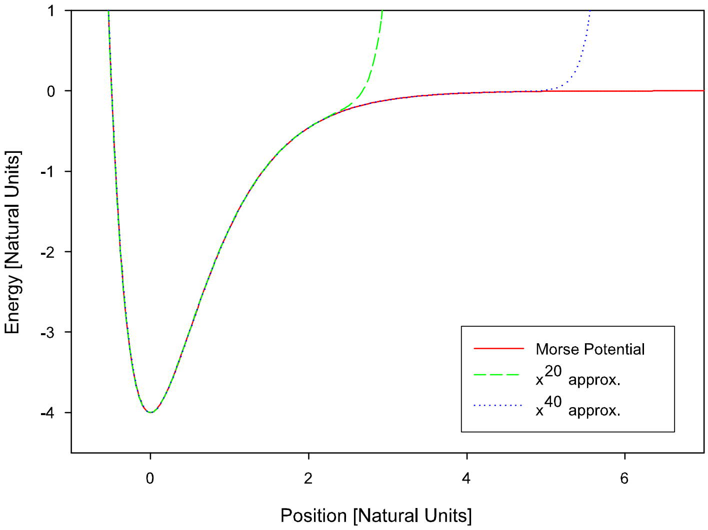


Figure 5.4:

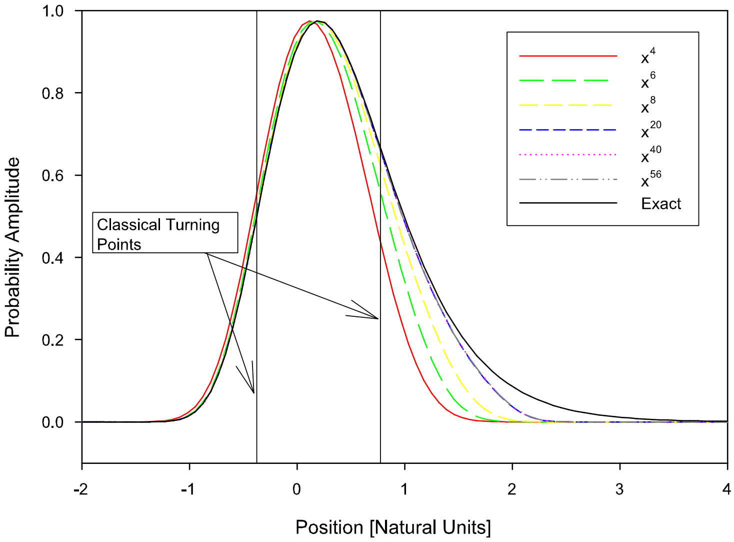


Figure 5.5: Approximations to the ground state as the order of the polynomial built from the Taylor series of the Morse potential increases. The graph is for the cases with $\delta = 6$ and $\alpha = 0.001$.

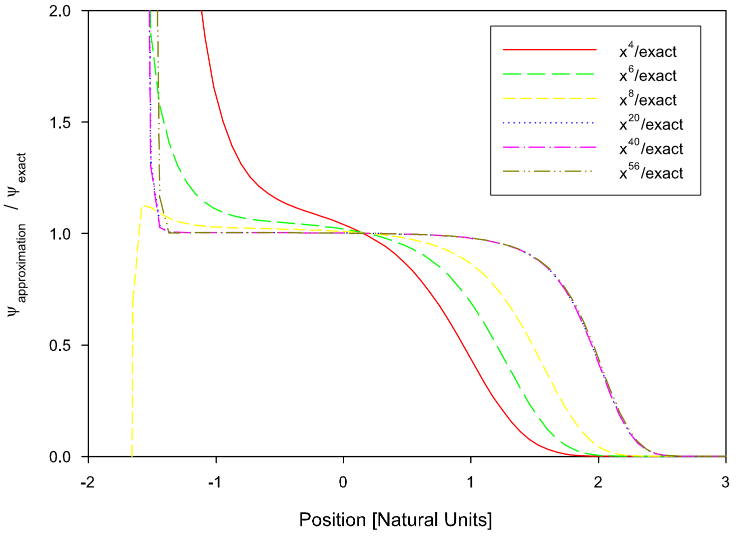


Figure 5.6: Approximations to the ground state as the order of the polynomial built from the Taylor series of the Morse potential increases. The graph is for the case with $\delta = 6$ and $\alpha = 0.001$.

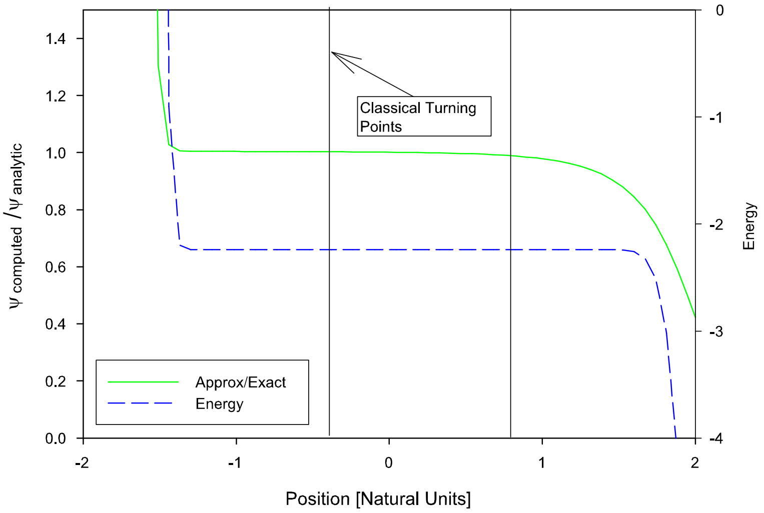


Figure 5.7: Graph showing that the area in x over which the resultant wave function is equal to the actual wave function roughly corresponds to the area over which the resultant energy is constant. The graph is for the cases with $\delta = 6$ and $\alpha = 0.001$.

5.6 The Undiscovered County

We have seen that the first order Iteration Operator was unable to give an approximation that was equal to the actual ground state eigenfunction over the classically allowed region of space. Going to higher orders in x in the Taylor polynomial of the potential does not seem to be the answer since the form of the resultant wave function does not change appreciably after twenty orders in x. We find also that going to higher orders in x in the truncation scheme used in the operator, we were at sixty orders in x for much of what was presented here, does not do much for us either.

In fact, in raising the number of terms we keep in the truncation scheme of the operator we end up hitting the limit as to how many terms this method can do using Maple and get an answer that make sense. We might be able to get around this though through going to a higher order Iteration Operator.

