Finite Difference Application to 1-D Schrödinger Equation:

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Outline of Talk:

- Basic quantum terminology and introduction to Schrödinger equation.

- Introduction to Finite Difference Methods (FDM) and computational methods.

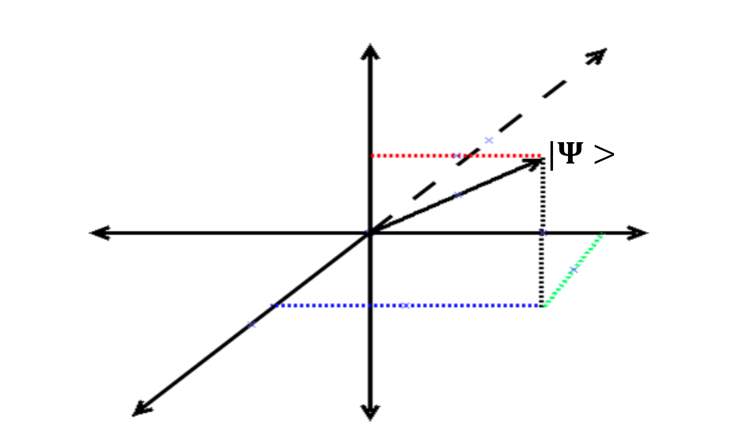
- Results of FDM applied to Time Dependent Schrödinger Equation (TDSE):
  - Normalization
  - Energy Conservation
  - Tunneling

- Future Work

Q: What is a wavefunction/ket?

- A wavefunction (written either as a function $\Psi(x)$, or a ket $|\Psi >$) is a collection of all possible states a particular state can be in.
  - Ψ is the function label or the ket label, it can be called anything we want! (Next slide will be $|t >$)
- This ket can be seen as a column vector.
  - Like any other vector, it resides in a vector space.
  - This space is known as the Hilbert Space .

$$|\Psi\rangle = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \vdots \\ \Psi_N \end{pmatrix} \rightarrow \Psi(x)$$



Q: What is the Schrödinger Equation:

- Consider an operator that has the sole purpose of taking a particular ket $|t_0 >$ to $|t_0 + \Delta t >$. We call this the time evolution operator and is denoted by $\hat{U}(t, t_0)$.
    - Properties we want:
        - $\hat{U}(t, t_0)^\dagger \, \hat{U}(t, t_0) = 1$ (Unitarity condition)
        - $\hat{U}(t_2, t_1) \, \hat{U}(t_1, t_0) = \hat{U}(t_2, t_0)$
        - $\hat{U}(-t, t_0) = \hat{U}^{-1}(t, t_0)$
        - $\lim_{t \to t_0} \hat{U}(t, t_0) = 1$
- Proposed Solution: $1 - \frac{i\hat{H}\Delta t}{\hbar}$ will sufficiently satisfy all these conditions if we assume non-linear time increments are negligible.

Quick Derivation:

$$\hat{U}(t,t_0) = 1 - \frac{i\hat{H}\Delta t}{\hbar} \qquad \hat{U}(t,t_0)|t> = |t+\Delta t>$$

$$\left(1 - \frac{i\hat{H}\Delta t}{\hbar}\right)|t> = |t+\Delta t>$$

$$|t> - \frac{i\hat{H}\Delta t}{\hbar}|t> = |t+\Delta t>$$

$$\lim_{\Delta t\to 0} \hat{H}|t> = \lim_{\Delta t\to 0} i\hbar\frac{|t+\Delta t> - |t>}{\Delta t}$$

$$\hat{H}|t> = i\hbar\partial_t|t>$$

$$\frac{-\hbar^2}{2m}\nabla^2|t> + V|t> = i\hbar\partial_t|t>$$

We are left with an interpretation of the Schrödinger equation.

- The purpose of this equation is to describe how a ket is taken from some time $|t>$ to some later time $|t+\Delta t>$. This is time evolution.
- One way to envision this is the ket is moving through a trajectory in its Hilbert space, and that trajectory is governed by the Schrodinger equation. This is Schrödinger's picture.
- Can see this as a quantum analogue to $F = ma$.

