

Time Evolution in Diffusion and Quantum Mechanics

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April 29, 2005

Abstract

The Diffusion and Time dependent Schrödinger equations were solved using both a Fourier based method and the method detailed in John Richardson's paper^[3]. The time evolution of the wave-packets interacting with a variety of different potentials were displayed graphically and the two methods were compared qualitatively.

1 Introduction

It is common knowledge^[1] that particles actually have a *dual wave/particle nature*. This is true to the point where we can treat all particles as waves if we should choose to; an example of this is the use of De Broglie's wavelength of an electron (which is commonly perceived as being a classical 'particle') as part of an explanation for electron diffraction.

The description of a 'particle' is given in the *Time dependent Schrödinger equation*:

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t)$$

where ' \hat{H} ' is the *Hamiltonian* and is defined as:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$$

where ' m ' is the mass of the particle and ' V ' is the potential.

This is analogous to the *Diffusion equation* which describes the flow of heat through a material:

$$\frac{\partial\Psi(x,t)}{\partial t} = \frac{1}{D}\frac{\partial^2\Psi(x,t)}{\partial x^2}$$

where ' D ' is the 'diffusivity' of the material.

Given the initial conditions of the wave (either the heat wave or the probability wave of the particle), we wish to be able to design a computer program that will determine the time evolution of a *Gaussian wave-packet*. We have chosen to use a Gaussian wave-packet, as this is a good model of a quantum mechanical particle that can be reduced to a solution to the Diffusion equation. A Gaussian wave-packet is illustrated in figure 1.

A Gaussian Wave Packet

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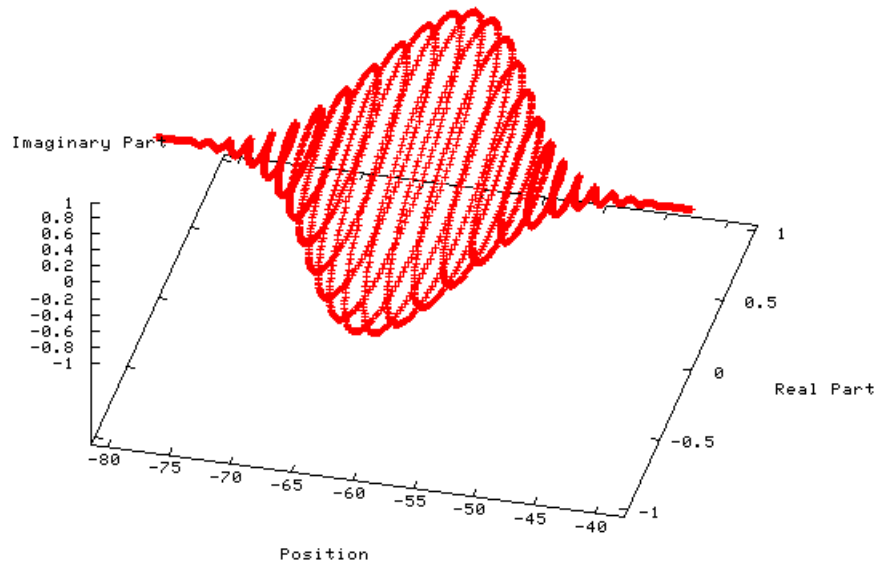


Figure 1: A wave-packet in a 3-dimensional complex space.

2 Method

2.1 Fourier Method^[2]

As previously mentioned, we chose a Gaussian wave packet as the solution to both the Time dependent Schrödinger equation and the Diffusion equation. In the case of the particle:

$$\psi(x, 0) = Ae^{\frac{(x-x_0)^2}{2\sigma^2}} e^{ik_0(x-x_0)}$$

where ‘ A ’ is a constant, ‘ x_0 ’ is the starting position of the peak of the Gaussian and ‘ k_0 ’ is the *principle wave-number*.

We recognised that we needed to ‘add’ the time dependence to our Gaussian wave packet. To do this we performed a Fourier Transform on the wave packet distribution and then multiplied by the time dependent term.

