Comparison of Finite Differences and WKB Method for Approximating Tunneling Times of the One Dimensional Schrödinger Equation

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Overview

The goal of this research was to examine the quantum mechanical phenomenon of tunneling with respect to the Schrödinger Equation. A quantum mechanical wave is said to "tunnel" when it travels (propagates) through a classically forbidden region. In a more physical interpretation, it is when the energy (E) of the wave is lower than the potential at a specific point V(x). [A point where V(x) is greater than E is referred to as a classical turning point.] The phenomenon of a tunneling was examined in a double-well potential. Another goal of this project was to compare two methods for approximating the tunneling time of a wave packet. The two methods used were the finite differences (numerical) and WKB (analytical) approximation methods. In order to compare a potential that experienced tunneling and one that did not, the solution to a quadratic potential was also solved.

Theory

Schrödinger Equation Theory:

The one dimensional Schrödinger equation is given as follows:

$$\hat{H}\psi(x,t)=E\psi(x,t) \tag{1.1}$$

Where $\hat{H}$ is the Hamiltonian operator, ψ is the wave function, and E is the energy.

In atomic units, the Hamiltonian operator for a particle in a potential is:

$$\hat{H} = -\nabla^2 + V(x) \tag{1.2}$$

The time-independent Schrödinger equation (TISE) bounded inside a potential becomes:

$$-\varphi_{xx}(x, 0) + V(x)\varphi(x,0) = E\varphi(x,0) \tag{1.3}$$

(φ is the time-independent wave function)

As stated, this equation is an eigenevalue problem where the operator returns the wave function multiplied by some eigenvalue, E.

This amounts to solving for the stationary states (normal modes) of the system by finding the set of eigenvalues and eigenvectors given a known potential V(x).

The time dependent Schrödinger equation (TDSE), bounded inside of a potential is:

$$i\psi_t(x, t) + \psi_{xx}(x, t) + V(x)\psi(x,t) = 0 \quad \text{(t is time)} \tag{1.4}$$

The TDSE becomes the TISE when t=0. The relationship between the two is:

$$i\psi_t = -E\varphi \quad \text{or} \quad \psi_t = -iE\varphi \tag{1.5}$$

Since t is 0, $\psi = \varphi$

Thus, to satisfy this equality, the solutions for the wave function become rotating complex exponentials:

$$\psi(x,t) = \varphi(x)e^{-iEt} \tag{1.6}$$

The time evolution, u(x,t), of the Schrödinger equation is given by a normalized, linear combination of stationary states (normal modes):

$$u(x,t) = a_1\psi_1(x)\, e^{-iE_1 t} + a_2\psi_2(x)\, e^{-iE_2 t} + a_3\psi_3(x)\; e^{-iE_3 t} \ldots\ ,\ \sum_n a_n^2 = 1 \tag{1.7}$$

The average energy (expectation value), <E>, of such a linear combination being:

$$\langle E\rangle = \sum_n a_n^2 E_n \tag{1.8}$$

The examined linear combinations were always of the type:

$$\frac{1}{\sqrt{2}}\left[\psi_a(x)\; e^{-iE_a t} + \psi_b(x)\; e^{-iE_b t}\right] \tag{1.9}$$

They were centered directly between the two combined normal modes.

Tunneling time amounts to ½ the period of this linear combination and is given by

$$t_{tun} = \pi/\Delta E \tag{1.1}$$

$$\text{Where } \Delta E = E_b - E_a \tag{1.11}$$

The two investigated potentials were the harmonic, quadratic potential and the double well potential:

$$V(x) = kx^2 \text{ (quadratic)} \tag{1.1}$$

$$V(x) = ux^4 - kx^2 + bh \text{ (double well)} \tag{1.1}$$

bh = barrier height between the two wells

Methods:

Finite Differences

The majority of the work was done using a finite differences approximation. Finite differences is a numerical method for solving partial an ordinary differential equations. For the Schrödinger equation, this is accomplished by spatial discretization (marching along in steps of Δx) and a matrix representation for the Hamiltonian (Equation 1.2). This approximation is:

$$K = \frac{-1}{(\Delta x)^2}\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & -2 & 1 \\ & & 1 & -2 \end{bmatrix} + \begin{bmatrix} v_1 & & & \\ & v_2 & & \\ & & v_3 & \\ & & & v_4 \end{bmatrix} \tag{2.1}$$

Where the v_ns along the diagonal represent the potentials evaluated at the points x_n. The diagonalization of this matrix yield two matrices [V,D] where V are the eigenvectors of the K matrix stacked in columns (normal modes/stationary states -- ψ) and D is a the diagonal matrix that contain the eigenvectors ("energies" -- E) associated with the normal modes (stationary states).

