Computationally Modeling Propagation of a Wave Packet

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Abstract

To calculate expected values of physical observables such as dipole moment, velocity, and acceleration, I represented a wave packet with a Gaussian envelope as a vector in discrete space and solve a linear systems problem to compute propagations at different time steps using the implicit propagation scheme. The wave packet is in a box, whose size emulates infinte space. Certain consequences of discretizing space and time are assessed. Using different parameters, particularly the center wave number and width of a potential well, I discovered that computational calculations for transmission in a system with a finite square potential well might align with the analytically derived transmission coefficient.

Contents

List of Figures

Introduction

Computationally studying a physical observable of a single-electron atom may require the use of a wave function represented in a computer. To compute the expected value of any physical quantity, one may make use of the probability distribution function (PDF) definition of expected value. The square magnitude of a solution to the Schrödoinger equation over position at a given time may be used as a PDF if it is normalized. It is very difficult to determine the state of a wave function at a given time in a certain system by analytical methods, so computational modeling of the wave functions is used.

I used the implicit scheme given an initial discretized wave function to propagate the wave function through discrete time. The implicit scheme and discretization of time and space introduces some limitations, but these limitations are predictable. This will allow for easier computation of expected values for physical quantities of interest, such as dipole acceleration, on an atomic level, which can be rescoped to a macro-level system using Maxwell's equations. This process can aid in understanding and manipulating certain atomic and molecular processes when combined with experimental methods such as utilizing high harmonic generation to create attosecond pulses of light.

The programs implement a basic particle-in-a-box system. The wave packet was constructed by multiplying a Gaussian function by a plane wave equation, and its evolution over time was computed iteratively by the implicit scheme of propagation. We investigate a system with constant potential energy as well as a potential well. The programs are verified by comparing computationally calculated expected values to those which were analytically calculated as well as assessing the autocorrelation. The results of different condidtions are examined graphically, and physical and mathematical explanations to those results are provided.

Theory

Storage and memory on computers are finite, so a wave function or packet and the dynamics of it must be represented discretely. Both time and space are discretized into a grid with units δt and δx, respectively, and we work within one dimension of space. We choose units such that $\hbar$ equal to one, and we assume that mass is one. Unless stated otherwise, change is assumed to be with respect to time.

Implicit Scheme of Propagation

I chose to implicitly propegate a wave function by virtue of computational simplicity. We start with the time-dependent Schrödinger equation.

$$\hat{H}\Psi(x,t) = \hat{E}\Psi(x,t)$$

where $\hat{H} = \frac{\hat{p}^2}{2} + V(x)$. We may express the energy operator explicitly and then solve differential equation for Ψ.

$$\begin{aligned}
\hat{H}\Psi(t) &= i\frac{\partial}{\partial t}\Psi(t) \\
\frac{\partial}{\partial t}\Psi(t) &= -i\hat{H}\Psi(t) \\
\Psi(t) &= e^{-i\hat{H}t}\Psi(0) \\
\Psi(t) &= \frac{e^{-i\hat{H}\frac{t}{2}}}{e^{i\hat{H}\frac{t}{2}}}\Psi(0)
\end{aligned}$$

We expand both the numerator and the denomenator of the operator into a first degree Maclaurin series.

$$\left(1 + i\hat{H}\frac{t}{2}\right)\Psi(t) \approx \left(1 - i\hat{H}\frac{t}{2}\right)\Psi(0)$$

Considering that we are working in discrete space and time, we have

$$\left(1 + iH\frac{\delta t}{2}\right)\vec{\Psi}(\delta t) \approx \left(1 - iH\frac{\delta t}{2}\right)\vec{\Psi}(0) \tag{1}$$

where H is the matrix representation of the Hamiltonian operator and $\vec{\Psi}(t)$ is the column vector representation of $\Psi(t)$ such that $\vec{\Psi}(t)_j$ is the value of $\Psi(t)$ at $x = j \cdot \delta x$. The wave function at the next time step is computed by solving the linear system through forward elimination and backsubstitution.

Total Energy Suppose we have a wave fuction representing a plane wave, $\psi(x) = e^{ikx}$. Assuming $\hat{H} = \frac{\hat{p}^2}{2}$, we have, in discrete space, from the time-independent Schödinger equation

$$-\frac{1}{2}\vec{\psi}_x'' = E\vec{\psi}_x.$$

Now we take the numerical second derivative of $\vec{\psi}_x$ by calculating the sum of the Taylor series expansions for $\vec{\psi}_{x-\delta t}$ and $\vec{\psi}_{x+\delta t}$ and then solve for E.

$$\begin{aligned}
-\frac{\vec{\psi}_{x-\delta t} - 2\vec{\psi}_x + \vec{\psi}_{x+\delta t}}{2\delta t^2} + \mathcal{O}\left[\delta t^2\right] &= E\vec{\psi}_x \\
-e^{ikx}\left(\frac{e^{-ik\delta t} + e^{ik\delta t} - 2}{2\delta t^2}\right) &\approx Ee^{ikx} \\
-\frac{2\cos(k)\delta t - 2}{2\delta t^2} &\approx E
\end{aligned}$$