Chapter 6

The 2-D Harmonic Oscillator

6.1 The 2-D SHO Potential

The 2-D simple harmonic oscillator potential is defined by

$$V(x,y) = \frac{1}{2}x^2 + \frac{1}{2}y^2 \tag{6.1}$$

6.2 Introduction to the 2-D Iteration Operator

As with first working with the SHO for the 1-dimensional Iteration Operator the 2-D harmonic oscillator seems to be the natural choice for developing the 2-dimensional Iteration Operator. Notably, the symmetry of the wave function allows us to see if the iteration operator will give a solution that is functionally symmetric. By this we mean that if the result $\psi(x)$ has a term such as:

$$\psi(x) = \ldots .181267714410^{-27} * x^{14} * y^{10} \ldots, \tag{6.2}$$

then it also has a corresponding term

$$\psi(x) = \ldots .181267714410^{-27} * y^{14} * x^{10} \ldots . \tag{6.3}$$

Due to the fact that (at least in Maple) we can only make truncations in one variable at a time, we lose the functional symmetry if we use Equation 1.12 and then truncate the result of each iteration first in x and then in y. We thus need to use Equation 1.12 twice once with truncating in one order on the first one, truncating in the reverse order on the second one, and then add the two results together. Of course we can multiply it all by a factor of one-half, but that can always be taken care of in normalization.

As an example of such an operation we will perform the first few iterations of one of these computations. We will use the following forms for the Iteration Operator and initial function:

$$I_p = [\,\psi_{initial} - \frac{\alpha}{2}(x^2 + y^2)\psi_{initial} + \frac{\alpha}{2}(\,\frac{\partial^2 \psi_{initial}}{\partial x^2} + \frac{\partial^2 \psi_{initial}}{\partial y^2}\,)\,]^p, \tag{6.4}$$

$$\psi_{initial} = e^{-\beta x^2 - \beta y^2}. \tag{6.5}$$

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

$$\begin{aligned} \psi_1 &= (0.9976 + 0.00044\,x^2 + 0.00044\,y^2)\,e^{-0.6x^2 - 0.6y^2}, \\ \psi_2 &= (0.99520752 + 0.000875776\,x^2 + 0.000875776\,y^2 + 3.872 * 10^{-7}\,y^2x^2 \\ &\quad + 1.936 * 10^{-7}\,x^4 + 1.936 * 10^{-7}\,y^4)\,e^{-0.6x^2 - 0.6y^2}. \end{aligned}$$

6.3 Results for The 2-D SHO

Figure 6.1 gives an example of the wave function with its fitness and Figure 6.2 gives an example of the energy generated by the Iteration Operator Method.

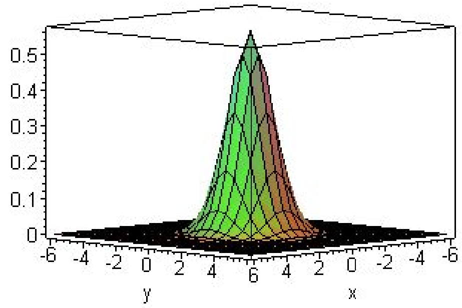
Results were also obtained for asymmetric trial functions. For example the following initial function was used in one instance

$$\psi_{initial} = y\,e^{-0.6(x^2 + y^2)}, \tag{6.6}$$

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 6.1.

6.4 The Addition of An Asymmetric Potential

We also included different polynomial functions $\tilde{V}(x, y)$, of order equal to or less than two, are added to the 2-D SHO potential. A list of the functions $\tilde{V}(x, y)$ and the resultant energies is given in Table 6.2. The resultant wave functions are stretched and contracted according to the way in which the potential is changed; see Figure 6.3



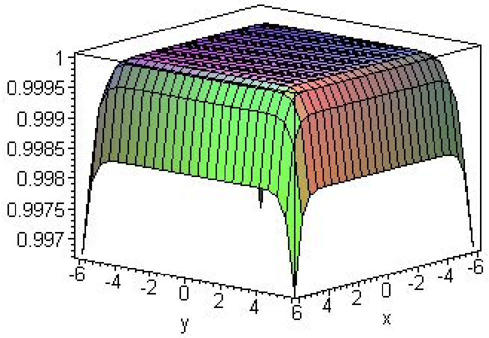


Figure 6.1: **Top:** Normalized resultant wave function for the case where $\psi(x, y) = exp(-0.6 * (x^2 + y^2))$ and $\alpha = 0.002$. **Bottom:** Closeness of fit for the same case.

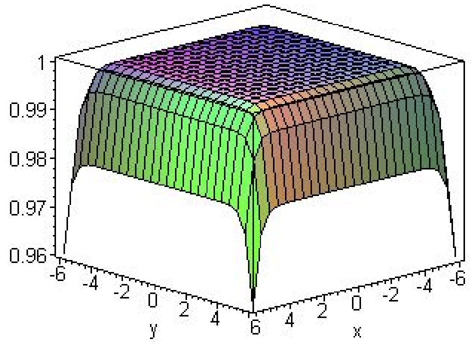


Figure 6.2: Energy eigenvalue approximation for the case where $\psi(x, y) = exp(-0.6 * (x^2 + y^2))$ and $\alpha = 0.002$.

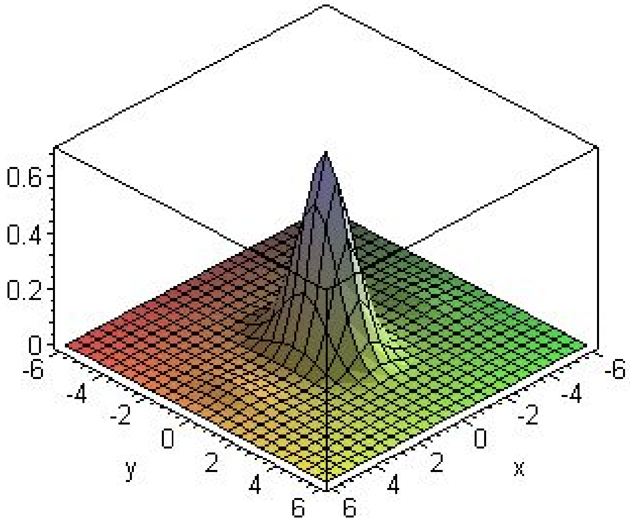


Figure 6.3: Resultant wave function for the added potential $\tilde{V}(x, y) = 2x^2$.

g(x,y)	Energy [Natural Units]
$-xy$	3.000000002
xy^2	2.000000002
x^2y	2.000000003
x^3y	3.000000004
x	2.000000004
xy	3.000000007
y	2.000000002
x^2y^2	1.000000000

Table 6.1: Results of the Iteration Operator acting on the initial function $\psi_{initial} = g(x,y)\, e^{-0.6x^2}$ with the iteration coefficient $\alpha = 0.006$.

$\tilde{V}(x,y)$	Energy [Natural Units]
$0.2x^2$	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

Table 6.2: Table of results for the potential $V(x,y) = \frac{1}{2}(x^2+y^2) + \tilde{V}(x,y)$ with the trial function $\psi(x) = e^{-0.6(x^2+y^2)}$ and the iteration coefficient $\alpha = 0.004$.

6.5 Insights on the Iteration Operator

An interesting feature of the iteration operator is that as the iteration coefficient increases, to somewhere around $\alpha = 0.005$, the energy draws closer to the ground state eigenvalue. Table 6.3 gives an example of how the energy decreases as the iteration operator increases. It appears that this is a general pattern. Another related feature is that the energy increases as α increases when the Gaussian Coefficient $\eta < \frac{1}{2}$ and the energy decreases as α increases when $\eta > \frac{1}{2}$.