The time independent Fourier Transform is:

$$g(k, 0) = \int \psi(x, 0)e^{-ikx} dk$$

The time dependent Fourier Transform can then be obtained by multiplying on the time dependence:

$$g(k, t) = g(k, 0)e^{-k^2t}$$

Then, once we had a time dependent solution in Fourier space, we simply had to transform back to arrive at our final time dependent solution.

This time dependent solution could then be plotted to display how the wave propagated and how the probability density spread over time and space.

However, whilst this sounds straightforward enough, the fact that a computer is limited to discrete mathematics means that we are forced to use a lattice approximation for our wave function.

To achieve a very good approximation we need to meet a number of prerequisites. Firstly, to use a region of space which was very large compared to the width of the wave packet. Secondly, the width of the Gaussian wave packet must be large enough to enclose a sufficiently large number of wavelets. Finally, we had to use enough points within the region of space as to provide a high enough ‘resolution’ of the wave packet.

2.1.1 Transmission and Reflection^[4]

When a particle approaches a potential obstacle of some description it can be reflected or transmitted. In terms of probability waves, this is analogous to

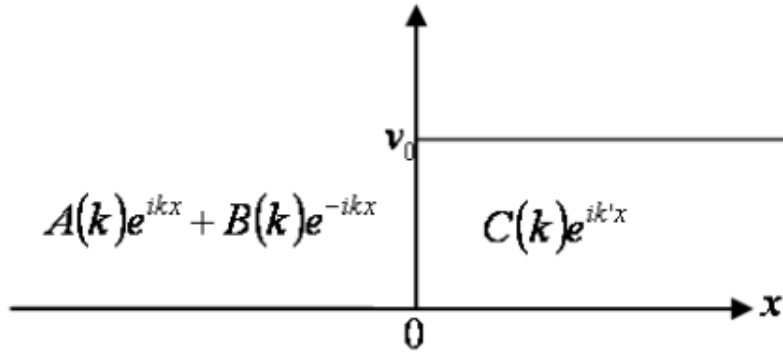


Figure 2: A positive potential step.

saying that the initial wave is split in two, a reflected wave moving from the obstacle and a transmitted wave moving through the obstacle. Depending upon the specifics of the initial wave and the obstacle these two resulting waves are produced in different proportions.

The amplitudes of the initial and reflected waves depend upon the particular situation. We define the reflection probability as being the ratio of the reflected wave's amplitude to the initial wave's amplitude, $R = |B/A|$. In a similar fashion, the transmission probability is $T = |C/A|$. In actual fact we are not interested in these probabilities, but we can use these fractions to find 'B' and 'C' as a function of the wave numbers 'k' and 'k'' and the amplitude of the initial wave, 'A'.

$$\begin{aligned}
 k &= \sqrt{\frac{2mE}{\hbar^2}} \\
 k' &= \sqrt{\frac{2m(E - V_0)}{\hbar^2}}
 \end{aligned}
 \tag{1}$$

This is done by equating the expressions for the wave functions and their spatial derivatives at the boundaries of the potential obstacle. The reason for only equating these two and not any further derivatives is due to the fact that all of our potential obstacles have perfectly 'vertical' boundaries.

These vertical boundaries create a discontinuity (at each spatial position of the boundary) in the first derivative and so as a result the second derivative does not exist. Therefore, it is by virtue of the fact that the higher derivatives do not exist that we are not required to consider them.

2.2 Richardson’s Method^[3]

Everything that has been described thus far is what we have come to know as the ‘Fourier method’ (named for its obvious use of Fourier Transformations). The Fourier method is a perfectly valid method; however it is best used for simple potentials (i.e. those with definite ‘edges’). The Fourier method also has the risk of *failing to conserve unitarity*¹, making the result nonsensical.

To deal with general potentials, the Fourier method would be both computationally inefficient and an analytical nightmare. Instead Richardson’s method is a much more versatile approach.