We examine the behavior of energy as the time step becomes small.

$$\begin{aligned}
\lim_{\delta t \to 0} E &\approx \lim_{\delta t \to 0} -\frac{\cos k\delta t - 1}{\delta t^2} \\
&\approx \lim_{\delta t \to 0} \frac{k \sin k\delta t}{2\delta t} \\
&\approx \lim_{\delta t \to 0} \frac{k^2 \cos k\delta t}{2} \\
&\approx \lim_{\delta t \to 0} \frac{k^2 \left(1 - \frac{(k\delta t)^2}{2}\right) + \mathcal{O}\left[\delta t^4\right]}{2} \\
E &\approx \frac{k^2}{2} \qquad (2)
\end{aligned}$$

Note that the energy in discrete space varies with the time step and will never be exactly $\frac{k^2}{2}$ as stored in the computer. Additionally, the maximum energy of the wave is given by $\frac{2}{\delta x^2}$.

Error In our derivation of equation (1), we approximated the exponential operators by truncating the Taylor series expansions of them. Note that $e^{-i\hat{H}t} \approx \frac{1-iH\frac{\delta t}{2}}{1+iH\frac{\delta t}{2}}$. If we expand the left side of the approximate equation to its Maclaurin series and multiply both sides by $1 + iH\frac{\delta t}{2}$, then we arrive at

$$1 - i\hat{H}\frac{\delta t}{2} - i\hat{H}^3\frac{\delta t^3}{12} \approx 1 - iH\frac{\delta t}{2}$$

so the error for the propagation operator is on the order of $\hat{H}^3\delta t^3$. This error will propagate through time.

Unitary Operator Because of the numerical second derivative, we know that H is a tridiagonal real matrix, so it is Hermitian as an operator. In order to use the wave function to calculate expected values, the squared magnitude of the wave function must be a PDF over x. Therefore, the wave function's squared magnitude integrated over all x (or in discrete space, the norm) must equal to one for all time, so our operator in equation (1) should be unitary.

$$\begin{aligned}\left(\frac{1-iH\frac{\delta t}{2}}{1+iH\frac{\delta t}{2}}\right)^{\dagger}\left(\frac{1-iH\frac{\delta t}{2}}{1+iH\frac{\delta t}{2}}\right) &= \frac{\left(1+iH^{\dagger}\frac{\delta t}{2}\right)\left(1-iH\frac{\delta t}{2}\right)}{\left(1-iH^{\dagger}\frac{\delta t}{2}\right)\left(1+iH\frac{\delta t}{2}\right)} \\ &= \frac{\left(1+iH\frac{\delta t}{2}\right)\left(1-iH\frac{\delta t}{2}\right)}{\left(1-iH\frac{\delta t}{2}\right)\left(1+iH\frac{\delta t}{2}\right)} \\ &= 1\end{aligned}$$

Model Boundary Conditions and Parameters

We model a one-dimensional particle in a box, where the wave packet is in an infinite potential well bounded at $x = 0, R$, where R is large enough to emulate an infinite x space for the wave packet. By taking the limit of a wave functions value as the potential energy tends toward infinity, we see that the magnitude of the wave function is equal to 0 at at the x boundaries. To reiterate, the grid spacing for time and space is given by δt and δx respectively. Finally, we propagate for a definite time. Also note the the parameters for a Gaussian wave packet such as the wave number and standard deviation.

Computer Representation of the Hamiltonian and Wave Function

Wave Function as a Column Vector A wave packet is a superposition of plane waves that have a nonzero range in wave number and angular frequency which forms a Gaussian envelope. For a given time, it can be created by the form

$$\Psi(x) = G(x)e^{ikx}$$

where Ψ is a wave packet, G a gaussian function, and e^{ikx} a plane wave expression. For storing on a machine, I represented $\Psi(x)$ as

$$\vec{\Psi}(t) = \begin{bmatrix}\Psi(1\delta x, t) \\ \Psi(2\delta x, t) \\ \vdots \\ \Psi(N\delta x, t)\end{bmatrix} = \begin{bmatrix}\Psi_1(t) \\ \Psi_2(t) \\ \vdots \\ \Psi_N(t)\end{bmatrix}$$

where N is the number of grid spaces on x.

The Propagator Matrix Let us denote $V(j\delta x)$ as V_j. Equation (1) can be expanded to

$$\Psi_j(\delta t) + i\frac{\delta t}{2}\left(-\frac{\Psi_{j-1}(\delta t)-2\Psi_j(\delta t)+\Psi_{j+1}(\delta t)}{2\delta x^2} + V_j\Psi_j(\delta t)\right) = \Psi_j(0) - i\frac{\delta t}{2}\left(-\frac{\Psi_{j-1}(0)-2\Psi_j(0)+\Psi_{j+1}(0)}{2\delta x^2} + V_j\Psi_j(0)\right)$$