Knowing that the energy follows this general pattern may be of use in obtaining a better initial function. In the case of the 2-D 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 than we can use this to obtain better values for these parameters.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy
0.6	0.00002	0	1.129782752
0.6	0.00004	0	1.085169262
0.6	0.00006	0	1.056295463
0.6	0.00008	0	1.037384696
0.6	0.0002	0	1.003330308
0.6	0.0004	1	1.000060612
0.6	0.0006	2	1.000001102
0.6	0.0008	2	1.000000019
0.6	0.002	2	1.000000000

Table 6.3: Pass[2] / Close [1] / Fail [0] results for the 2-D SHO. The computed energy of the approximation draws closer to the ground state eigenvalue as the iteration coefficient increases.

Chapter 7

Second Order Iteration Operator

7.1 Introduction

In the preceding chapters we concentrated on using the first order Iteration Operator obtain approximations of the states that we are looking at. Since the second order Iteration Operator contains a better approximation of $exp[-i(\hat{H} - E_o)t]$, we expect that it will give a better approximation of the desired eigenfunction.

The second order Iteration Operator for a SHO is given by

$$\hat{I}_p := (1-\alpha\hat{H}+\alpha^2\hat{H}^2)^p = (1-\frac{\alpha}{2}x^2+\frac{\alpha}{2}\frac{d^2}{dx^2}+\frac{\alpha^2}{4}x^4-\frac{\alpha^2}{2}x^4\frac{d^2}{dx^2}-\alpha^2 x\frac{d}{dx}-\frac{\alpha^2}{2}+\frac{\alpha^2}{4}\frac{d^4}{dx^4})^p. \tag{7.1}$$

Equation 7.1 is used on initial functions of the form of Equation 2.1.

7.2 Differences Between The First And Second Order Iteration Operators

The second order Iteration Operator Method does a better job of approximating the desired eigenfunction than the first order Iteration Operator (see Figure 7.1). Figure 7.2 shows how the second order operator obtains as good a fit to the SHO ground state as the first order operator but with several times fewer orders in x.

The drawback for using the second order Iteration Operator is that it takes longer to run, see Table 7.1. On the other hand it gives a better approximation in a more compact form, which has its uses when one wants to share the result, or use it to do more complicated computations.

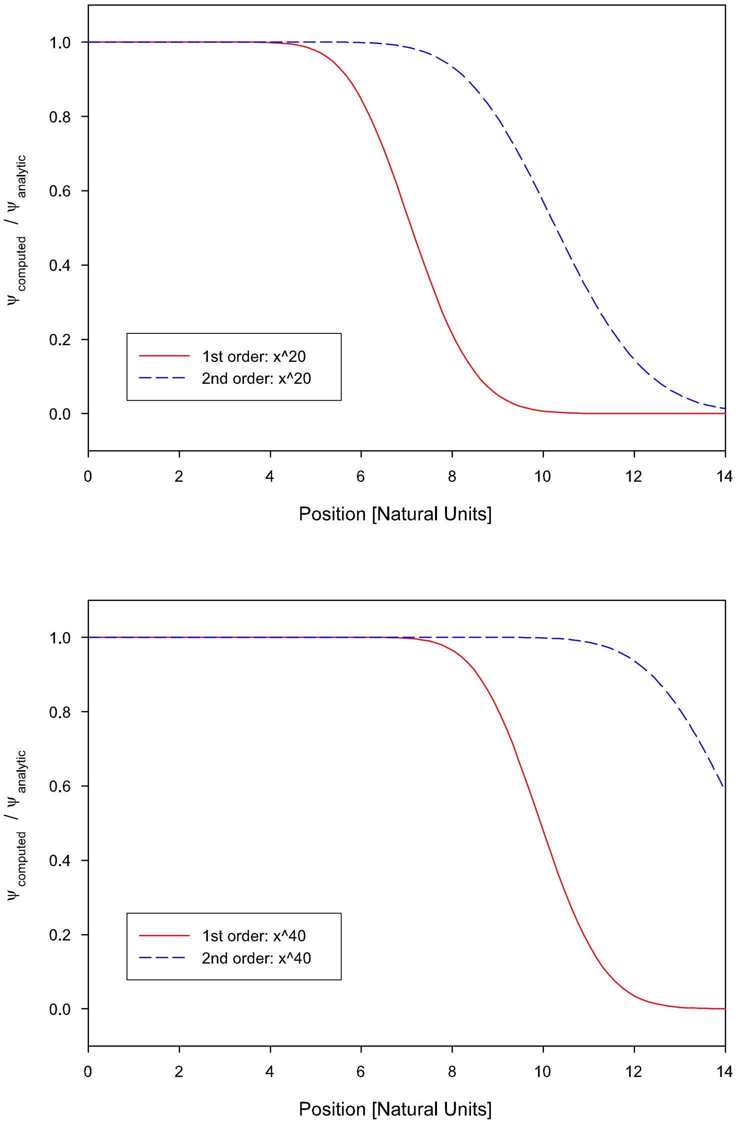


Figure 7.1: Closeness of fit graphs showing the difference in approximations between the first and second order Iteration Operators. The initial wave functions in each case is $e^{-0.6x^2}$ with $\alpha = 0.001$. **Top:** Twenty orders in x. **Bottom:** Forty orders in x.

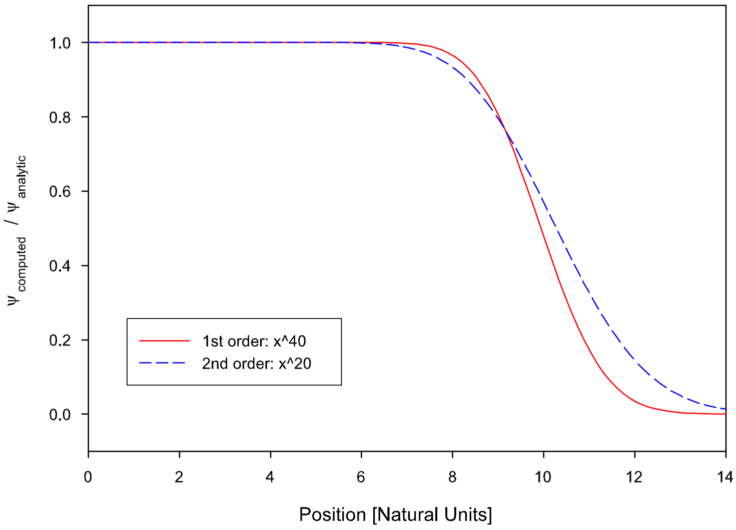


Figure 7.2: Closeness of fit graphs showing when the first and second order Iteration Operators give approximately the same result. The initial wave functions in each case is $e^{-0.6x^2}$ with $\alpha = 0.001$.

IO Order	Powers in x	Time Used [sec]	Memory Used [MB]
1	20	26.4	0.69
1	40	46.5	0.69
2	20	90.2	0.69
2	40	158.5	0.69

Table 7.1: Memory used and time spent on calculating 10000 iterations of the Iteration Operator with the SHO potential, the initial function $e^{-0.6x^2}$, and $\alpha = 0.001$.