Richardson’s method unlike the Fourier method makes use of the time stepping operator of Schrödinger’s equation, ‘ $e^{-\frac{it}{\hbar}\hat{H}}$ ’, where ‘ \hat{H} ’ is the Hamiltonian operator. ie.

$$\Psi(x, t) = e^{-\frac{it}{\hbar}\hat{H}}\Psi(x, 0) \quad (2)$$

The Hamiltonian is defined as, $\hat{H} = \hat{T} + V(x)$, and so we rewrite equation (2) in terms of the kinetic energy operator, ‘ \hat{T} ’, and the potential, ‘ V ’. We then split the kinetic energy operator² to produce a computable approximation for the time stepping operator.

For small enough decrements in time one can iterate over time using this operator on the wave-function to obtain the wave-function at a later time given the initial wave-function, ‘ $\psi(x, 0)$ ’, and an arbitrary potential, ‘ $V(x)$ ’.

3 Computational Implementation

3.1 Analysis of a Free Wave

If we were to consider a region where there is no potential, then the solution to this situation could represent either a particle travelling through free space (i.e. a solution to the Time dependent Schrödinger equation) or, if the principle wavenumber is zero, $k_0 = 0$, the flow of heat through a material (i.e. a solution to the diffusion equation). If this principle wavenumber is zero then the heat wave will not propagate like the particle does through space.

As in all of the situations, the initial wave is a Gaussian wave packet. As we time evolve this in our program we see that (see figure 3), for the more interesting particle, the wave packet traverses the one-dimensional space

¹Meaning the wave-function does not remain normalised.

²The maths for this is described in Richardson’s paper^[3] on visualising quantum scattering.

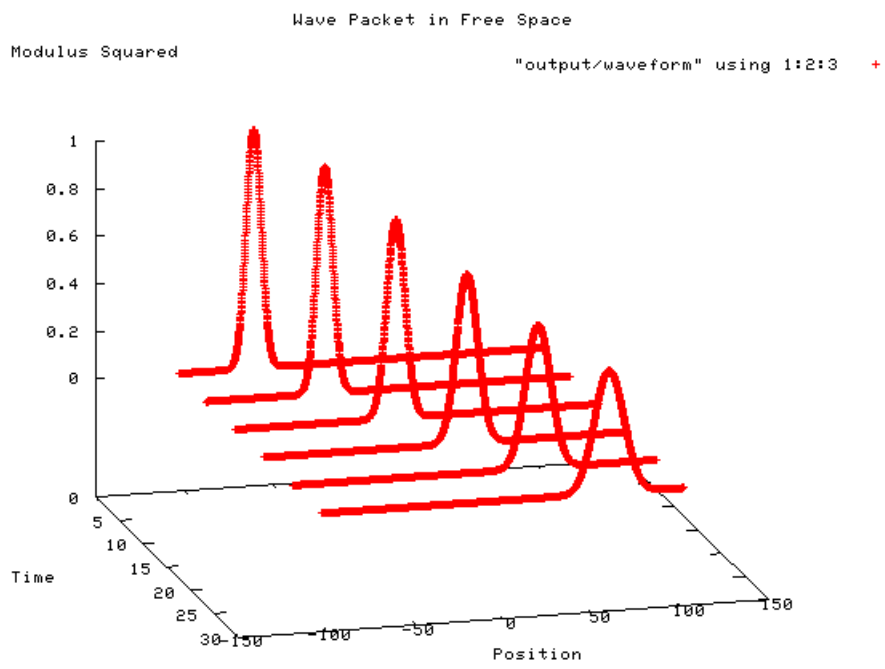


Figure 3: A space-time graph of a wave-packet propagating free of any potential.