$$\begin{bmatrix} 1+i\frac{\delta t}{2}\left(V_1+\frac{1}{\delta t^2}\right) & -i\frac{\delta t}{(2\delta x)^2} & 0 & 0 & 0 & \cdots & 0 \\ -i\frac{\delta t}{(2\delta x)^2} & 1+i\frac{\delta t}{2}\left(V_2+\frac{1}{\delta t^2}\right) & -i\frac{\delta t}{(2\delta x)^2} & 0 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & 0 & \cdots & 0 \\ \vdots & & & & & & \vdots \\ 0 & \cdots & \cdots & 0 & -i\frac{\delta t}{(2\delta x)^2} & 1+i\frac{\delta t}{2}\left(V_2+\frac{1}{\delta t^2}\right) & -i\frac{\delta t}{(2\delta x)^2} \end{bmatrix} \begin{bmatrix} \Psi_1(\delta t) \\ \Psi_2(\delta t) \\ \vdots \\ \Psi_N(\delta t) \end{bmatrix} = \vec{\phi}_j(0) \tag{3}$$

where the matrix in equation (3) is the propagator matrix. It is straightforward to guess the algorithm that is used to repeatedly propagate the wave function column vector through time.

Finite Square Potential Well

A potential well is a region where the wave packet experiences a lower amount of potential energy. A well can be modeled by defining the potential energy function $V(x)$ to include a region with a lower value.

In computer implementation, the well must be continuous due to the Gibbs phenomenon. A smooth square well that does not allow for the occurance of Gibbs phenomenon can be achieved by using a higher power Gaussian function. In my modeling, I set the width of the well to be smaller than the width of the wave packet, which will be discussed in more detail within the Results section.

Transmission Coefficient

As the wave propagates through the finite potential well, some of it is reflected backward, and some of it is transmitted through to the other side of the well.

Suppose a potential well has a width of $2a$ and is centered at $x = 0$, where the potential $V(x)$ is equal to $-V_0$ for $-a \leq x \leq a$ and 0 for $x > a$ and $x < -a$. We label the region corresponding to $x < -a$ as region I, to $-a < x < a$ as region II, to $x > a$ as region III. During our meetings we solved for the one-dimentional time-independent Schrödinger equation for when $E > V(x)$ and $E < V(x)$, obtaining

$$\Psi_{\mathrm{I}}(x) = Ae^{ikx} + Be^{-ikx}$$
$$\Psi_{\mathrm{II}}(x) = C\sin(lx) + D\cos(lx)$$
$$\Psi_{\mathrm{III}}(x) = Fe^{ikx}$$

where $l = \sqrt{2(E+V_0)}$, $k = \sqrt{2E}$, and the subscript of the denotation of each function indicates over which region the function is defined. The requirements to stitch the three functions into one function which is defined for all x follows the properties of a valid solution to the Schrödinger equation:

We compute the transmission coefficient (T) by definition ($T^{-1} = \frac{|A|^2}{|F|^2}$), substituting F with equivalent expression in terms of the energy of the wave (E) and the depth of the potential well. We choose units such that $\hbar = 1$ and asuume $m = 1$.

The requirements to stitch the three wave functions into one follows the properties of a valid solution to the Schrödinger equation:

$$Ae^{-ika} + Be^{ika} = -C\sin(la) + D\cos(la) \tag{4}$$
$$C\sin(la) + D\cos(la) = Fe^{ika} \tag{5}$$
$$ik(Ae^{-ika} - Be^{ika}) = l(C\cos(la) + D\sin(la)) \tag{6}$$
$$l(C\cos(la) - D\sin(la)) = ikFe^{ika} \tag{7}$$

Now we solve for F in terms of l, k, a, and A. From equation (5), we solve

$$C = \frac{Fe^{ika} - D\cos(la)}{\sin(la)} \tag{8}$$

and substitute into equation (7) to solve for

$$Fe^{ika}\left(\frac{ik}{l}\sin(la) - \cos(la)\right) = -D(\cos^2(la) + \sin^2(la))$$
$$D = Fe^{ika}\left(\cos(la) - \frac{ik}{l}\sin(la)\right)$$

Then we substitute D in terms of F into equation (8) and simplify. Note $1-\cos^2(la) = 1-\frac{1}{2}(1+\cos(2la)) = 1-\frac{1}{2}(1+1-2\sin^2(la)) = \sin^2(la)$.

$$C = \frac{Fe^{ika}(1-\cos^2(la)+\frac{ik}{l}\cos(la)\sin(la))}{\sin(la)} = Fe^{ika}\left(\frac{1-\cos^2(la)}{\sin(la)} + \frac{ik}{l}\cos(la)\right)$$

$$C = Fe^{ika}\left(\sin(la) + \frac{ik}{l}\cos(la)\right)$$

Note $\cos^2(la) - \sin^2(la) = \cos(2la)$ and $2\cos(la)\sin(la) = \sin(2la)$. Substituting D and C in terms of F into equation (4), we get

$$\begin{aligned} Ae^{-ika} &= Fe^{ika}\left(-\sin^2(la) - \tfrac{ik}{l}\cos(la)\sin(la) + \cos^2(la) - \tfrac{ik}{l}\sin(la)\cos(la)\right) - Be^{ika} \\ &= Fe^{ika}\left(\cos(2la) - \frac{ik}{l}\sin(2la)\right) - Be^{ika}. \end{aligned} \tag{9}$$