Chapter 8

Conclusion

The Iteration Operator method, as with many approximation methods, has the ability to give a "good" approximation to the lowest order state with a given symmetry assuming that appropriate choices for the initial function (or trial function) and value of the iteration coefficient. We have seen that the Iteration Operator method might also converge to an incorrect solution as was the case for the SHO in Section 2.2.

In the choosing of the parameter E used in Equation 1.12 we have found a few guide lines:

1. If $V(x) \geq 0 \ \forall \ x \,\epsilon\, \mathbb{R}$ then set $E = 0$.

2. If $V(x) < 0$ for some region $x = \{x_a, x_b\}$ then set $E = \inf V(x)$ or to some value $\inf V(x) \leq E \leq E_o$.

We have seen that the ability for this method to give the proper energy approximation is dependent on the number of terms kept. In order to make sure that enough terms are kept when doing the approximation, one must run it with several different orders in position, say x^{20}, x^{30}, and x^{40}. Then increase the number of terms until the energy approximation stabilizes.

It may be that the number of orders in x that are needed is somehow dependent on the simplicity of the potential as well as on its symmetry. For the SHO we only needed x^{10}, for the QPW we needed x^{20}, and for the an-harmonic potential we needed x^{40}.

Finally, it appears that this method is capable of obtaining approximate solutions to problems for which other methods do not work. We have seen it obtain solutions to many systems for which perturbation methods will not work; for example the QPW of Equation 3.1, or the oscillator systems of Table 6.2.

8.1 Where Do We Go From Here?

This is a method that can take LARGE amounts of memory and time. With that in mind it seems reasonable that if one is going to try to solve an involved problem with this method then they will need a method of calculation that will allow them to make use of supercomputers or of distributive computing.

One problem that is conspicuously missing from this thesis is a $\frac{1}{r}$ potential. A few quick attempts were attempted at using the Iteration Operator to find the excited states of the hydrogen atom, but time constraints prevented us from continuing work on this particular potential. Further work is planned on the hydrogen atom; we would also like to look at atoms with more than one electron in the valence shell.

Appendix A

Tables

The following tables are not an exhaustive list of all of the cases that I had to do in order to find a case that worked, but I have tried to explain the pitfalls that I found in the preceding chapters and feel that it would not be instructive to give table after table of cases where I went down the wrong track. Most of the problem I found was starting off with the wrong trial function. What the following tables contain though are the cases where a right trial function was used and if the combination of that trial function with a particular α, after a sufficient number of iterations, gave the correct energy eigenvalue over a range of position.

Due to the large number of cases used for each system information that would be most naturally in one table will have to be split into two tables.

κ	Pass/Close/Fail	Energy [Natural Units]
0	2	.5000000005
1	2	1.500000003
2	2	.4999999966
3	2	1.500000000
4	2	.4999999932
5	2	1.499999996
6	2	.4999999900
7	2	1.499999992
8	2	.4999999856
9	2	1.499999988
20	2	.4999999646
21	2	1.499999973
22	2	.4999999649
23	0	NR
24	0	NR
25	0	NR
26	0	NR

Table A.1: Table of pass [2] fail [0] results for SHO with the trial function $\psi(x) = x^{\kappa}e^{-0.6x^2}$. The NR in the energy column stands for "No Result".

Guassian Coefficient	Iteration Coefficient	Pass/Close/Fail
0.2	0.00002	0
0.2	0.00005	0
0.2	0.0002	1
0.2	0.002	2
0.2	0.004	2
0.2	0.005	2
0.2	0.01	2
0.2	0.02	2
0.2	0.03	2
0.2	0.04	2
0.2	0.05	2
0.2	0.06	0
0.2	0.07	0
0.4	0.0002	0
0.4	0.002	2
0.4	0.005	2
0.4	0.02	2
0.4	0.0242	2
0.4	0.05	2
0.45	0.02	1
0.6	0.0002	0
0.6	0.0005	0
0.6	0.0002	1
0.6	0.001	2
0.6	0.01	2
0.6	0.02	2
0.6	0.03	2
0.6	0.04	2
0.6	0.05	2
0.6	0.06	2
0.6	0.07	0

Table A.2: **Part 1:**Table of pass [2] close [1] fail [0] results for SHO with all cases being ran for 10000 iterations and 20 orders in x.

Guassian Coefficient	Iteration Coefficient	Pass/Close/Fail
0.8	0.00002	0
0.8	0.00005	0.5
0.8	0.0002	1
0.8	0.001	1
0.8	0.002	2
0.8	0.004	1
0.8	0.005	2
0.8	0.01	2
0.8	0.02	2
0.8	0.03	2
0.8	0.04	2
0.8	0.05	0
0.8	0.06	0
0.8	0.07	0
1	0.002	2
1	0.005	2
1	0.04	0
1	0.05	0
2	0.005	2
10	0.02	0

Table A.3: **Part 2:**Table of pass [2] close [1] fail [0] results for SHO with all cases being ran for 10000 iterations and 20 orders in x.

Iteration Coefficient	Iterations	Pass/Close/Fail	Energy [Natural Units]
0.00002	20000	0	0.5835274080
0.0002	20000	1.5	0.5000574288
0.001	20000	2	0.5000000121
0.002	20000	2	0.5000000123
0.003	20000	2	0.5000000123
0.004	20000	2	0.5000000131
0.005	20000	2	0.5000000130
0.006	20000	2	0.5000000128
0.007	20000	2	0.5000000124
0.008	20000	2	0.5000000120
0.009	20000	2	0.5000000123
0.01	20000	2	0.5000000126
0.02	20000	2	0.5000000130
0.03	20000	2	0.5000000130
0.04	20000	2	0.5000000124
0.05	20000	0	40.255551960
0.06	20000	0	40.256059360
0.07	20000	0	40.256060230
0.00002	30000	0	0.5544889115
0.0002	30000	2	0.5000010642
0.001	30000	2	0.5000000128
0.002	30000	2	0.5000000127
0.003	30000	2	0.5000000132
0.004	30000	2	0.5000000124
0.005	30000	2	0.5000000131
0.006	30000	2	0.5000000124
0.007	30000	2	0.5000000122
0.008	30000	2	0.5000000124
0.009	30000	2	0.5000000130
0.01	30000	2	0.5000000118
0.02	30000	2	0.5000000127
0.03	30000	2	0.5000000130
0.04	30000	2	0.5000000129
0.05	30000	0	40.256156930
0.06	30000	0	40.256058900
0.07	30000	0	40.256060340

Table A.4: **Part 1:** Table of pass [2] close [1] fail [0] results for SHO with the trial function $\psi(x) = e^{-0.7071x^2}$. The resultant functions are truncated at 20 orders in x.