WKB Method

The tunneling time for the finite differences approach was compared to the WKB (Wentzel-Kramers-Brillouin) approximation method:

Unlike finite differences, the WKB approximation is analytic, not numerical. It works under the assumption that "the quantum wavelength not change appreciably over the distance of one wavelength" (Liboff 232).

The change in wavelength with respect to the change in distance is given by:

$$\delta\lambda = \frac{d\lambda}{dx}\delta x \tag{2.2}$$

After one wavelength the change becomes:

$$\delta\lambda = \frac{d\lambda}{dx}\lambda \tag{2.3}$$

The WKB assumption is that $\delta\lambda << \lambda$, adding this criterion into the previous equation yields:

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{d\lambda}{dx}\right| << 1 \tag{2.4}$$

This consequence is examined with respect to momentum (p):

$$\left(\frac{h}{\lambda}\right)^2 = p^2 = 2m(E-V) \tag{2.5}$$

$$\frac{d(\lambda^2)}{dx} = -\frac{h^2}{p^4}\frac{d(p^4)}{dx} = -\frac{h^2}{p^4}\left(-2m\frac{dV}{dx}\right) \tag{2.6}$$

or

$$\frac{d\lambda}{dx} = \frac{mh}{p^3}\frac{dV}{dx} \tag{2.7}$$

This momentum combined with the WKB approximation that $\delta\lambda << \lambda$ becomes:

$$\left|\frac{\delta\lambda}{\lambda}\right| = \left|\frac{mh}{p^3}\frac{dV}{dx}\right| << 1 \tag{2.8}$$

This approximation can be applied to the Schrödinger equation if we take into account a slowly varying potential.

If the potential varies slowly, then the solution becomes very near to a free-particle problem where we look for solutions of the form:

$$\varphi(x) = Ae^{ikx} = Ae^{ipx/\hbar} \tag{2.9}$$

So, we are looking for solutions of the following form:

$$\varphi(x) = Ae^{iS(x)/\hbar} \tag{2.10}$$

Substitution in equations 1.2 yields:

$$-i\hbar\frac{\partial^2 S}{\partial x^2} + \left(\frac{\partial S}{\partial x}\right)^2 = p^2(x) \tag{2.1}$$

Next, the limit of $\hbar \to 0$ is examined. In this limit, the "Gaussian packet reduces to the classical particle" (Liboff 234). Thus, we can expand S(x) in powers of $\hbar$:

$$S(x) = S_0(x) + \hbar S_1(x) + \frac{\hbar^2}{2}S_2(x) + \ldots \tag{2.1}$$

Combining this with equation 2.11:

$$0 = \left[\left(\frac{\partial S_0}{\partial x}\right)^2 - p^2\right] + 2\hbar\left(\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} - \frac{i}{2}\frac{\partial^2 S_0}{\partial x^2}\right) + O(\hbar^3) \tag{2.1}$$

Since this equation must hold true for any small value $\hbar$, the powers must vanish independently. Thus, two important equalities come out of this equation.

$$\left(\frac{\partial S_0}{\partial x}\right)^2 = p^2 \tag{2.14}$$

and

$$\frac{\partial S_0}{\partial x}\frac{\partial S_1}{\partial x} = \frac{i}{2}\frac{\partial^2 S_0}{\partial x^2} \tag{2.15}$$

The first of these equalities becomes the following upon integration:

$$S_0(x) = \pm\int_{x_0}^{x} p(x)dx \tag{2.16}$$

For the tunneling condition, this amounts to integration across the barrier of $\sqrt{V(x)-E}$ [2m=1](the imaginary potential). Thus, inserting this back into equation 2.10:

$$\varphi(x) = Ae^{i\pm\int_{x_0}^{x}\sqrt{V(x)-E}dx} \tag{2.17}$$

In atomic units, A = a prefactor

We can use this result to get the energy splitting of near-degenerate eigenvalues of the double well potential:

$$\Delta E = \frac{\hbar\omega}{\sqrt{e\pi}}\exp\left[-\int_{-a}^{a}\frac{|p|}{\hbar}dx\right] \quad \text{(Garg 431)} \tag{2.18}$$