Now we substitute this result and D and C in terms of F into equation (6) and solve for B.

$$\begin{aligned} Fe^{ika}\left(-\tfrac{ik}{l}\sin(2la) + \cos(2la)\right) - 2Be^{ika} &= \tfrac{l}{ik}Fe^{ika}\left(2\cos(la)\sin(la) + \tfrac{ik}{l}\cos^2(la) - \tfrac{ik}{l}\sin^2(la)\right) \\ -2B &= F\sin(2la)\left(\frac{l}{ik} + \frac{ik}{l}\right) \\ B &= i\frac{\sin(2la)}{2kl}(l^2-k^2)F \end{aligned}$$

To solve for F in terms of A we substitute B, C, and D into equation (9).

$$\begin{aligned} Ae^{-ika} &= Fe^{ika}\left(\cos(2la) - \frac{ik}{l}\sin(2la) - i\frac{\sin(2la)}{2kl}(l^2-k^2)\right) \\ Ae^{-2ika} &= Fe^{ika}\left(\cos(2la) - \left(\frac{ik}{l} + \frac{i(l^2-k^2)}{2lk}\right)\sin(2la)\right) \\ F &= \frac{e^{-2ika}A}{\cos(2la) - i\left(\frac{k^2+l^2}{2kl}\right)\sin(2la)} \end{aligned}$$

Finally, we compute T^{-1} and rewrite it in terms of E and V_0.

$$T^{-1} = \frac{|A|^2}{|F|^2} = \frac{|A|^2}{\frac{\left|e^{-2ika}\right|^2|A|^2}{\left|\cos^2(2la)+i\left(\frac{k^2+l^2}{2kl}\right)\sin(2la)\right|^2}} = \cos^2(2la) + \left(\frac{(k^2+l^2)^2}{4k^2l^2}\right)\sin^2(2la)$$

$$= 1 - \sin^2(2la) + \left(\frac{(k^2+l^2)^2}{4k^2l^2}\right)\sin^2(2la) = 1 + \left(\frac{k^4 - 2k^2l^2 + l^4}{4k^2l^2}\right)\sin^2(2la)$$

$$= 1 + \left(\frac{4E^2 - 8E(E+V_0) + 4(E^2 + 2EV_0 + V_0^2)}{16E(E+V_0)}\right)\sin^2(2a\sqrt{2(E+V_0)}$$

$$\boxed{T = \frac{1}{1 + \left(\frac{V_0}{4E(E+V_0)}\right)\sin^2(2a\sqrt{2(E+V_0)}}}$$

Note that T oscillates with changes in the width of the well and the energy of the wave.

Expected Values over Time

In the Verifying Implementation subsection, I will be numerically calculating the expected values of certain physical observables of the wave packet through time to gain confidence in correctness of my programs. In this section, we will study the theoretic evolution of those values, and the potential energy functions of interest are determined by systems which were modeled computationally.

Both systems are closed, so energy is conserved and the value of the Hamiltonian does not change.

Constant Potential Energy

From (2), we can deduce that $p \approx k$. As the wave packet approaches a wall, the expected momentum will decrease as some of the wave packet will have been reflected backward, while the rest of the wave packet is still moving forward. The expected momentum will continue to decrease until the wave packet has been fully reflected, at which point $p \approx -k$.

Recall that a wavepacket is a superposition of eigenstates, and that it has multiple, distinct k values. One may calculate the distribution of the k

values from a Fourier transform, and would notice that it corresponds to the Gaussian envelope of the wave packet. The components of the wave packet with larger corresponding wave numbers will have larger momentum than those with smaller corresponding wave numbers, so at every reflection, change in momentum after the inflection point is less drastic.

The expected momentum is proportional to the change in the expected position (in our case, it exactly describes the motion of the wave packet because we assume that mass is one), so the expected x would increase to a certain point linearly, then decrease linearly to a certain point, and so on. Because of the range of wave numbers discussed above, the change in x of the wave packet becomes larger, and the maxiumum expected x for each period is less than that for the previous period.

Finite Square Potential Well

Just as in a system with a constant potential function, the momuntum of the wave packet is initially approximately k in a system with a finite potential well. However, once the wave packet passes the region with lower potential, part of it is transmitted as a wave packet whose momentum has the same sign as the momentum of the original wave packet, and the rest reflected as another wave packet whose momentum has the opposite sign as the momentum of the original wave packet. Otherwise, it is negative. The larger the probability of the particle that is localized by the wave packet being past the potential well after transmission, the larger the expected momentum will be. If more of the wave packet is transmitted, the momentum between the time of finishing transmission and reflection off the boundaries of the infinite square well is positive.

Of course, the behavior of the momentum at reflection off the boundaries of the box is consistent with that within a box with constant potential, and the consequences of the wave packet having a range of wave numbers holds in this system. Again, the change of the expected position is proportional to the momentum.