Iteration Coefficient	Iterations	Pass/Close/Fail	Energy [Natural Units]
0.00002	40000	0	0.5358800368
0.0002	40000	2	0.5000000310
0.001	40000	2	0.5000000125
0.002	40000	2	0.5000000125
0.003	40000	2	0.5000000129
0.004	40000	2	0.5000000118
0.005	40000	2	0.5000000124
0.006	40000	2	0.5000000130
0.007	40000	2	0.5000000118
0.008	40000	2	0.5000000128
0.009	40000	2	0.5000000130
0.01	40000	2	0.5000000128
0.02	40000	2	0.5000000128
0.03	40000	2	0.5000000124
0.04	40000	2	0.5000000127
0.05	40000	0	40.255660310
0.06	40000	0	40.256060900
0.07	40000	0	40.256059400

Table A.5: **Part 2:** Table of pass [2] close [1] fail [0] results for SHO with the trial function $\psi(x) = e^{-0.7071x^2}$. The resultant functions are truncated at 20 orders in x.

Iteration Coefficient	Order in x	Pass/Close/Fail	Energy [Natural Units]
0.0002	10	2	3.782689188
0.0005	10	2	3.772511036
0.002	10	2	3.772511053
0.003	10	2	3.772511044
0.004	10	2	3.772511056
0.005	10	2	3.77251104
0.006	10	2	3.772511024
0.007	10	2	3.772511042
0.008	10	2	3.772511037
0.009	10	2	3.772511047
0.01	10	2	3.772511044
0.02	10	2	3.772511039
0.00005	20	0	7.439852694
0.00007	20	0	6.132226524
0.00008	20	0	5.410423235
0.00009	20	0	10.2246224
0.0001	20	0	4.0944651
0.0002	20	1	2.423828576
0.0003	20	2	2.394811616
0.0004	20	2	2.394355266
0.0005	20	2	2.394355412
0.001	20	2	2.394355274
0.002	20	2	2.394355261
0.003	20	2	2.394355253
0.004	20	2	2.394355257
0.005	20	2	2.394355268
0.006	20	2	2.394355261
0.007	20	2	2.394355272
0.008	20	2	2.394355271
0.009	20	2	2.394355262
0.01	20	2	2.394355275
0.015	20	2	2.394355271
0.0175	20	2	2.394355273
0.0185	20	2	2.394355274
0.01875	20	0	104.5166223
0.019	20	0	104.51739
0.02	20	0	104.5148402

Table A.6: **Part 1:** Table of pass [2] close [1] fail [0] results for the QPW with the trial function $\psi(x) = e^{-0.4714(x^2+6)^{\frac{3}{2}}}$. The resultant functions are truncated at 20 orders in x.

Iteration Coefficient	Order in x	Pass/Close/Fail	Energy [Natural Units]
0.03	20	0	104.5147889
0.04	20	0	104.5147891
0.05	20	0	104.5147892
0.06	20	0	104.5147891
0.07	20	0	104.5147891
0.00002	30	0	8.97865467
0.00005	30	0	7.439847475
0.0002	30	1	2.388460789
0.0005	30	2	2.35864383
0.002	30	2	2.35864375
0.003	30	2	2.358643686
0.004	30	2	2.358643717
0.005	30	2	2.358643708
0.006	30	2	2.358643694
0.007	30	2	2.35864369
0.008	30	2	2.3586437
0.009	30	2	2.358643705
0.01	30	2	2.358643708
0.02	30	0	144.2858642
0.00002	40	0	8.978654655
0.00005	40	0	9.254371903
0.0002	40	1	2.387232338
0.0005	40	2	2.357286644
0.002	40	2	2.357286544
0.003	40	2	2.357286538
0.004	40	2	2.357286542
0.005	40	2	2.357286504
0.006	40	2	2.357286523
0.007	40	2	2.357286526
0.008	40	2	2.357286544
0.009	40	2	2.35728653
0.01	40	2	2.357286526
0.02	40	0	202.0392889

Table A.7: **Part 2:** Table of pass [2] close [1] fail [0] results for the QPW with the trial function $\psi(x) = e^{-0.4714(x^2+6)^{\frac{3}{2}}}$. The resultant functions are truncated at 20 orders in x.

δ	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
2	0.0002	1	2.417136034
2	0.0005	2	2.393230412
2	0.002	2	2.393230352
2	0.005	2	2.393230344
2	0.02	2	2.393230348
4	0.0002	1	2.563022648
4	0.0005	2	2.537303815
4	0.002	2	2.537303828
4	0.005	2	2.537303818
4	0.02	2	2.537303837
6	0.0002	1	2.423828576
6	0.0005	2	2.394355412
6	0.002	2	2.394355261
6	0.005	2	2.394355268
6	0.02	0	104.5148402
8	0.0002	1	3.157282397
8	0.0005	2	3.135980986
8	0.002	2	3.135980952
8	0.005	2	3.135980897
8	0.02	0	143.292045

Table A.8: Table of pass [2] close [1] fail [0] results for the QPW with the trial function $\psi(x) = e^{-0.4714(x^2+\delta)^{\frac{3}{2}}}$. The resultant functions are truncated at 20 orders in x.

Iteration Coefficient	Power in x	δ	Pass/Close/Fail	Energy [Natural Units]
0.001	10	4	2	4.105823427
0.006	10	4	2	4.105823425
0.001	20	4	2	-1.80233961
0.006	20	4	2	-1.802339545
0.06	20	4	0	96.30639868
0.001	30	4	2	-4.186397702
0.006	30	4	2	-4.186397715
0.001	40	4	2	-4.592865187
0.006	40	4	2	-4.592865215
0.001	50	4	2	-4.592865209
0.006	50	4	0	-41.96511852
0.006	10	6	2	5.085141872
0.00001	20	6	0	9.85162792
0.00006	20	6	0	6.757886194
0.0001	20	6	0	1.101384417
0.0006	20	6	2	-0.826611028
0.001	20	6	2	-0.826611032
0.002	20	6	2	-0.826611048
0.006	20	6	2	-0.826611015
0.01	20	6	2	-0.826611032
0.06	20	6	0	113.6502622
0.006	30	6	2	-3.782656525
0.006	40	6	2	-4.542952913
0.006	50	6	2	-4.609590692
0.006	20	8	2	0.04995267549
0.006	30	8	2	-3.298337573
0.006	40	8	2	-4.438446728
0.006	50	8	2	-4.603577252

Table A.9: Table of pass [2] close [1] fail [0] results for the An-harmonic oscillator with the initial function $\psi(x) = e^{-0.4714(x^2+\delta)^{\frac{3}{2}}}$.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.2	0.00002	0	0.553666593
0.2	0.0002	2	0.984420189
0.2	0.002	2	0.999197513
0.2	0.02	2	0.999197514
0.4	0.00002	0	0.861367267
0.4	0.00004	0	0.904902409
0.4	0.00006	0	0.935243809
0.4	0.00008	0	0.956129003
0.4	0.0004	2	0.9999259278
0.4	0.0006	2	0.9999986574
0.4	0.0008	2	0.9999999774
0.4	0.001	2	0.9999999992
0.4	0.002	2	0.9999999996
0.4	0.02	2	0.9999999990
0.4	0.04	2	0.9999999998
0.4	0.06	0	71.12002828
0.4	0.8	0	14.87584853
0.6	0.00002	0	1.129782752
0.6	0.00004	0	1.085169262
0.6	0.00006	0	1.056295463
0.6	0.00008	0	1.037384696
0.6	0.0002	0	1.003330308
0.6	0.0004	1	1.000060612
0.6	0.0006	2	1.000001102
0.6	0.0008	2	1.000000019
0.6	0.002	2	1.000000000
0.6	0.004	2	1.000000000
0.6	0.006	2	1.000000001