Where $\pm a$ = the points at which <E> crosses the barrier

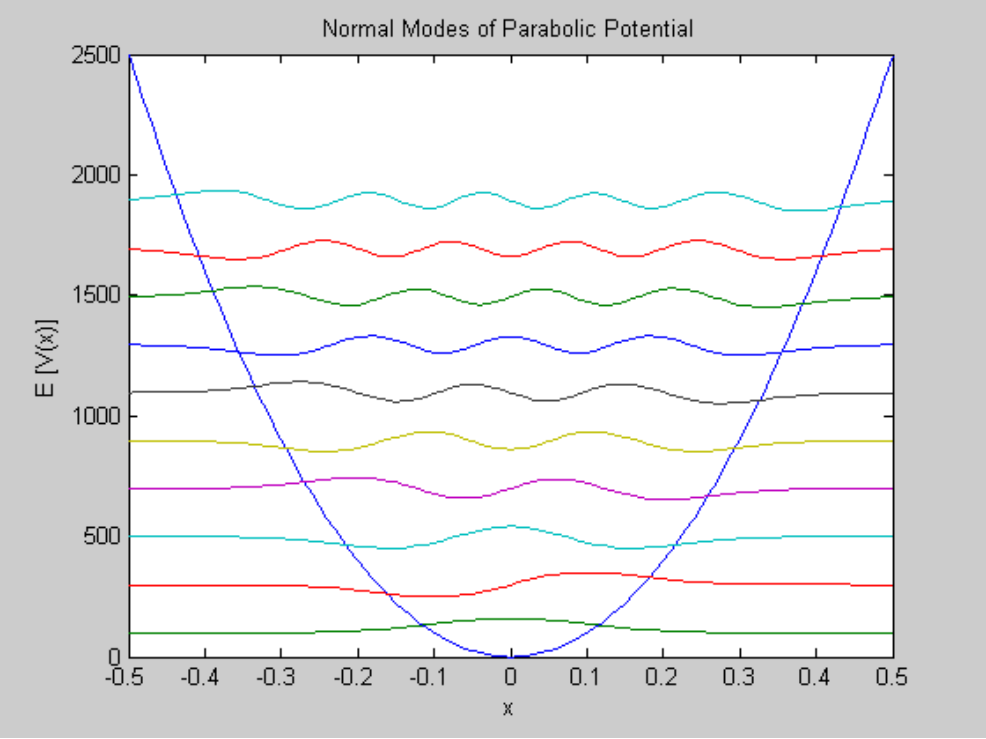
ω for a double well potential of the form in equation 11 is given by

$$\omega = \sqrt{8k} \text{ (Garg 434)} \tag{2.19}$$

Results and Discussion:

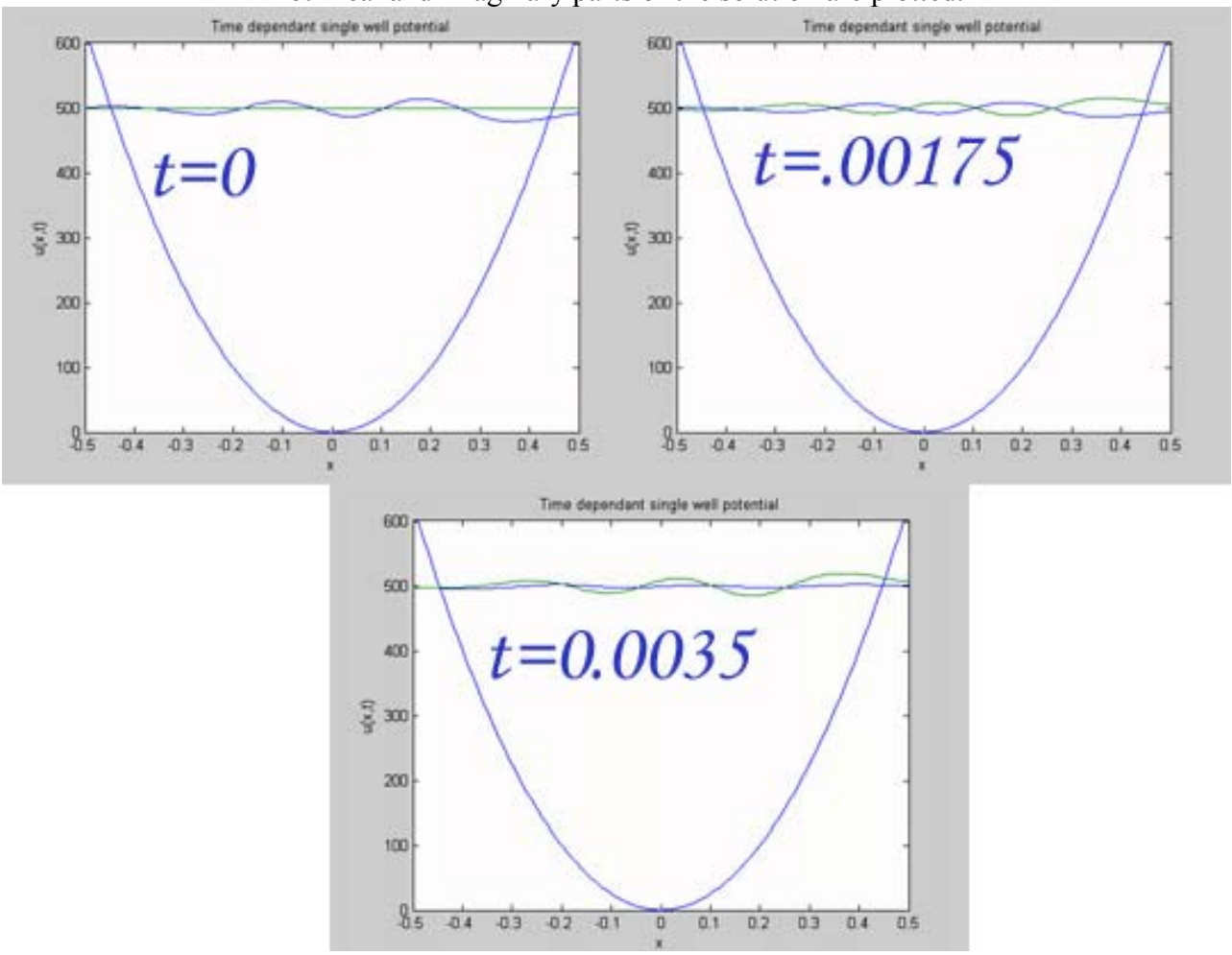
Using the finite differences methods the solutions to the Schrödinger equation were approximated by different methods. For the quadratic potential (*See figure 1*), the eigenvalues (energies) were equally spaced and each successive normal mode had one more node than the previous (the first normal mode, corresponding to the first eigenvalue, had the lowest energy and no nodes)