Effects of Changing Well Width and Energy We know that the behavior of expected momentum and position in a finite square well are contingent on the transmission of the initial wave packet(s) and that the transmission changes with the width of the well and the energy of the wave packet. Thus

the behavior of the those expected values change with the width of the well and the energy of the wave packet. Changing the value of either with the other held constant oscillates the value of the transmission coefficient, and the changes with respect to the width of the well and the energy of the wave packet in the evolution of expected momentum and expected position follow from the descriptions detailed above.

Results

All the necessary concepts in the theory for the model have been covered, so we are free to fully discuss the computational portion.

Verifying Implementation

Before we invesigate the results of the computational modeling, we gain confidence in the correctness of the programs by checking values over time. We also use autocorrelation to further support the correctness of the propagation.

Examining Expected Values

First, we check if my implemetned operator is unitary. For all graphs, the x axis is displaying time unless specified otherwise. The final time is not changed.

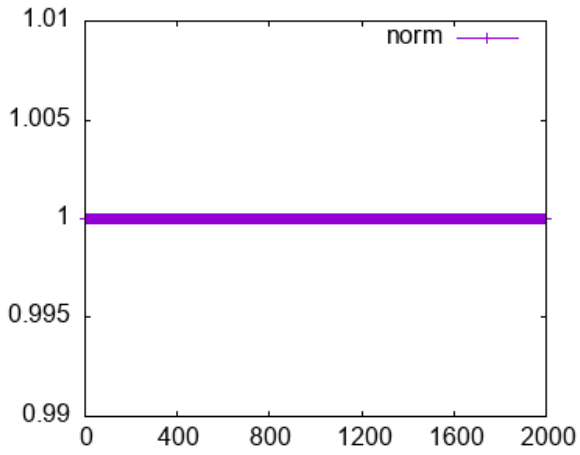

Figure 1: The `norm` axis indicates the sum of all the elements of $\vec{\Psi}(t)$.

The norm is one through all our time steps, so the implemented operator is unitary, as we calculated. Now we examine the expected total energy, momentum, and position for different k values for a system with a constant potential function and a potential well.

Constant Potential

We check to see if $\langle H \rangle \approx \frac{k^2}{2}$ and $\left|\frac{d}{dt}\langle x \rangle\right| = |\langle p \rangle| \approx k$, and that they behave roughly as explained in the Expected Values over Time section.

For $k = 0.59$, I computed with the programs the following values.

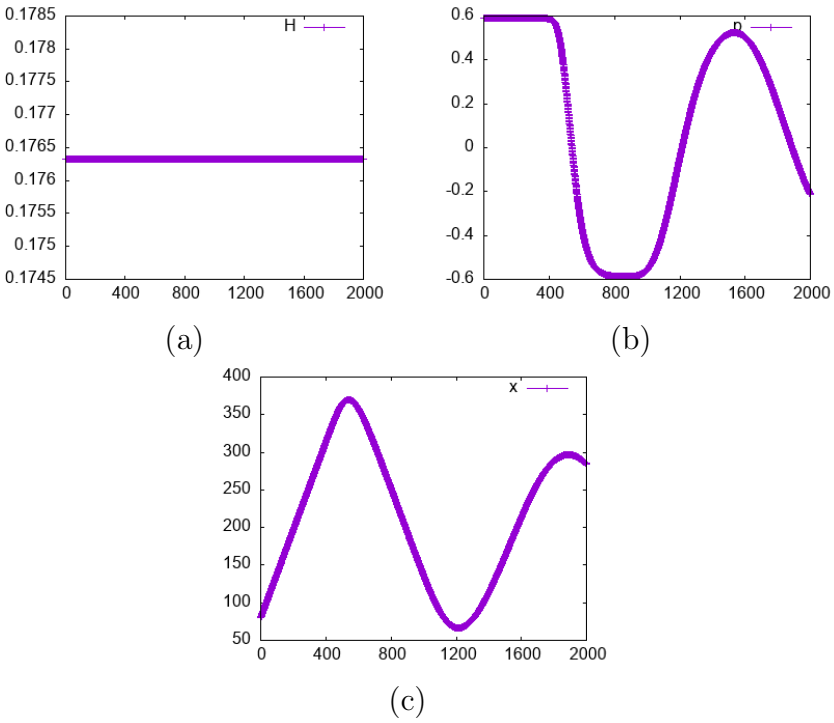

Figure 2: The three plots display the expected values over time for $k = 0.59$. The y-axis in plot (a) indicates the total energy of the system. The y-axis in plots (b) and (c) indicate the expected momentum and expected position of the wave packet, respectively.

The value $\frac{d}{dt}\langle x \rangle$ is equal to the slope in plot (c) in Figure 2, which can be computed using the coorindates $(x, t) = (0, 80), (81, 127.34)$ from the datafile: $\frac{d}{dt}\langle x \rangle \approx 0.58 \approx k$. The computational expectation values for the total energy of the system and momentum of the wave packet are consistent with the theory.

Now for $k = 1$, the programs output the following data.