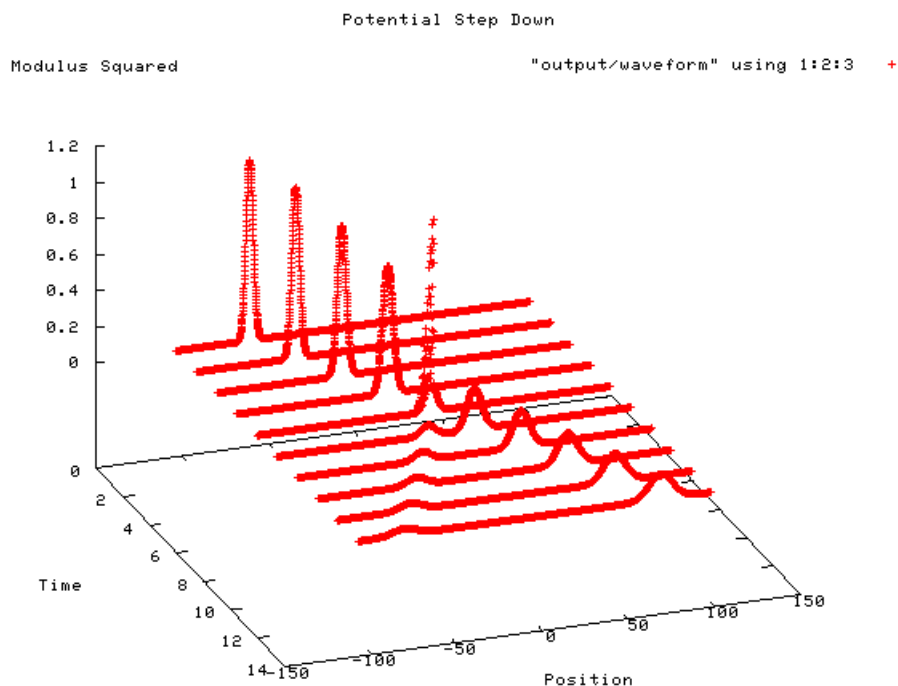


Figure 4: A space-time graph of a wave-packet hitting a negative potential step.

and that its width increases as it does so. This ‘spreading out’ must be counteracted by a reduction in height to conserve unitarity.

3.2 Analysis of Potential Steps

We distinguish between two types of potential steps, a step down and a step up. In actual fact these two potential obstacles are treated in exactly the same way mathematically to provide very similar coefficients for the reflected and transmitted waves.

First we split the one-dimensional space into two distinct regions (as shown in figure 2); the region that includes the potential obstacle and the region that does not. By convention, the initial wave starts on the ‘left hand’ side of the one-dimensional space and travels to the right heading towards the potential obstacle.

In the region of space to the left of the obstacle, the resulting wave is a superposition of the initial wave and the wave that is reflected from the barrier. By contrast, the resulting wave in the region of space to the right

of the obstacle is purely the transmitted wave. Figure 4 shows the simplest case of a finite step.

As previously mentioned, the wave function and its first spatial derivative must be continuous across the boundary of the potential obstacle.

Equating the wave-functions we find:

$$A(k)e^{ik'x} + B(k)e^{-ik'x} = C(k)e^{ikx}$$

Equating the derivatives we find:

$$k'A(k)e^{ik'x} - k'B(k)e^{-ik'x} = kC(k)e^{ikx}$$

(Obviously these equations are only valid for a boundary at $x = 0$.)

Solving these simultaneous equations gives the coefficients of the reflected and transmitted wavelets in terms of the wave-numbers and the amplitudes of the initial wavelets.

$$B(k) = \frac{k - k'}{k + k'}A(k)$$

$$C(k) = \frac{2k}{k + k'}A(k)$$

The potential step down is a simpler situation than the potential step up because of one fact; in the step up the wavelets can have either more or less energy than the obstacle, depending upon their particular wave-number. This means that in the region containing the potential step, the wavelets can have an imaginary wave-number.

This imaginary wavenumber has one major consequence; within the potential barrier, the wavelets, with less energy than the potential of the barrier, are transmitted form a wave that decays exponentially. These wavelets are superposed with those that had a greater energy than the barrier to form the transmitted wave.