Figure 1: Normal Modes of a Quadratic Potential, $V(x) = 20000x^2$ [Blue]



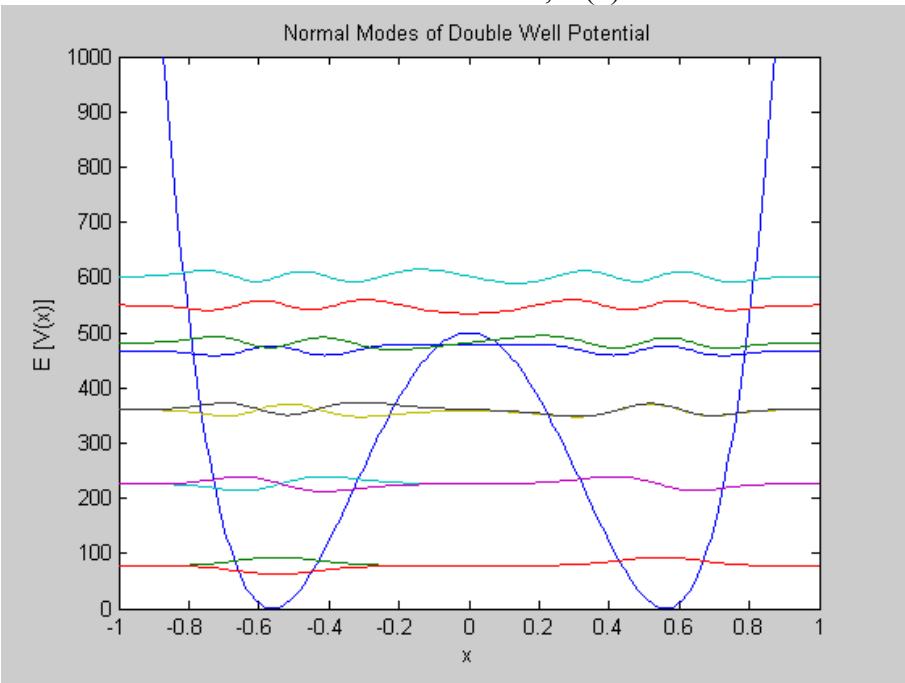
The TDSE of the quadratic potential remained inside the given potential, V(x), and did not 'tunnel' or 'go through' the potential. Instead, the wave packed turned at the classic turning points on either side of the potential (An example of a solution to the TDSE is found in *figure 2*).

Figure 2: One solution to the TDSE. t=0 is at start of period, t=.0035 is halfway through period. Both real and imaginary parts of the solution are plotted.