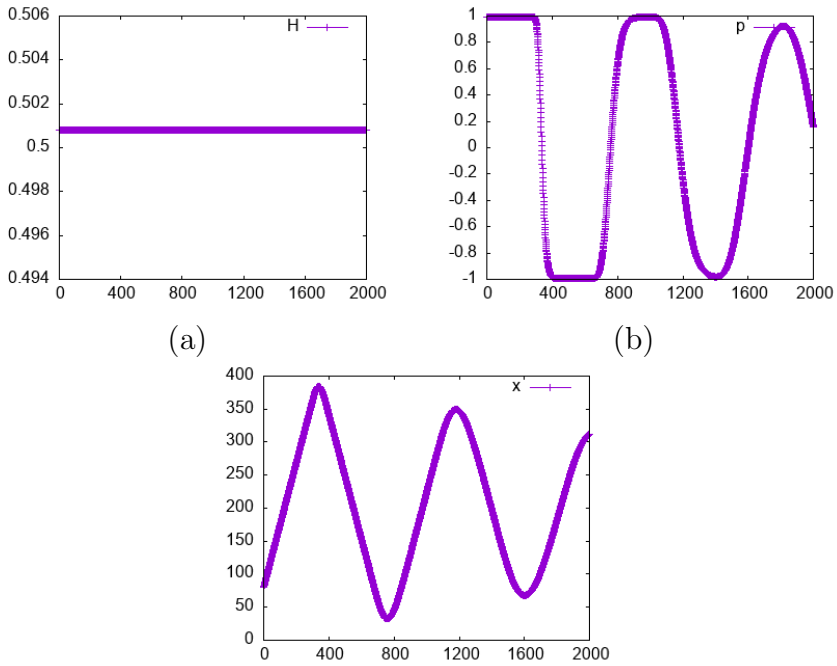

Figure 3: The three plots display the expected values over time for $k = 1$. The y-axis in plot (a) indicates the total energy of the system. The y-axis in plots (b) and (c) indicate the expected momentum and expected position of the wave packet, respectively.

The value $\frac{d}{dt}\langle x\rangle$ is equal to the slope in plot (c) in Figure 3, which can be computed using the coorindates $(x, t) = (0, 80), (81, 156.43)$ from the datafile: $\frac{d}{dt}\langle x\rangle \approx 0.94 \approx k$. The wave packet moves over more distance in the same amount of time for a larger k. The computational expectation values are consistent with the theory.

Finite Potential Square Well

I used the following potential well.

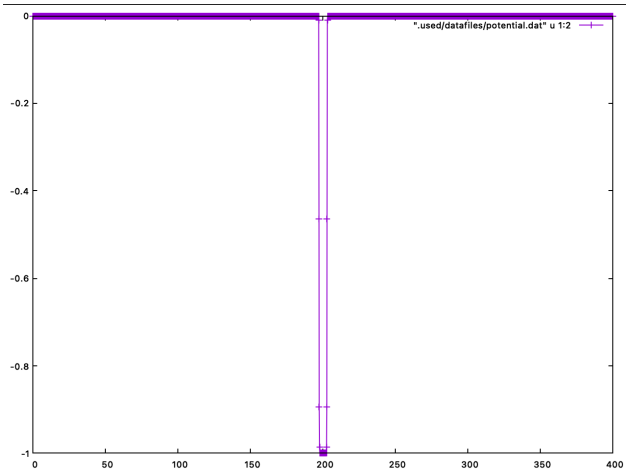

Figure 4: The y-axis represents the potential energy, and the x-axis represents the position within the box.

We check to see if $\langle H \rangle \approx \frac{k^2}{2}$ and if initially $\left|\frac{d}{dt}\langle x \rangle\right| = |\langle p \rangle| \approx k$, and that they behave roughly as explained in the Expected Values over Time section. The width of the well used was $0.01R$, and the full width at half maximum (FWHM) of the Gaussian scalar function of the initial wave packet used is $20\sqrt{2\log(2)}$ in x space.

Figure 5 on the next page shows the numerical computations of the expected value of each of the physical quantities for $k = 0.59, 1$, as calculated by the programs.

