1. Introduction

We are going to be solving and implementing the **Time dependent Schrödinger equation**, which tells us how quantum particles behave.

Goal: We want to simulate and visualize a quantum particle (like an electron) moving in 3D space over time.

1.1. The main equation

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$$

Meaning symbols

- $\boldsymbol{\psi}$ **(psi)** = the "wavefunction" — describes where the particle might be
- $\boldsymbol{t}$ = time
- $\boldsymbol{\hbar}$ **(h-bar)** = Planck's constant ÷ 2π (a fundamental constant in quantum mechanics)
- $\boldsymbol{\widehat{H}}$ **(H-hat)** = Hamiltonian (the total energy operator)
- $\boldsymbol{i}$ = the imaginary number $\sqrt{-1}$

The Hamiltonian has two parts:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r}, t)$$

Meaning Parts

- $\boldsymbol{-\frac{\hbar^2}{2m}\nabla^2}$ = kinetic energy (energy from motion)
  - $\boldsymbol{m}$ = mass of the particle
  - $\boldsymbol{\nabla^2}$ = Laplacian operator (measures how the wavefunction curves in space)
- $\boldsymbol{V(r,t)}$ = potential energy (energy from forces, like electric fields)

Probability: The quantity $|\psi|^2$ tells you the probability of finding the particle at each location.

1.1.1. Simplified Units

To make the math easier, we will for now set $\hbar = 1$ and $m = 1$. This gives us:

$$i\frac{\partial\psi}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V(\boldsymbol{r}, t)\right]\psi$$

We can convert back to real units later by putting $\hbar$ and m back in.

1.2. How to Solve It: The Split-Step Method

We want to move the wavefunction forward in time by small steps Δt.

The exact solution would be:

$$\psi(t + \Delta t) = \exp\Big(-i\hat{H}\Delta t/\hbar\Big)\psi(t)$$

But this is hard to compute directly! So we **split** the Hamiltonian into two easier parts:

- $\widehat{\boldsymbol{T}}$ = kinetic energy part = $-\frac{\hbar^2}{2m}\nabla^2$
- $\widehat{\boldsymbol{U}}$ = potential energy part = $V(\boldsymbol{r}, t)$

The **Strang splitting** method says we can approximate one time step as:

[half kinetic step] → [full potential step] → [half kinetic step]

Mathematically:

$$\exp\Big(-i\hat{H}\Delta t/\hbar\Big) \approx \exp\left(-i\hat{T}\frac{\Delta t}{2\hbar}\right) \cdot \exp\left(-i\hat{U}\frac{\Delta t}{\hbar}\right) \cdot \exp\left(-i\hat{T}\frac{\Delta t}{2\hbar}\right)$$

This is accurate to order Δt^2 (very good for small time steps).

1.3. Why Use FFTs? (The Clever Trick)

The Problem: The kinetic and potential energy parts are hard to compute in the same space.

The Solution: Use different spaces for each part!

1.3.1. Potential Energy (Easy in Real Space)

In regular 3D space (where x, y, z are positions), applying the potential energy is simple multiplication:

$$\psi_{\text{new}(\boldsymbol{r})} = \exp(-iV(\boldsymbol{r}, t)\Delta t/\hbar) \cdot \psi_{\text{old}(\boldsymbol{r})}$$

You just multiply each point by a phase factor.

1.3.2. Kinetic Energy (Easy in Momentum Space)

In **Fourier space** (also called k-space or momentum space), the kinetic energy is also simple multiplication:

$$\tilde{\psi}_{\text{new}(\boldsymbol{k})} = \exp\left(-i\frac{\hbar\ |\boldsymbol{k}|^2}{2m}\Delta t\right) \cdot \tilde{\psi}_{\text{old}(\boldsymbol{k})}$$

Where $\boldsymbol{k}$ is the wave vector (related to momentum by $\boldsymbol{p} = \hbar\boldsymbol{k}$).

1.3.3. The Bridge: Fast Fourier Transform (FFT)

- **FFT** converts from real space (x, y, z) to momentum space $\left(k_x, k_y, k_z\right)$
- **IFFT** (inverse FFT) converts back

So the algorithm alternates:
1. Real space → FFT → momentum space → apply kinetic energy
2. IFFT → real space → apply potential energy
3. Repeat

1.4. Setting Up the Grid

We simulate on a 3D box with dimensions $L_x \times L_y \times L_z$, divided into $N_x \times N_y \times N_z$ grid points.

1.4.1. Real Space Grid

- Spacing: $\Delta x = L_x/N_x$, $\Delta y = L_y/N_y$, $\Delta z = L_z/N_z$
- Points: $x_i = -L_x/2 + i\Delta x$, for $i = 0, 1, ..., N_x - 1$
- (Same for y and z)

1.4.2. Momentum Space Grid

The FFT gives you momentum values:

$$k_{x(p)} = \frac{2\pi}{L_x} \times \{0, 1, 2, ..., N_x/2 - 1, -N_x/2, ..., -1$$

(Same pattern for k_y and k_z)

The squared magnitude is:

$$k^2 = k_x^2 + k_y^2 + k_z^2$$

Precompute these grids once at the start!

