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# Mini Project:
# Solving the time-dependent Schrödinger equation

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## 1 Project Summary

In this project the time-dependent Schrödinger Equation has been solved using the 'Finite Domain Time Difference Method' for different simple static potential wells for a Gaussian wave packet.

The behaviour of the particle waves exhibits the inherently quantum mechanical behaviour that is expected. The animations generated allow to gain physical intuition.

## 2 Theory

The equation to solve is the **time-dependent Schrödinger Equation** (TDSE):

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = H(x)\Psi(x,t) \tag{1}$$

with $H(x)$ the static Hamiltonian. For simplicity here a static potential was chooses.

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

The TDSE can be rewritten applying the standard "Finite Time Difference Method" (see here):

$$\frac{\partial\Psi(x,t)}{\partial t} = \frac{\Psi(x,t+\Delta t) - \Psi(x,t)}{\Delta t} \tag{3}$$

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = \frac{\Psi(x,t+\Delta t) - 2\Psi(x,t) + \Psi(x-\Delta x,t)}{\Delta x^2} \tag{4}$$

Substituting this into the TDSE yields:

$$\Psi(x,t+\Delta t) = \Psi(x,t) - \frac{\Delta t\hbar}{2i(\Delta x)^2 m}\left[(x+\Delta x,t) - 2\Psi(x,t) + \Psi(x-\Delta x,t)\right] + \frac{\Delta t}{i\hbar}V(x)\Psi(x,t) \tag{5}$$

where we define the constants as

$$c_1 = \frac{\Delta t}{2(\Delta x)^2 m} \tag{6}$$

and

$$c_1 = \frac{\Delta t}{\hbar} \tag{7}$$

Then taking the real and imaginary parts of the wavefucntion one finally arrives at the equations used for the calculation:

$$\boxed{\Phi_R(x,t+\Delta t) = \Phi_R(x,t) - c_1\left[\Phi_I(x+\Delta x,t) + 2\Phi_I(x,t) + \Phi_I(x-\Delta x,t)\right] + c_2 V(x)\Phi_I(x,t)} \tag{8}$$

$$\boxed{\Phi_I(x,t+\Delta t) = \Phi_I(x,t) + c_1\Big[\Phi_R(x+\Delta x,t) + 2\Phi_R(x,t) + \Phi_R(x-\Delta x,t)\Big] + c_2 V(x)\Phi_R(x,t)} \tag{9}$$

These two equations are the core of the simulation. For the purpose of generating a meaningful animation the constants $c_1$ and $c_2$ have been slightly adapted.[1]

The **wavefunction** defining the particle to simulate is chosen to be an well defined electron. In order to define the particle well a Gaussian wave packet is chosen. For a Gaussian wavepacket a single wavevector can be defined as its Fourier transform frequencies are clustered around that single wave vector. This allows to define a somewhat localized particle. The Gaussian wavepacket is:

$$\Psi(x,0) = \Phi_0(x) = \frac{1}{\sqrt{\sigma\sqrt{\pi}}} e^{-\frac{x^2}{2*\sigma^2}} \tag{10}$$

let us define the normalisation as $\sqrt{\sigma\sqrt{\pi}} = A$. Then the modulated real and imaginary parts are

$$\Phi_R(x,0) = \frac{1}{A} e^{-\frac{1}{2}\left(\frac{x-x_0}{s}\right)^2} cos[k(x-x_0)] \tag{11}$$

$$\Phi_I(x,0) = \frac{1}{A} e^{-\frac{1}{2}\left(\frac{x-x_0}{s}\right)^2} sin[k(x-x_0)] \tag{12}$$

where the normalization constant can be found by integration according to the Born Rule:

$$1 = \int_{-\infty}^{\infty} |\Psi(x,t)|^2 \, dx \tag{13}$$

The particles momentum is specified using the deBroglie relations:

$$p = \hbar k \tag{14}$$

where $k$ is the wavevector defines as:

$$k = \frac{2\pi}{\lambda} \tag{15}$$

The **potentials** chosen to present here are all finite potentials:

- finite square well
- finite step well
- quadratic/harmonic well

The default particle presented has a wavelength $\lambda = 30nm$ and a rest mass $m = m_e$. Therefore the energy of the chosen electron particle has a kinetic energy as a free particle given by the deBroglie relation as:

$$E = \hbar\omega = \frac{hc}{\lambda} \approx 6.625 * 10^{-18} J \approx 41.35 eV \tag{16}$$

Therefore to explore the interesting behaviour of a bound particle we choose the welldepth or wellheight to be 80eV.

# 3 Aims & Objectives

## 3.1 Aims

- solve the time dependent Schrödinger equation using the 'Finite Domain Time Difference Method'
- demonstrate the working method on a few potentials
- comment on physical intuition gained

### 3.2 Objectives

- discretize space and time
- implement a physical potential parameters
- implement physical particle/wave parameters
- generate potential wells: free, square, harmonic, step
- demonstrate potential wells

## 4 Method

All of the method is self contained and described the Mathematica notebook. Please see the Notebook.

## 5 Usage of Code

This the Mathematica notebook contains all the calculations and some interactive animations.

For convenience all animation produced have been exported for ease of viewing as some calculations may take a few moments. Find the animations in the *\animations* folder.
All cells have been evaluated already to show the results. To rerun the calculations please evaluate all essential cells and user inputs cell consecutively. Note the color coding:

- **light blue** cells are essential to be run
- **yellow cells** require user input
- **white cells** are optional
-  **cells** with a watch face mark may take 1-3 minutes to evaluate

In case errors occur please rerun the notebook in consecutive order. Note that occasionally the notebook may require time to reformat, a message will show **Formatting Notebook Contents**.

## 6 References

[1] A fast explicit algorithm for the time-dependent Schrödinger equation Computers in Physics 5, 596 (1991); https://doi.org/10.1063/1.168415 P. B. Visscher