Table A.10: **Part 1:** Pass[2] / Close [1] / Fail [0] results for the 2-D SHO.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.8	0.00002	0	1.365984306
0.8	0.00004	0	1.231353736
0.8	0.00006	0	1.149370173
0.8	0.00008	0	1.097707892
0.8	0.0002	0	1.008475642
0.8	0.0006	2	1.000003431
0.8	0.0008	2	1.000000678
0.8	0.002	2	1.00000063
0.8	0.004	2	1.000000633
0.8	0.006	2	1.000000632
0.8	0.008	2	1.000000631
0.8	0.02	2	1.000000632
0.8	0.06	0	94.37723002
0.8	0.08	0	94.37722974
2	0.00002	0	2.345471458
2	0.0002	2	1.031642642
2	0.002	2	1.015689546
2	0.02	0	257.1460311

Table A.11: **Part 2:** Pass[2] / Close [1] / Fail [0] results for the 2-D SHO.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.2	0.0001	0	0.4452226566
0.2	0.0005	2	0.5211323215
0.2	0.001	2	0.5221702600
0.2	0.005	2	0.5209937794
0.2	0.01	2	0.5195730670
0.2	0.05	2	0.5107134840
0.4	0.0001	0	0.4851813284
0.4	0.0005	2	0.5000002416
0.4	0.001	2	0.5000053560
0.4	0.005	2	0.5000050944
0.4	0.01	2	0.5000047678
0.4	0.05	2	0.5000023324
0.6	0.0001	0	0.5124603688
0.6	0.0005	2	0.5000055832
0.6	0.001	2	0.5000014251
0.6	0.005	2	0.5000013550
0.6	0.01	2	0.5000012660
0.6	0.05	2	0.5000002510
0.8	0.0001	0	0.5124603700
0.8	0.0005	2	0.5000055825
0.8	0.001	2	0.5000014250
0.8	0.005	2	0.5000013552
0.8	0.01	2	0.5000012665
0.8	0.05	2	0.5000002514

Table A.12: Pass[2] / Close [1] / Fail [0] results for the Second Order Iteration Operator on the SHO truncated at after 10 orders in x.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.2	0.0001	0	0.4451650064
0.2	0.0005	2	0.4996028134
0.2	0.001	2	0.4996076464
0.2	0.005	2	0.4996420716
0.2	0.01	2	0.4996823549
0.2	0.05	2	0.4998794365
0.4	0.0001	0	0.4851812684
0.4	0.0005	1	0.4999949159
0.4	0.001	2	0.4999999998
0.4	0.005	2	
0.4	0.01	2	0.5000000005
0.4	0.05	2	
0.6	0.0001	0	0.5124603346
0.6	0.0005	1	0.5000041605
0.6	0.001	2	0.5000000004
0.6	0.005	2	0.4999999997
0.6	0.01	2	0.5000000000
0.6	0.05	0	31.89363446
0.8	0.0001	0	0.5322486840
0.8	0.0005	2	0.5000108625
0.8	0.001	2	0.5000003095
0.8	0.005	2	0.5000002810
0.8	0.01	2	0.5000002390
0.8	0.05	2	0.5000002395

Table A.13: **Part 2:** Pass[2] / Close [1] / Fail [0] results for the Second Order Iteration Operator on the SHO truncated at after 20 orders in x.

Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.2	0.0001	0	0.4451649737
0.2	0.0005	2	0.4999866822
0.2	0.001	2	0.5000067785
0.2	0.005	2	0.5000059270
0.2	0.01	2	0.5000049670
0.2	0.05	2	0.5000014314
0.4	0.0001	0	0.4851812728
0.4	0.0005	1	0.4999949172
0.4	0.001	2	0.4999999992
0.4	0.005	2	0.4999999998
0.4	0.01	2	0.4999999994
0.4	0.05	0	29.99474335
0.6	0.0001	0	0.5124603410
0.6	0.0005	1	
0.6	0.001	2	0.5000000002
0.6	0.005	2	0.4999999996
0.6	0.01	2	0.5000000000
0.6	0.05	0	49.15714714
0.8	0.0001	0	0.5322486668
0.8	0.0005	1	0.5000105575
0.8	0.001	2	0.5000000003
0.8	0.005	2	0.5000000000
0.8	0.01	2	0.5000000002
0.8	0.05	0	73.99477645

Table A.14: Pass[2] / Close [1] / Fail [0] results for the Second Order Iteration Operator on the SHO truncated at after 30 orders in x.