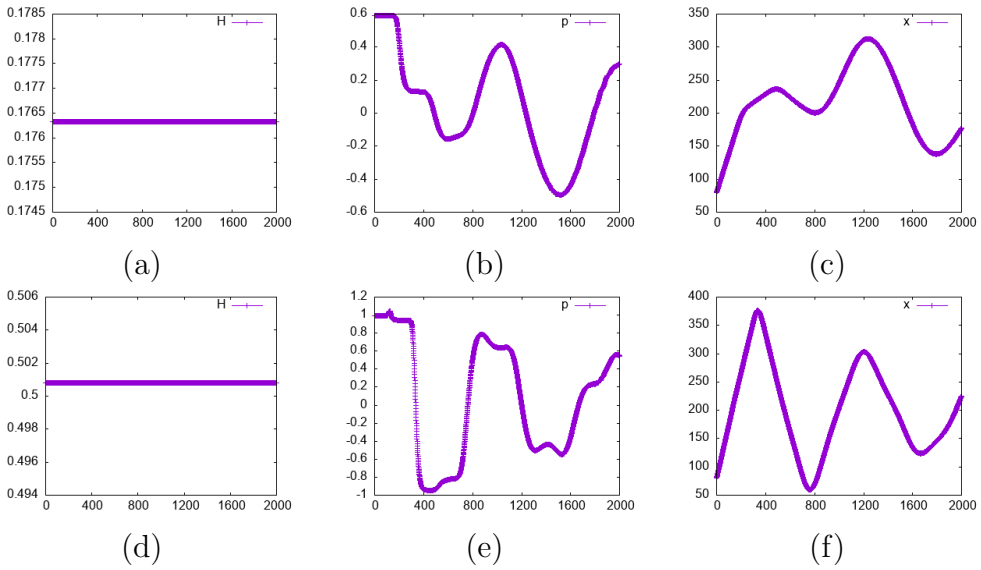

Figure 5: The top three plots display the expected values over time for $k = 0.59$, and the bottom three for $k = 1$. The y-axis in plots (a) and (d) indicates the total energy of the system. The y-axis in plots (b) and (e) indicates the expected momentum, and the y-axis in plots (c) and (f) indicates the expected position of the wave packet.

Although we will not compute the initial slope of plots (c) and (f), we may notice that the predicted change in the expected position is represented in the graphs, so the computational expected values are consistent with the theory. The discrepancies between the graphs for $k = 0.59$ and $k = 1$ will be discussed in further detail in the Numerical Calculations of the Transmission Coefficient subsection.

Autocorrelation for $|\Psi|^2$ through Negative Time

We assess correctness with autocorrelation by checking if it is approximately equal to one. The following is the schema for measuring autocorrelation, where $n \in \mathbb{Z}$.

$$\Psi(n\delta t) = \left(\frac{1 - iH\frac{\delta t}{2}}{1 + iH\frac{\delta t}{2}}\right)^n \Psi(0)$$
$$\tilde{\Psi}_n(0) = \left(\frac{1 - iH\frac{-\delta t}{2}}{1 + iH\frac{-\delta t}{2}}\right)^n \Psi(n\delta t)$$
$$\text{autocorrelation} = \int_0^R \Psi(0)^* \tilde{\Psi}(0) dx$$

To implement this measure using the implicit scheme of propagation, I propagated forward in time by n time-steps, and backward in time by the same number of time steps. The integral was calculated by summing the product of each element of $\vec{\Psi}(0)$ and the complex conjugate of its corresponding element of $\vec{\tilde{\Psi}}(0)$.

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autocorr norm: 1.000000
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Figure 6: The output for the autocorrelation for $\delta t = 0.9$ and the $n = 2222$.

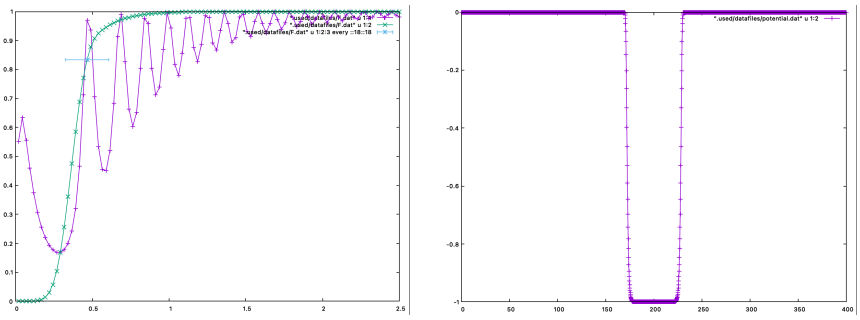
The autocorrelation is exactly equal to one because the error in forward propagation is equal to the negative of the backward negative operator because a factor of the propagator error, δt^3, is odd with respect to δt.

Numerical Calculations of the Transmission Coefficient

I numerically calculated the transmission coefficient by

$$\sum_{j=A}^{N} \vec{\Psi}_j(t_f)$$

where A is the number of spacial steps that corresponds to the approximate edge of the well that is on the side opposite of the starting position of the wave packet, N is again the total number of spacial steps. This summation is computed at t_f, corresponding to a time after the full transmission through the well has occured.



(a) (b)

Figure 7: The x-axis represents k. The transmission coefficient as calculated analytically is plotted in purple and as computed numerically is plotted in turquoise. The length of each side of the error bar is the half width of the wave packet in k space, calculated by $\frac{2}{\sqrt{2\sigma^2}}$ where σ is the standard deviation parameter for the Gaussian envelope.

We see that the numerical computation does not match the analytical solution. If we recall that the analytical solution is for an eigenstate, and that a wave packet is superposition of many eigenstates, it is then reasonable to guess that the plot of the numerical solution appears as sort of an S-curve because the transmission of all plane waves composing the wave packet, each of which corresponds to its own k value, are summed, and that the center of the k distribution is larger than one oscillation in the analytical solution. We must reduce the width of the wave packet in k-space in order for the numerical plot to resemble the analytical plot. This corresponds to a decrease in the width of the wave packet in x-space, which at this point we may reduce the width of the well to maintain an approximately infinitely large box*. The graph (a) in Figure 7 uses a well width of $0.1R$, seen in graph (b). The following figure uses a well width of $0.01R$, seen in Figure 4.

*The relation between the well width in x-space and k-space is calculated by Fourier transform and FWHM of the wave packet.