As you can see in figure 5, the transmitted wave appears more like a Gaussian wave packet. This is due to the exponentially decaying terms being greatly outnumbered by the Gaussian wavelets that are transmitted.

3.3 Analysis of a Potential Barrier

The analysis of the potential barrier is much like the above analysis for the potential step. The considerations of the continuity of the wave function and its spatial derivative at the boundaries of the barrier are exactly the same. However unlike the potential step, the barrier has two sides that must both

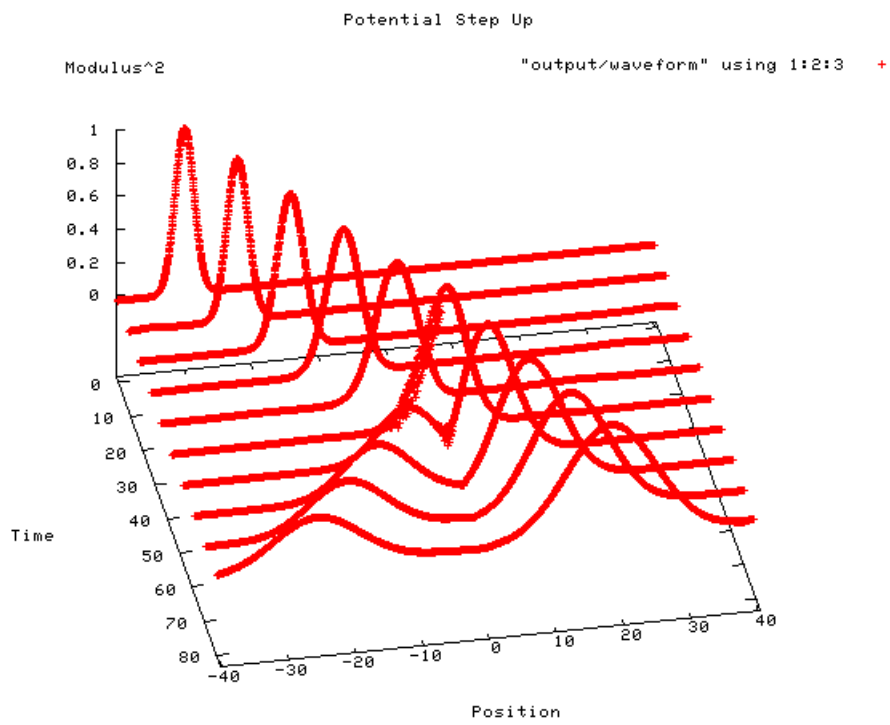


Figure 5: A space-time graph of a wave-packet hitting a positive potential step.