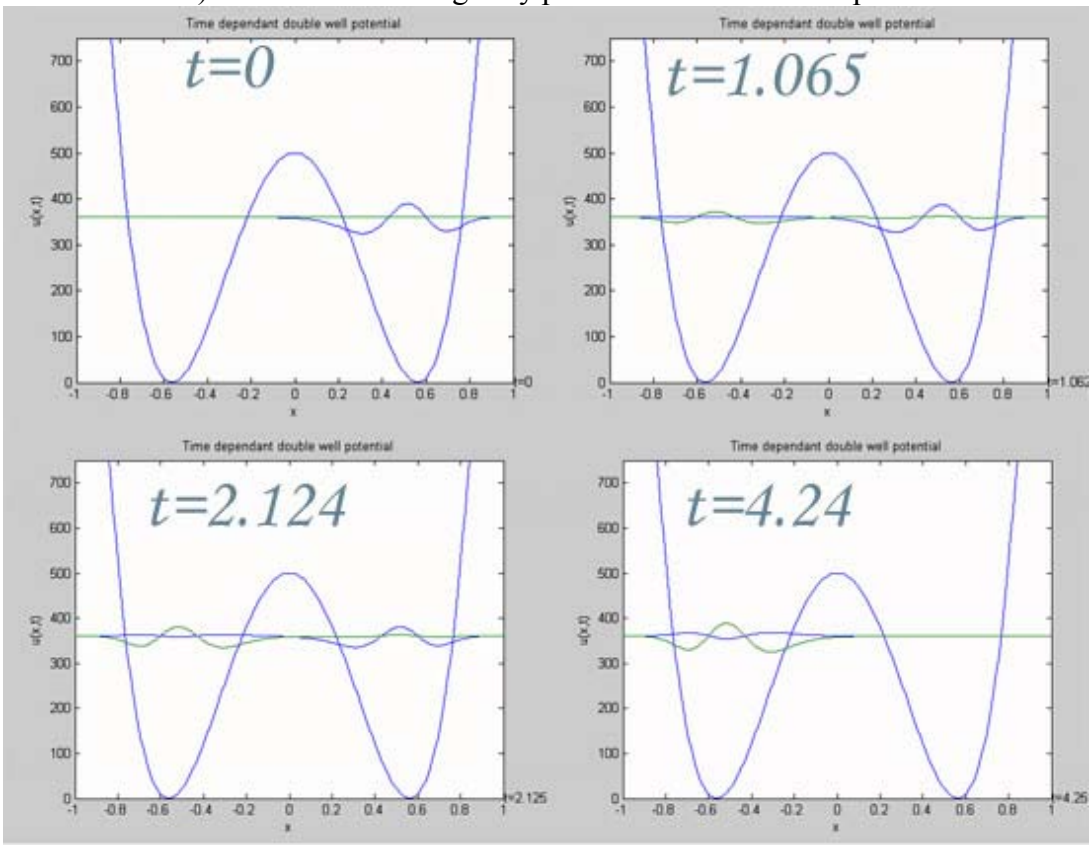
The double well (quartic) potential's normal modes had several different characteristics as compared to the double well. Firstly, the energy levels existed in pairs of closely spaced (*See figure 3*), nearly-degenerate doublets. These doublets in the stationary state solution arose because of the two separate wells. One of each degenerate pairs occupied one or the other well. However, they were not completely degenerate because one had to be symmetric and one had to be antisymmetric. Therefore, the symmetric level was slightly lower in energy because it had one less node than the corresponding antisymmetric level. Another interesting characteristic was the spacing of successive doublets. The spacing between successive doublets decreased as the energy was increased because of the slight anharmonicity (non-symmetric nature) of the well around the barrier. The spacing between the doublets, however, increased with increased energy until the point when E > bh when the spacing between the doublets became so large that they could be considered to be discrete normal modes.