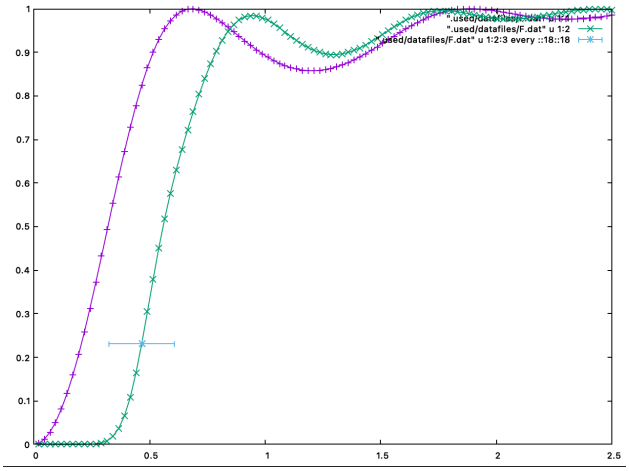


Figure 8: The plots are the same as in Figure 7.

We see now that the error bar is smaller than one oscillation in the analytical plot, and that both functions match with an offset of some phase constant.

Revisiting the graphs for the expected values over time for a system with a finite potential well (Figure 5), we noted the differences in the expected values over $k = 0.59$ and $k = 1$. If we compare those to the graphs in Figures 2 and 3, we see that the expected values behave more similarly between a constant potential and a potential well for $k = 1$ than $k = 0.59$. This is because there is a larger transmission at $k = 0.59$, which is supported by the analytical plot.

Extended Verification

We extend our verification process by examining the wave packet and transmission over time over k. We notice a reflection and transmission in Figure 9, and an oscillation in transmission (equal to the plateau since the initial wave packet is normalized) through k in Figure 10.

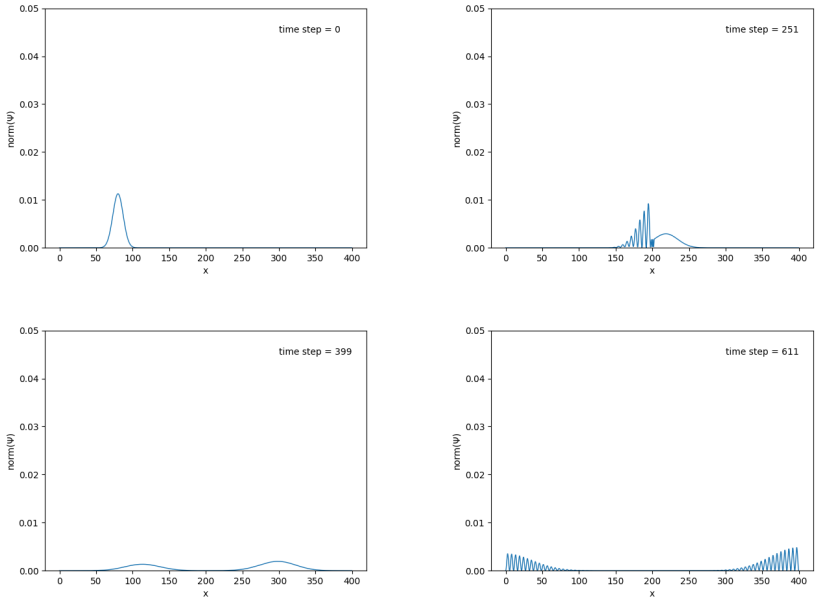


Figure 9: The squared magnitude of the wave packet at four different time steps

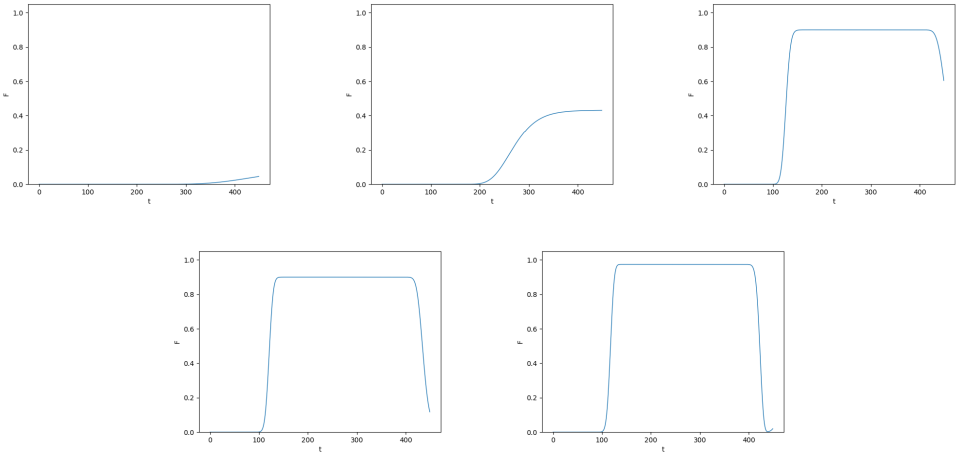


Figure 10: The probability of the localized particle being transmitted (F) over time for increasing k