1.5. The Complete Algorithm (Step-by-Step)

1.5.1. Setup (do once):

1. Compute the k-space grid values $\left(k_x, k_y, k_z, \text{and } k^2\right)$
2. Precompute the kinetic factor:

$$K(\boldsymbol{k}) = \exp(-ik^2\Delta t/4)$$

(half-step with $\hbar = m = 1$)

3. Precompute the potential factor:

$$P(\boldsymbol{r}) = \exp(-iV(\boldsymbol{r})\Delta t)$$

(if V doesn't change in time)

1.5.2. Each Time Step (repeat many times):

1. First half kinetic step (in momentum space):

- Transform: $\tilde{\psi} \leftarrow \text{FFT}[\psi]$
- Multiply: $\tilde{\psi} \leftarrow K(\boldsymbol{k}) \cdot \tilde{\psi}$
- Transform back: $\psi \leftarrow \text{IFFT}\left[\tilde{\psi}\right]$

2. Full potential step (in real space):

- Multiply: $\psi \leftarrow P(\boldsymbol{r}) \cdot \psi$

3. Second half kinetic step (in momentum space):

- Transform: $\tilde{\psi} \leftarrow \text{FFT}[\psi]$
- Multiply: $\tilde{\psi} \leftarrow K(\boldsymbol{k}) \cdot \tilde{\psi}$
- Transform back: $\psi \leftarrow \text{IFFT}\left[\tilde{\psi}\right]$

1.5.3. Visualization:

After each time step (or every few steps), compute the probability density:

$$\rho(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2$$

This is what you display as a 3D volume or isosurface!

1.6. Key Points to Remember

- $\boldsymbol{\psi}$ **is complex:** It has real and imaginary parts (or magnitude and phase)
- $\boldsymbol{|\psi|^2}$ **is real:** This is what you see — the probability density
- **FFT is the speed trick:** It makes the kinetic energy easy to compute
- **Small time steps:** Smaller Δt gives more accurate results
- **Normalization:** The total probability should stay 1:

$$\int |\psi|^2 \, \mathrm{d}^3 r = 1$$

1.7. Summary

The split-step FFT method works by:

1. Splitting the problem into kinetic and potential parts

2. Using FFTs to switch between real space (good for potential) and momentum space (good for kinetic energy)
3. Taking small time steps, alternating between the two spaces
4. Visualizing $|\psi|^2$ to see where the particle is likely to be

This method is fast, accurate, and perfect for GPU implementation!

2. Implementation

2.1. On Setup

- Compute k-space grid values $\left(k_x, k_y, k_z, \text{and } k^2\right)$
- Compute kinetic factor:

$$K(\boldsymbol{k}) = \exp(-ik^2 \Delta t/4)$$

  (half-step with $\hbar = m = 1$)
- Compute the potential factor:

$$P(\boldsymbol{r}) = \exp(-iV(\boldsymbol{r})\Delta t)$$

  (if V doesn't change in time)
- Initialize guassian wavepacket (can use something else if wanted):

$$\psi(\boldsymbol{r}, t=0) = A \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2}{4\sigma^2} + i\boldsymbol{k}_0 \cdot \boldsymbol{r}\right)$$

Meaning

1. **Position part** (real Gaussian):

$$\exp\left(-\frac{r^2}{4\sigma^2}\right)$$

   - Centers the particle at position (x_0, y_0, z_0)
   - σ = width parameter (how spread out it is)

2. **Momentum part** (plane wave):

$$\exp(i\boldsymbol{k}_0 \cdot \boldsymbol{r}) = \exp\big(i\big(k_{0x}x + k_{0y}y + k_{0z}z\big)\big)$$

   - Gives the particle initial momentum
   - $\boldsymbol{k}_0 = \big(k_{0x}, k_{0y}, k_{0z}\big)$ = initial wave vector

3. **Normalization constant**:

$$A = \left(\pi\sigma^2\right)^{-3/4}$$

2.2. On Update

First half kinetic step (in Fourier space):

- Transform: $\tilde{\psi} \leftarrow \mathrm{FFT}[\psi]$
- Multiply: $\tilde{\psi} \leftarrow K(\boldsymbol{k}) \cdot \tilde{\psi}$
- Transform back: $\psi \leftarrow \mathrm{IFFT}\left[\tilde{\psi}\right]$

Full potential step (in real space):

- Multiply: $\psi \leftarrow P(\boldsymbol{r}) \cdot \psi$

Second half kinetic step (in Fourier space):

- Transform: $\tilde{\psi} \leftarrow \mathrm{FFT}[\psi]$
- Multiply: $\tilde{\psi} \leftarrow K(\boldsymbol{k}) \cdot \tilde{\psi}$
- Transform back: $\psi \leftarrow \mathrm{IFFT}\left[\tilde{\psi}\right]$

Visualizing

- After N steps we compute the probability density in 3D volume

$\rho(\boldsymbol{r}) = |\psi(\boldsymbol{r})|^2$