Figure 3: Normal Modes of a Double Well Potential, $V(x) = 5000x^4 - 3162x^2 + 500$ [Blue]



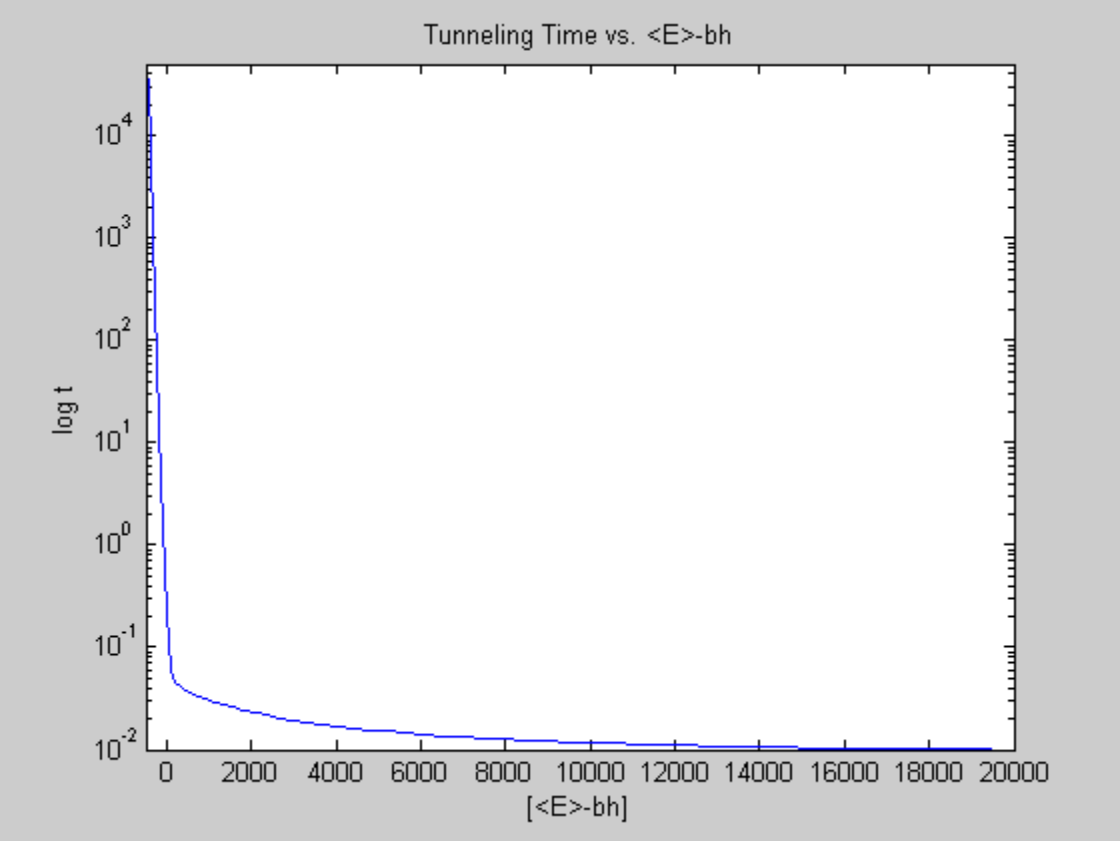
The time evolution of a linear combination of two nearly-degenerate states was approximated using the finite differences method. When <E> < bh the wave experienced tunneling. The time it took for the wave to travel completely from one well to the other well is given by equation 1.10. An illustration of this phenomenon is shown in *figure 4*.

Figure 4: One solution to the TDSE. t=0 is at start of period, t=4.24 is halfway through period (the tunneling time). Both real and imaginary parts of the solution are plotted.



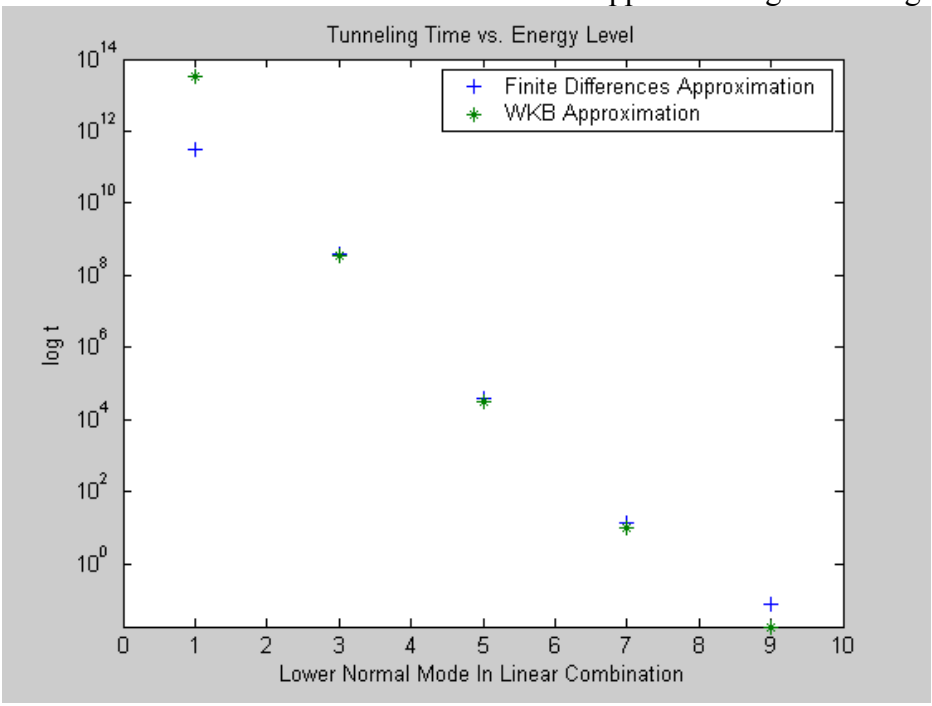
The tunneling time can be more closely examined by comparing tunneling time to the difference between <E> and the barrier height. In *figure 5*, a plot of tunneling time vs. <E>- bh is shown. When the difference is negative (expectation value is less than barrier height) the tunneling time is large because the wave cannot immediately cross the barrier. However, when the expectation value is larger than the barrier height (a positive difference) the 'tunneling time' tapers off very quickly. In this region, though the wave still 'feels' the potential increase at the barrier, it no longer is truly tunneling. This shift from tunneling to not tunneling is illustrated by the change in slope at the point when the expectation value equals the barrier height (x axis = 0 in *figure 5*).