How to Solve this Computationally:

- Finite difference methods (FDM) relates differentiation to difference quotients.
- Consider $f(x + \Delta x) = f(x_{i+1})$; $f(x) = f(x_i)$; $f(x - \Delta x) = f(x_{i-1})$

$$\boldsymbol{f(x + \Delta x) = f(x) + f_x(x)\Delta x + \frac{f_{xx}\Delta x^2}{2} + \frac{f_{xxx}\Delta x^3}{6} + O(\Delta x^4)}$$

$$\boldsymbol{f(x - \Delta x) = f(x) - f_x(x)\Delta x + \frac{f_{xx}\Delta x^2}{2} - \frac{f_{xxx}\Delta x^3}{6} + O(\Delta x^4)}$$

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$$\boldsymbol{f_{xx}(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{\Delta x^2} + O(\Delta x^2)}$$

- We apply this general idea to differential equations. First, we split the waveform into real and imaginary parts.

$$\boldsymbol{\Psi_n(t) = R_n + iI_n}$$

- Application of FDM on TDSE yields a system of ordinary differential equations.
- For stability purposes we get the TDSE into a symplectic form, allowing for leapfrog integration as an ODE solver.

$$\frac{dR_n}{dt} = -\frac{1}{2\Delta x^2} I_{n+1} + \left(\frac{1}{\Delta x^2} + U_n^m\right) I_n - \frac{1}{2\Delta x^2} I_{n-1} \rightarrow f_n(I, t)$$
$$\frac{dI_n}{dt} = -\frac{1}{2\Delta x^2} R_{n+1} + \left(\frac{1}{\Delta x^2} + U_n^m\right) R_n - \frac{1}{2\Delta x^2} R_{n-1} \rightarrow g_n(R, t)$$

- Leapfrog integration preserves physical quantities, and is well known for stability in Hamiltonian systems.

- As the wavefunction is propagated in time, we calculate expectation values at each time step.

Ex:

$$P_n^m(x,t) = |\Psi_n^m|^2$$

$$< x >^m = < \Psi_n^m | x_n^m | \Psi_n^m > = \int_a^b [(R_n^m)^2 + (I_n^m)^2] x_n^m dx$$

$$< p >^m = < \Psi_n^m | p_n^m | \Psi_n^m > = \int_a^b \left[R_n^m \frac{dI_n^m}{dx} - I_n^m \frac{dR_n^m}{dx} \right] dx$$

$$< K >^m = < \Psi_n^m \left| \frac{(p_n^m)^2}{2} \right| \Psi_n^m > = \int_a^b \left[\left(\frac{dR_n^m}{dx} \right)^2 - \left(\frac{dI_n^m}{dx} \right)^2 \right] dx$$

$$< U >^m = < \Psi_n^m | U_n^m | \Psi_n^m > = \int_a^b [(R_n^m)^2 + (I_n^m)^2] U_n^m dx$$

$$J_n^m = R_n^m \frac{dI_n^m}{dx} - I_n^m \frac{dR_n^m}{dx}$$

Key Features to Consider:

- Normalization Condition:

$$\frac{\partial < \Psi|\Psi >}{\partial t} = 0$$

- Uncertainty Principle:

$$\Delta x \Delta p \geq \hbar/2$$

- Conservation of Energy

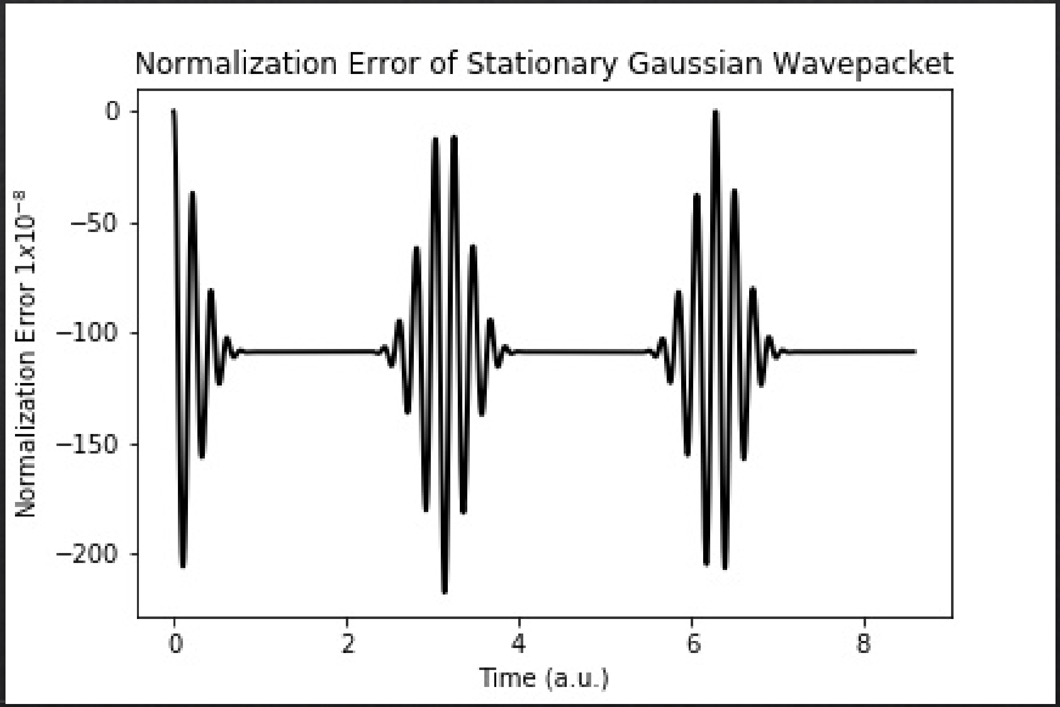
- Quantum phenomenon: Tunneling

Conditions and Constraints:

- We consider a Gaussian plane wave moving with a constant velocity v as our wavefunction.
  - The spread of the Gaussian is characteristic of the lack of certainty of it's position.
- For all of our simulations we use a periodic boundary condition (PBC).
  - Above all else, normalization must be conserved in quantum theory. This is the motivation for a PBC despite it's apparent unphysical traits.
- We consider:
  - A unit system that is characteristic of atomic scales the atomic units (a.u. scale)
  - Domain: $[-30,30]$ with 2048 divisions.
  - Central Velocity: Context dependent
  - $\boldsymbol{\Psi_n^0} = (\boldsymbol{\sigma}\sqrt{\boldsymbol{\pi}})^{-1/2}\, \boldsymbol{e}^{-\frac{(x-x_0)^2}{2\sigma^2}+ik_0x}$

Results I: Validation

Normalization Condition:

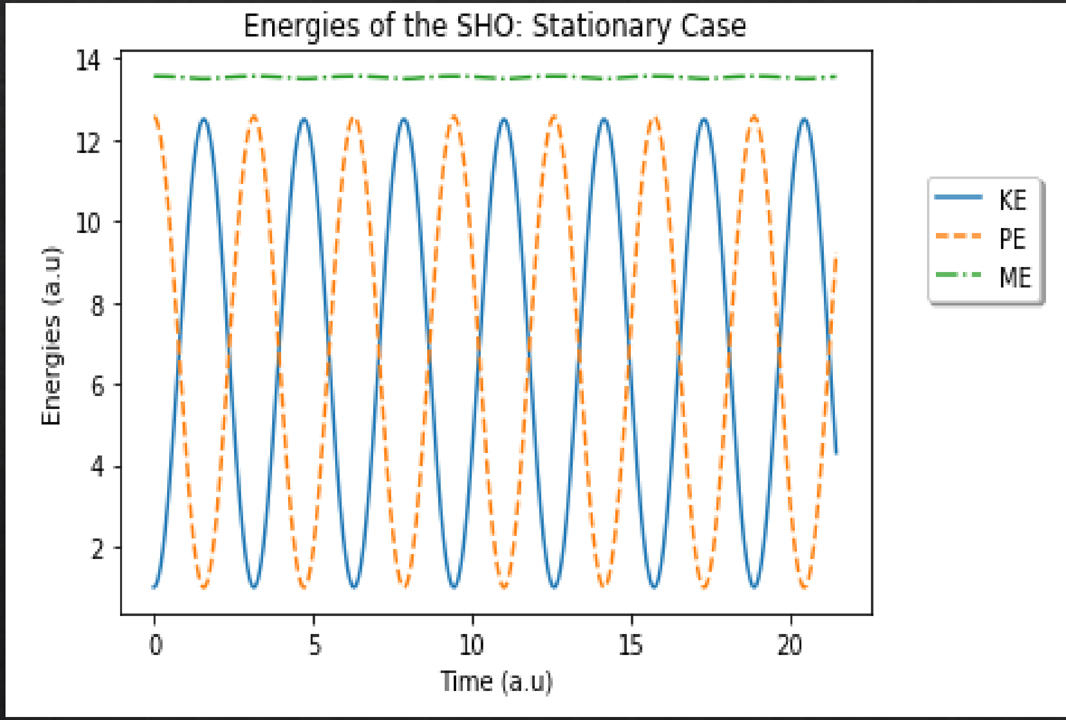


Importance of Normalization:

- Normalization can be attributed to conservation of probability.
  - Also seen as conservation of particle number.
- Any other simulations will have this error as a systematic error, so minimizing this is vital.
- This "beat" like pattern is characteristic of symplectic integration.

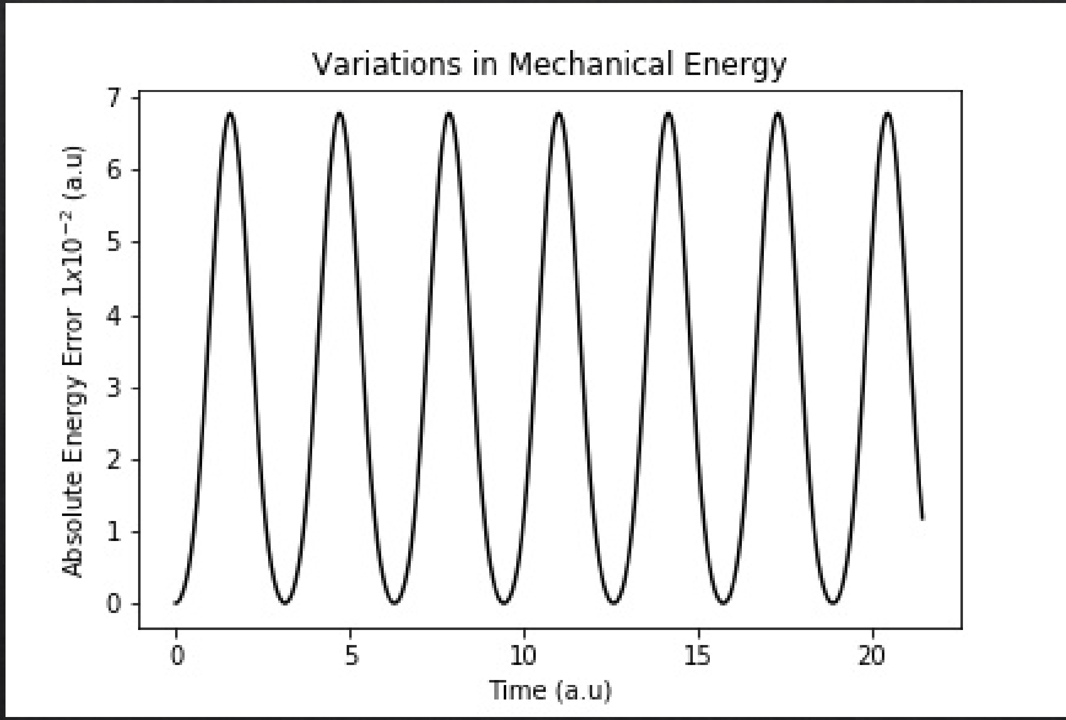
Result II: Validation

Energy Conservation (?):



An initial Gaussian packet with initial velocity $v = \sqrt{2}$ displaced $\Delta x = 5$ from the equilibrium position.