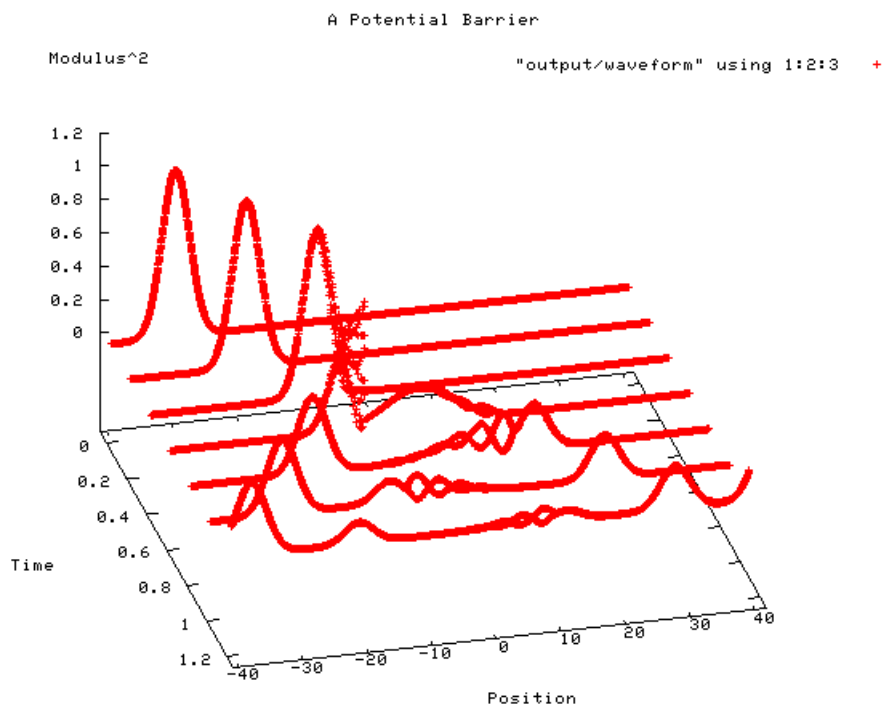


Figure 6: A space-time graph of a wave-packet hitting a potential barrier of width 20 centred at $x = 0$.

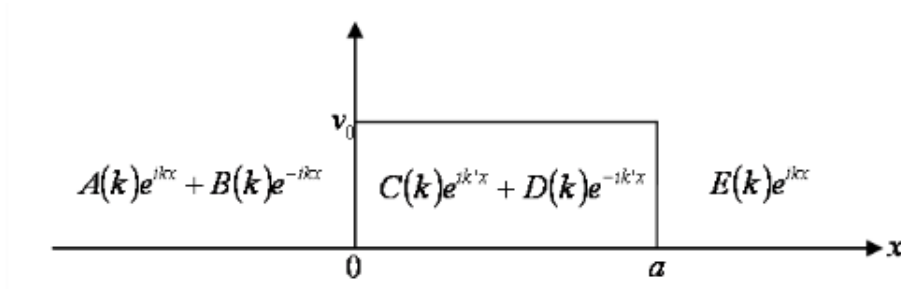


Figure 7: A potential barrier.

be considered to find the correct wave-functions. The situation is illustrated in figure 7.

After much similar mathematics to before, we find that:

$$\begin{aligned}
 B(k) &= \frac{(k^2 - k'^2)(1 - e^{2ik'a})}{(k + k')^2 - (k - k')^2 e^{2ik'a}} A(k) \\
 C(k) &= \frac{(k + k')e^{i(k-k')a}}{2k'} E(k) \\
 D(k) &= \frac{(k' - k)e^{i(k+k')a}}{2k'} E(k) \\
 E(k) &= \frac{4kk'e^{i(k'-k)a}}{(k + k')^2 - (k - k')^2 e^{2ik'a}} A(k)
 \end{aligned}$$

From equation (1) we see that, in a similar fashion to the potential step up, the potential barrier situation splits into two different problems, one where the energy of a wavelet is greater than the 'height' of the barrier and one where it is lesser. When the energy of a given wavelet, $\frac{k^2 \hbar^2}{2m}$, is lower than the potential of the barrier, we find that the wavenumber in the barrier is imaginary and so as a result, the wave function decays exponentially through the potential barrier.

However when the wave function exits the barrier, the imaginary wavenumbers become real again. The result of this is that inside the barrier, the wave function decays exponentially and then, upon exiting the barrier, again forms a Gaussian wave packet.

These characteristics are clearly seen in figure 6.

Notice that, at $t = 0.6$, just to the left the boundary of the potential at $x = -10$, $|\Psi|^2$ appears to fluctuate randomly. This characteristic is due to the superposition of the initial and reflected waves.