Figure 5: log (Tunneling time) vs. <E>-bh.



As explained in the methods section, the finite differences numerical approximation method and the WKB analytic approximation method were compared. The methods agreed with each other fairly (*See figure 6*) well expect for some key points. The most important disagreement is the linear combination of the lowest two doubly-degenerate pairs (x axis = 1). This is most likely due to the machine precision of the program used to calculate the energy spacing. At these low levels, the spacing between pairs is so small that the difference may only lie in the last digit or two of machine precision. This leads to less accurate energy splittings. The other important area of divergence is the area above the barrier (x-axis = 9) because the WKB approximation only holds under the barrier when the pairs are nearly-degenerate. In the region between these points, however, when the expectation value is less than the barrier height and the machine can calculate the energy splittings to several significant figures, the two methods correspond well and either can be used to determine the tunneling time fairly accurately.

Figure 6: WKB vs. Finite Differences Method for Approximating Tunneling Time



A convergence test for the ground state energy level as well as the first energy splitting was conducted. A plot of the ground state energy level convergence is found in *Figure 7*, and the first energy splitting between the ground state and its nearly-degenerate pair is found in *Figure 8*. For both convergences, it was found that the dx values were quadratically convergent. The value of dx (Δx) actually used in previous calculations was 0.01. Though the convergence for the actually energy of the ground state is within a very narrow relative range, the convergence for the splittings occurs over a much larger range of energies. This is because, as previously stated, machine precision makes the energy splitting somewhat inaccurate at the lower levels. Perhaps, if a smaller Δx was used, the WKB and finite differences approximations would correspond better at lower energy levels.

Figure 7: Convergence Test for Energy (Eigenvalue) of First Stationary State (Ground State) [Δx (dxs) vs. E]