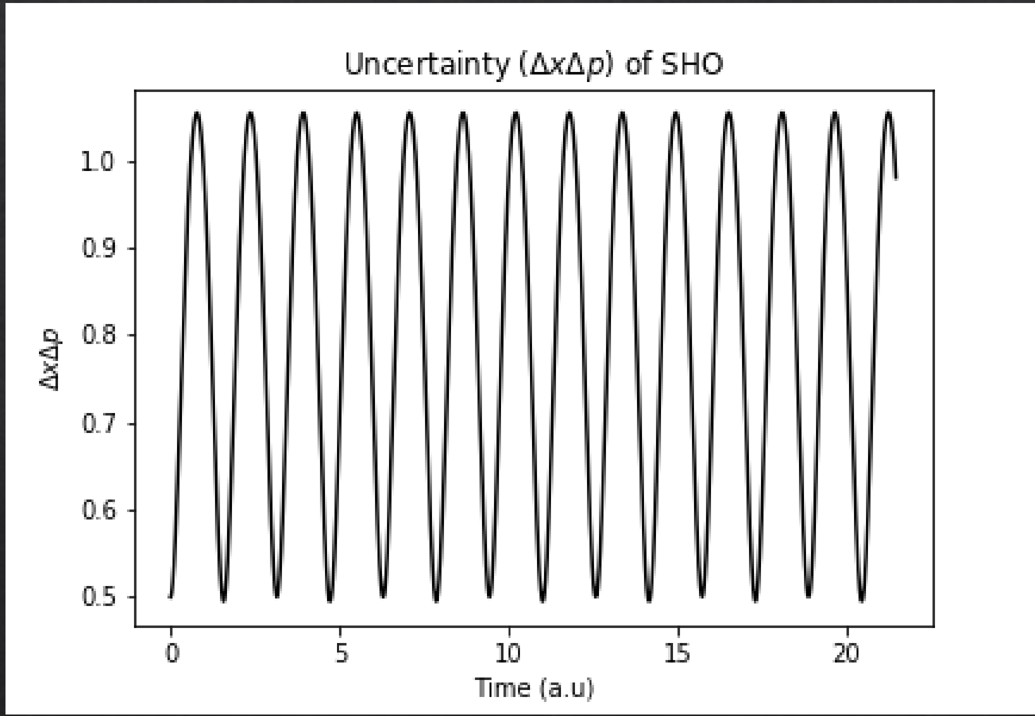
Deviation in Energy Conservation:



Deviations in mechanical energy (ME) by plotting total ME – initial energy.