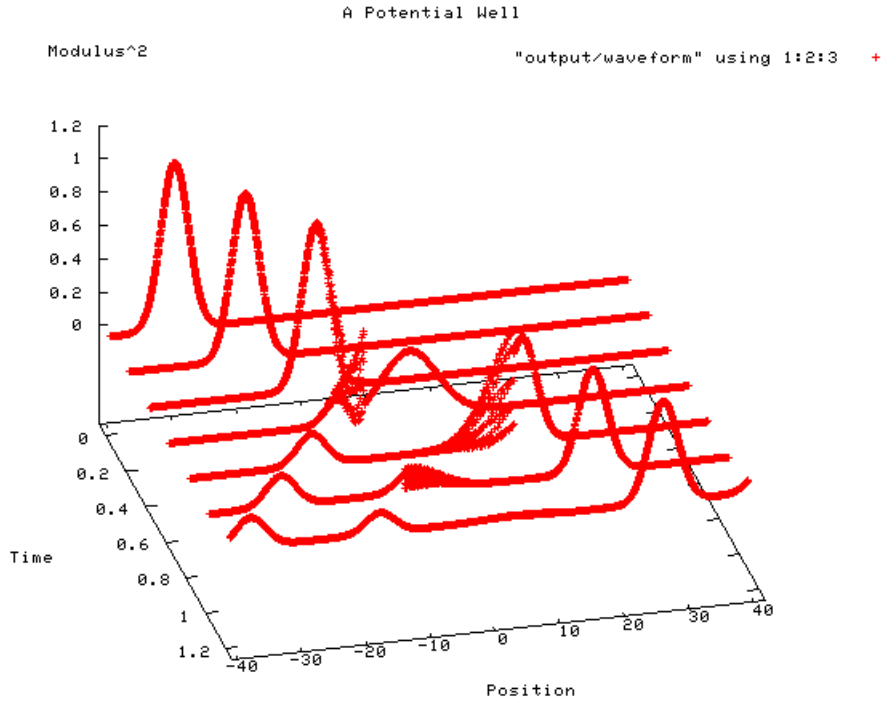


Figure 8: A space-time graph of a wave-packet hitting a potential well of width 20 centred at $x = 0$.

In a similar fashion, the activity within the barrier is due to the superposition of the wave that was transmitted through the left hand side of the step and the wave that was reflected from the right hand side of the barrier.

Also note that to the right of the barrier, the transmitted wave is again a Gaussian with decreasing amplitude and increasing width.

One can also see the second reflected wave packet, this is due to reflections off the right hand side of the barrier.

3.4 Analysis of a Potential Well

A potential well is a negative potential barrier and its effects on a wave-packet can be seen in figure 8. As for the potential barrier, notice that for the potential well, at $t = 0.6$, just to the left of the well, the superposition of the reflected and initial waves causes what appears to be a random interference. Also in this same time frame we can observe that the wavelets that enter the well form a propagating Gaussian wave packet again.

At the right hand side of the well, some of the wavelets are reflected back

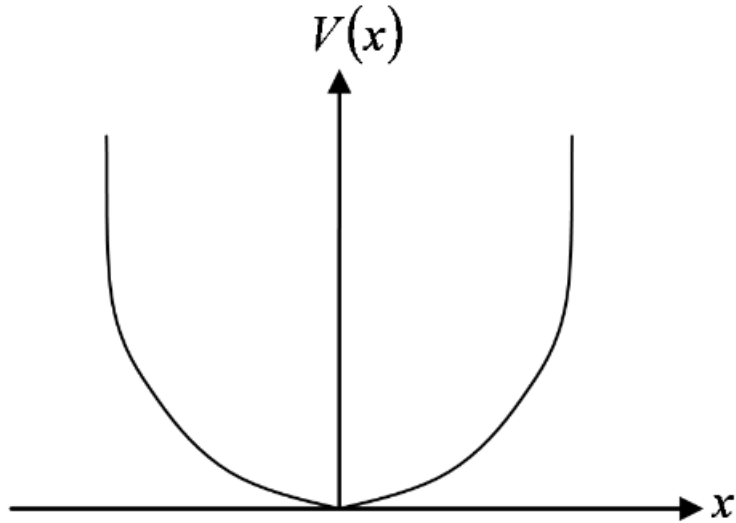


Figure 9: A parabolic SHM-like potential.

‘into’ the well and so in the $t = 0.8$ time frame we can see the superposition of the remainder of the initial wave (that is still in the well) and the reflected wave (that has been reflected from the exiting of the potential).

Once again we observe that after the potential has been traversed by the wave packet, the transmitted wave packet is a Gaussian with similar properties to the free particle previously observed.