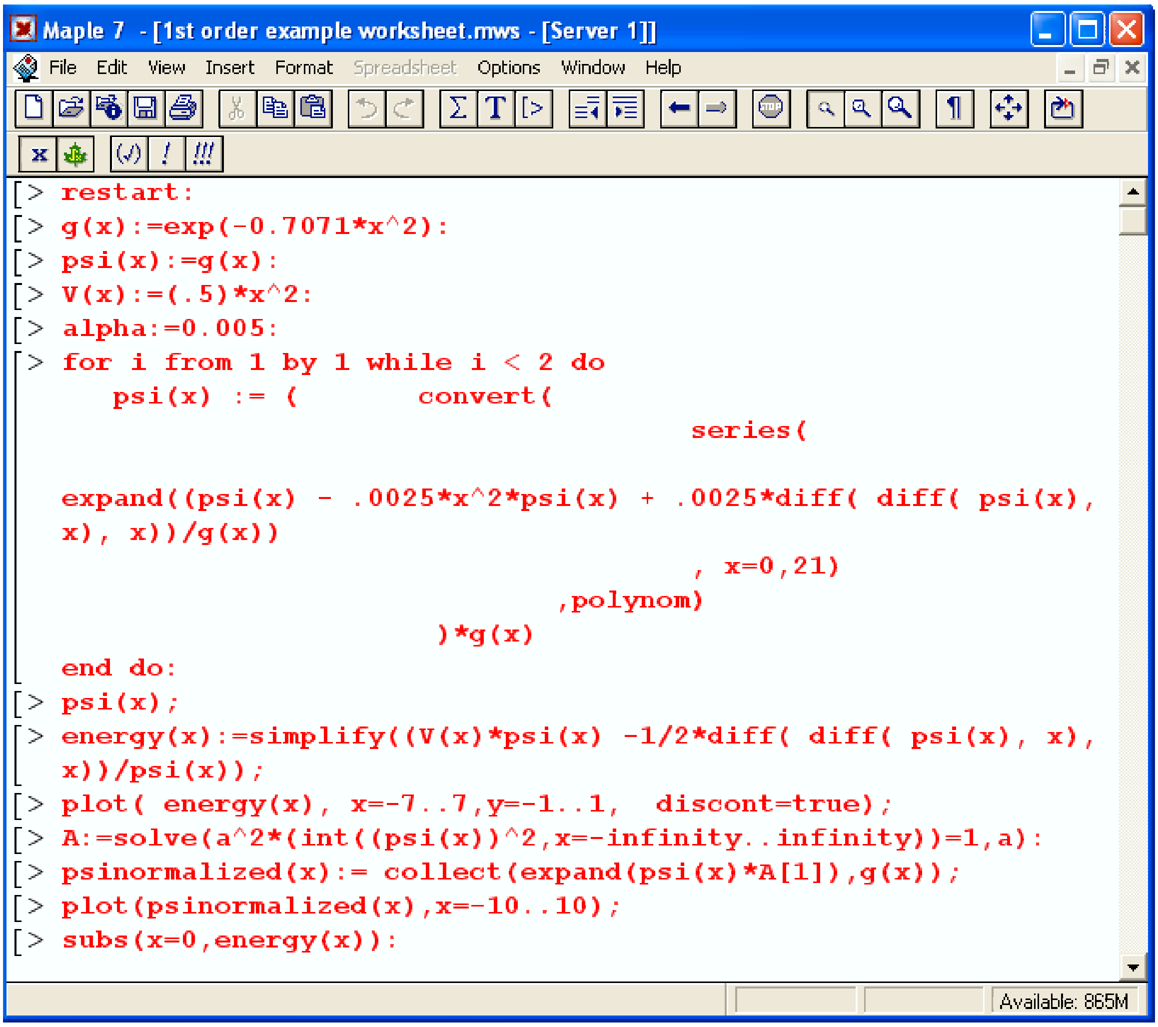
Gaussian Coefficient	Iteration Coefficient	Pass/Close/Fail	Energy [Natural Units]
0.2	0.0001	0	0.4451651846
0.2	0.0005	1	0.4999802908
0.2	0.001	2	0.4999998881
0.2	0.005	2	0.4999999073
0.2	0.01	2	0.4999999266
0.2	0.05	0	-6.581880416
0.4	0.0001	0	0.4851812684
0.4	0.0005	1	0.4999949152
0.4	0.001	2	0.4999999995
0.4	0.005	2	0.5000000001
0.4	0.01	2	0.5000000000
0.4	0.05	0	39.48218547
0.6	0.0001	0	0.5124603371
0.6	0.0005	1	0.5000041600
0.6	0.001	2	0.5000000002
0.6	0.005	2	0.5000000000
0.6	0.01	2	0.4999999999
0.6	0.05	0	66.55515042
0.8	0.0001	0	0.5322486563
0.8	0.0005	1	0.5000105558
0.8	0.001	2	0.4999999986
0.8	0.005	2	0.4999999994
0.8	0.01	2	-1.348235560
0.8	0.05	0	100.4686616

Table A.15: Pass[2] / Close [1] / Fail [0] results for the Second Order Iteration Operator on the SHO truncated at after 40 orders in x.

Appendix B

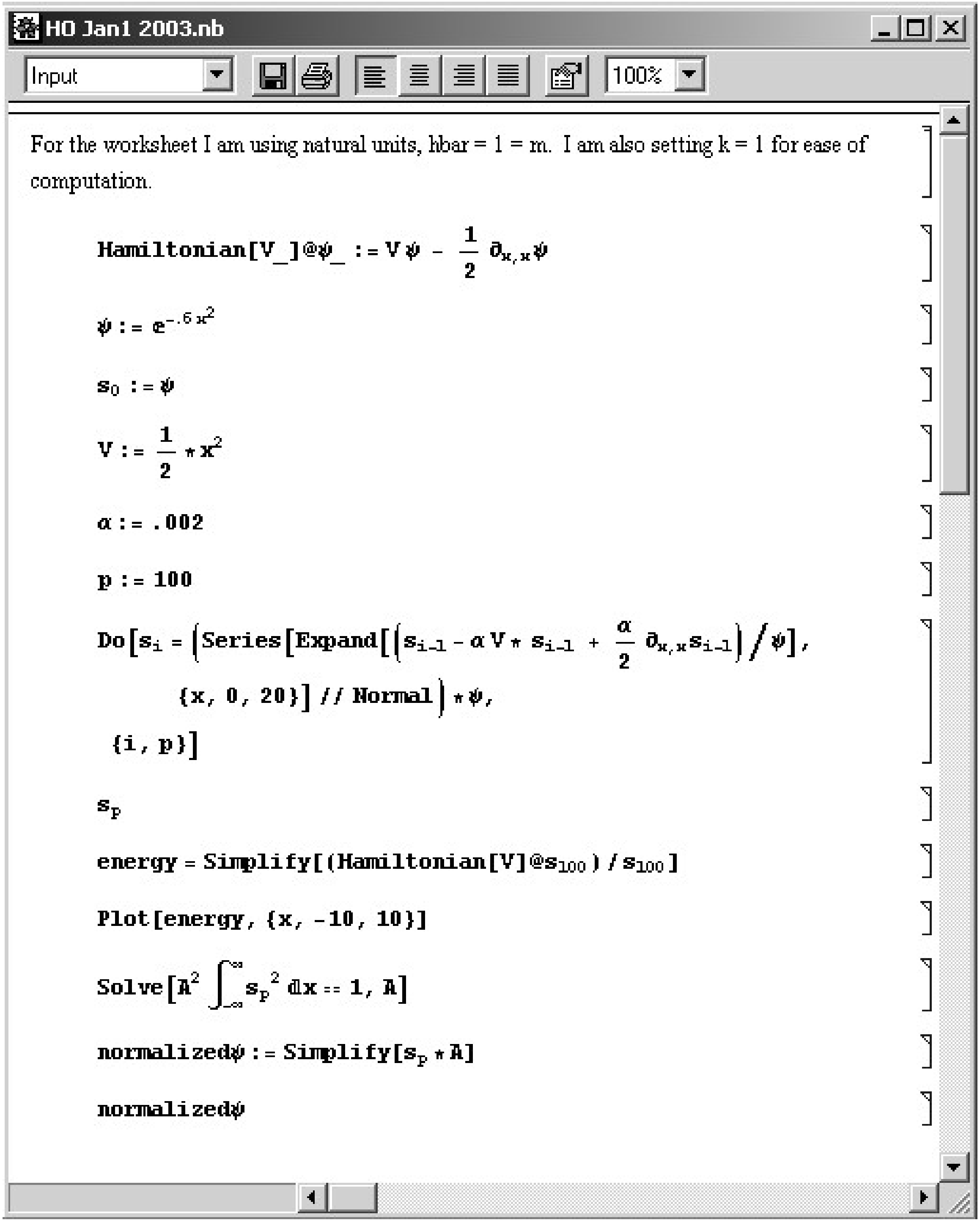
Examples of Implementation

The figures that follow hereafter are representations of the Maple®work sheets and the Mathematica®notebooks that were used.



```
> restart:
> g(x):=exp(-0.7071*x^2):
> psi(x):=g(x):
> V(x):=(.5)*x^2:
> alpha:=0.005:
> for i from 1 by 1 while i < 2 do
     psi(x) := (         convert(
                                         series(

  expand((psi(x) - .0025*x^2*psi(x) + .0025*diff( diff( psi(x),
  x), x))/g(x))
                                         , x=0,21)
                                  ,polynom)
                            )*g(x)
  end do:
> psi(x);
> energy(x):=simplify((V(x)*psi(x) -1/2*diff( diff( psi(x), x),
  x))/psi(x));
> plot( energy(x), x=-7..7,y=-1..1,  discont=true);
> A:=solve(a^2*(int((psi(x))^2,x=-infinity..infinity))=1,a):
> psinormalized(x):= collect(expand(psi(x)*A[1]),g(x));
> plot(psinormalized(x),x=-10..10);
> subs(x=0,energy(x)):
```