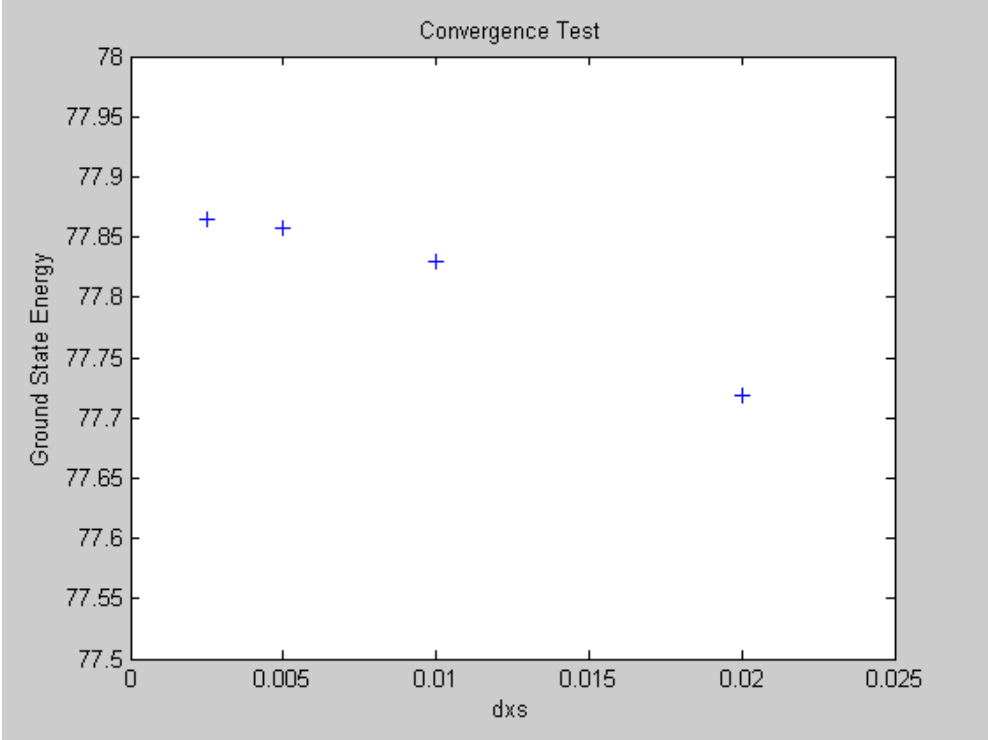
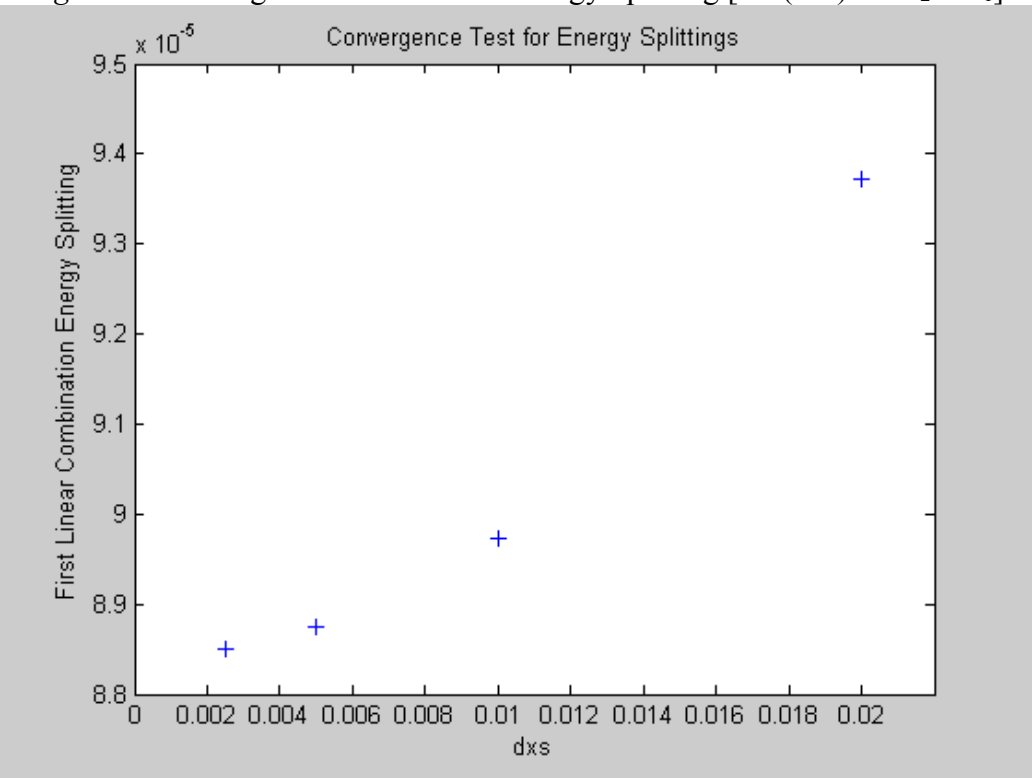


Figure 8: Convergence Test for First Energy Splitting [Δx (dxs) vs. $E_2 - E_1$]



Conclusion

The quantum mechanical phenomenon of tunneling can be examined using numerical and analytic methods of approximation. However, it may be useful to use both methods, depending on the conditions of the problem. In the region when the difference between the barrier height and the energy is large (lower energy states) the best method may be analytic method because of a lack of machine precision with such small energy gaps. However, when the spacing between the energy and the barrier height is very small, the better method is the numerical method because the assumptions of the analytical WKB method become no longer valid. It may also be crucial to take smaller Δx steps in order to increase the accuracy of the spacings between lower energy levels, thus increasing the accuracy of the numerical method.

References

Garg, Anupam. "Tunnel Splittings for One-Dimensional Potential Wells Revisited". American Journal of Physics. 68 (5), 2000. 430-437.

Liboff, Richard L. *Introductory Quantum Mechanics*. San Francisco: Cornell University Press, 1990.