3.5 Analysis of an SHM Potential

A wave-packet initially at the bottom of a *simple harmonic oscillator*-like potential with some kinetic energy is illustrated in figure 10. The actual Shape of this potential is a quadratic parabola that spans the entire width of the one-dimensional space (see figure 9). The parabolic walls of this potential well gradually reflect more and more of the wave packet as it propagates until the entire wave packet has been reflected. The wave packet is then completely contained within this well and continues to be reflected back and forth. The wave-packet undergoes Simple Harmonic Motion about the centre of the well ($x = 0$). The wave-packet will however continue to spread just like the free Gaussian did previously.

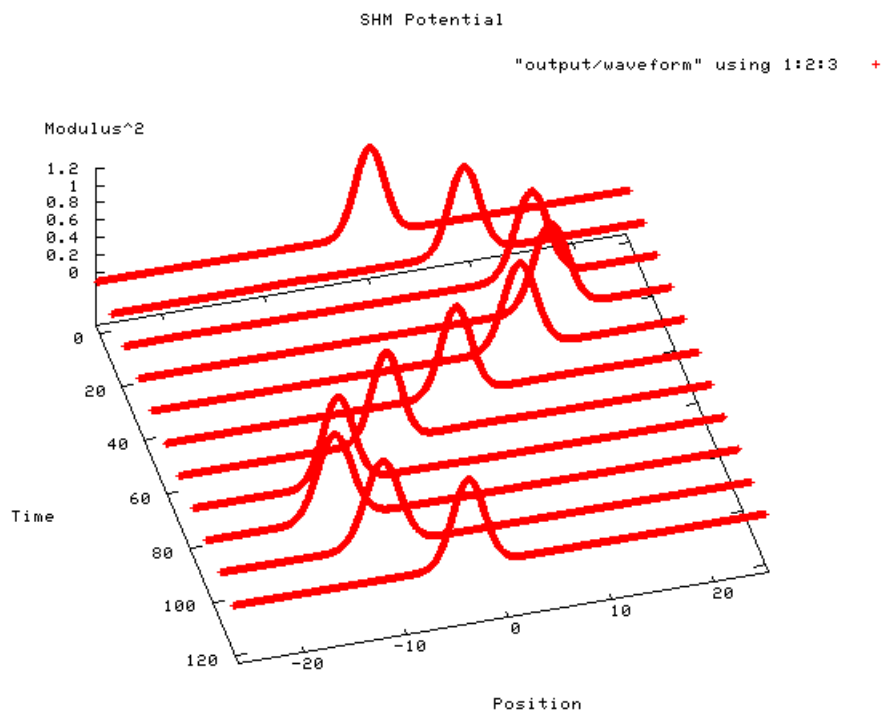


Figure 10: A space-time graph of a wave-packet oscillating in a parabolic (SHM-like) potential centred on $x = 0$.

4 Conclusion

The purpose of the project was to construct a computer program that could numerically find solutions to the Diffusion and Time dependent Schrödinger equations. This was accomplished using Fourier and Richardson's methods. This program's ability to handle 'standard' and more exotic potentials was then demonstrated graphically

As previously shown, the Richardson method can handle arbitrary potentials, but this method can only calculate the evolution of the wave packet by iterating through small increments in time. Therefore to calculate the state of the wave at a given time, Richardson's method must calculate all of the states up to that point in time. The Fourier method is not constrained in this way; it can calculate the required time frame in just one calculation.

5 Evaluation

This project has proved to be an interesting one both computationally and physically. The natural progression of the project would seem to be to expand into two or more dimensions. Richardson's method is well suited to this extension. However, visualising of such extensions becomes increasingly difficult; in two-dimensional space the representation would be a time evolving surface and in three dimensions we would require to display the evolution of a volume.

A different extension could be to attempt to overcome the disadvantages to the Richardson and Fourier methods so that a given time frame could be calculated for a general potential in just one calculation and still retain unitarity.

References

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