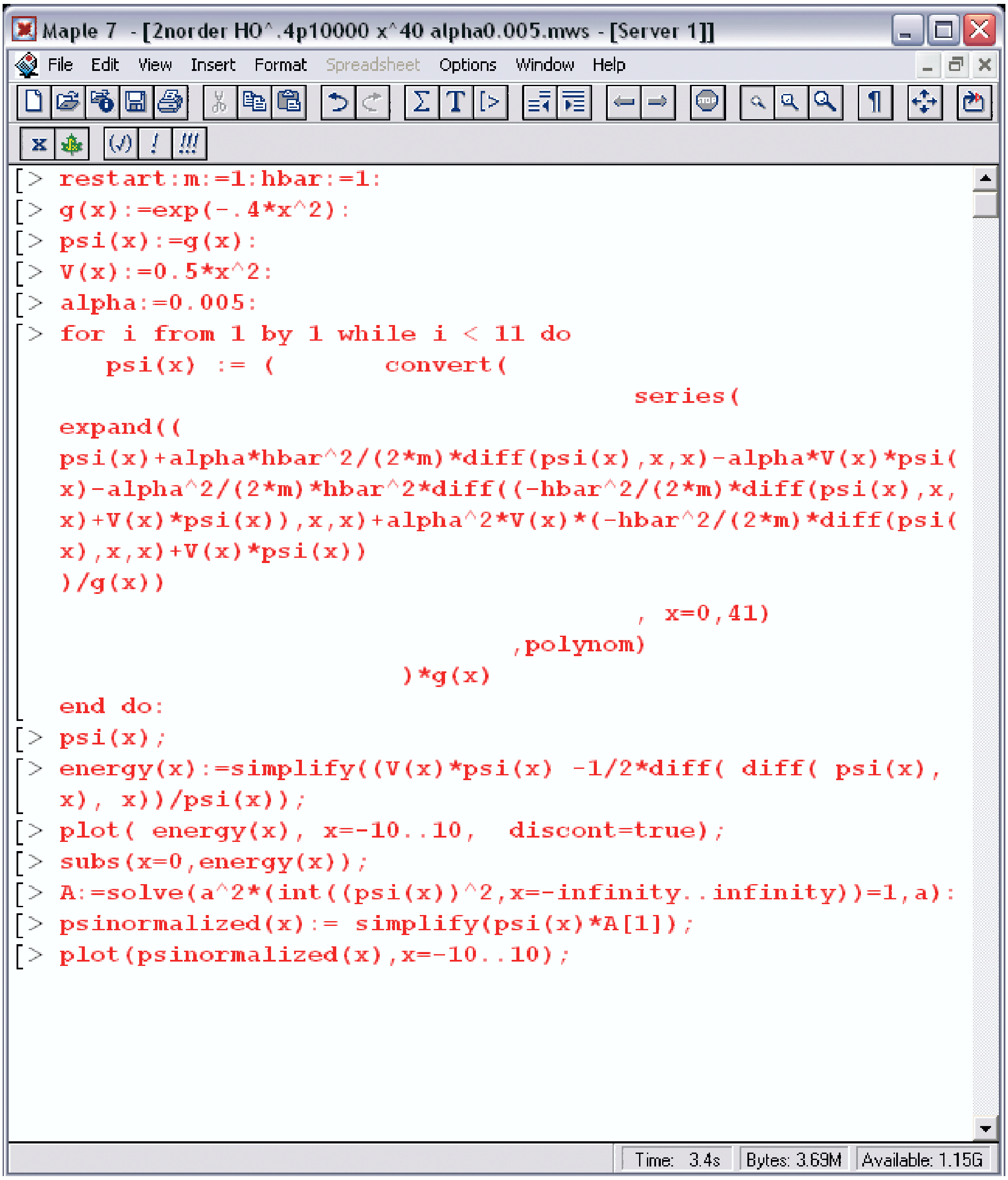
Figure B.1: Example worksheet for the Maple®implementation of the first order Iteration Operator.



For the worksheet I am using natural units, hbar = 1 = m. I am also setting k = 1 for ease of computation.

```
Hamiltonian[V_]@ψ_ := V ψ - 1/2 ∂x,x ψ

ψ := e^(-.6 x^2)

s0 := ψ

V := 1/2 * x^2

α := .002

p := 100

Do[si = (Series[Expand[(si-1 - α V * si-1 + α/2 ∂x,x si-1) / ψ],
        {x, 0, 20}] // Normal) * ψ,
  {i, p}]

sp

energy = Simplify[(Hamiltonian[V]@s100) / s100]

Plot[energy, {x, -10, 10}]

Solve[A^2 ∫-∞^∞ sp^2 dx == 1, A]

normalizedψ := Simplify[sp * A]

normalizedψ
```

Figure B.2: Example worksheet for the Mathematica® implementation of the first order Iteration Operator.



```
[> restart:m:=1:hbar:=1:
[> g(x):=exp(-.4*x^2):
[> psi(x):=g(x):
[> V(x):=0.5*x^2:
[> alpha:=0.005:
[> for i from 1 by 1 while i < 11 do
      psi(x) := (       convert(
                                        series(
   expand((
   psi(x)+alpha*hbar^2/(2*m)*diff(psi(x),x,x)-alpha*V(x)*psi(
   x)-alpha^2/(2*m)*hbar^2*diff((-hbar^2/(2*m)*diff(psi(x),x,
   x)+V(x)*psi(x)),x,x)+alpha^2*V(x)*(-hbar^2/(2*m)*diff(psi(
   x),x,x)+V(x)*psi(x))
   )/g(x))
                                        , x=0,41)
                                  ,polynom)
                            )*g(x)
   end do:
[> psi(x);
[> energy(x):=simplify((V(x)*psi(x) -1/2*diff( diff( psi(x),
   x), x))/psi(x));
[> plot( energy(x), x=-10..10,  discont=true);
[> subs(x=0,energy(x));
[> A:=solve(a^2*(int((psi(x))^2,x=-infinity..infinity))=1,a):
[> psinormalized(x):= simplify(psi(x)*A[1]);
[> plot(psinormalized(x),x=-10..10);
```

Figure B.3: Example worksheet for the Maple®implementation of the second order Iteration Operator.

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