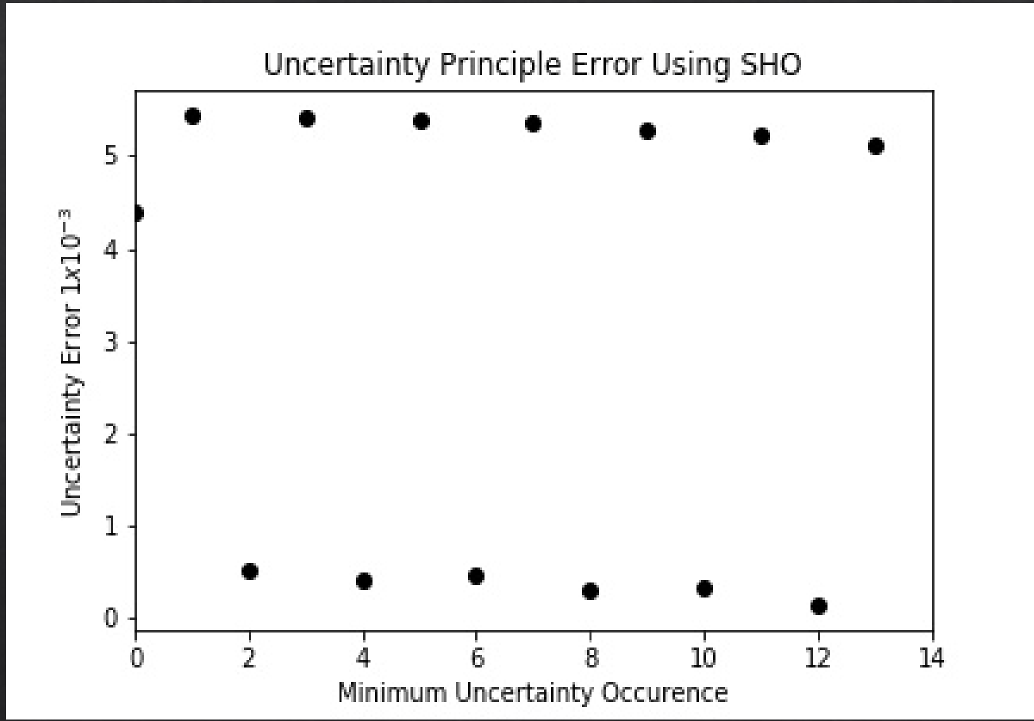
Results III: Validation

Uncertainty Principle:



Under the investigation of SHO this is the plot of $\Delta x \Delta p$ at each instant of time.

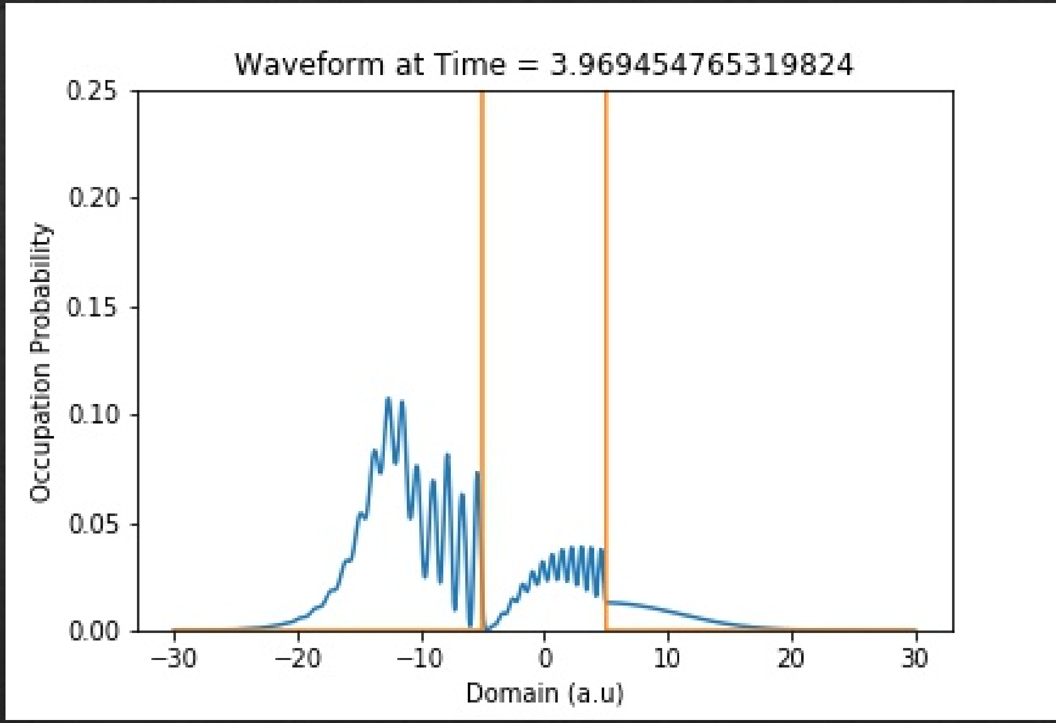
Deviation in Uncertainty Principle:



Quantifying the error by plotting the points of minimum uncertainty and plotting (1/2 – minimum.)

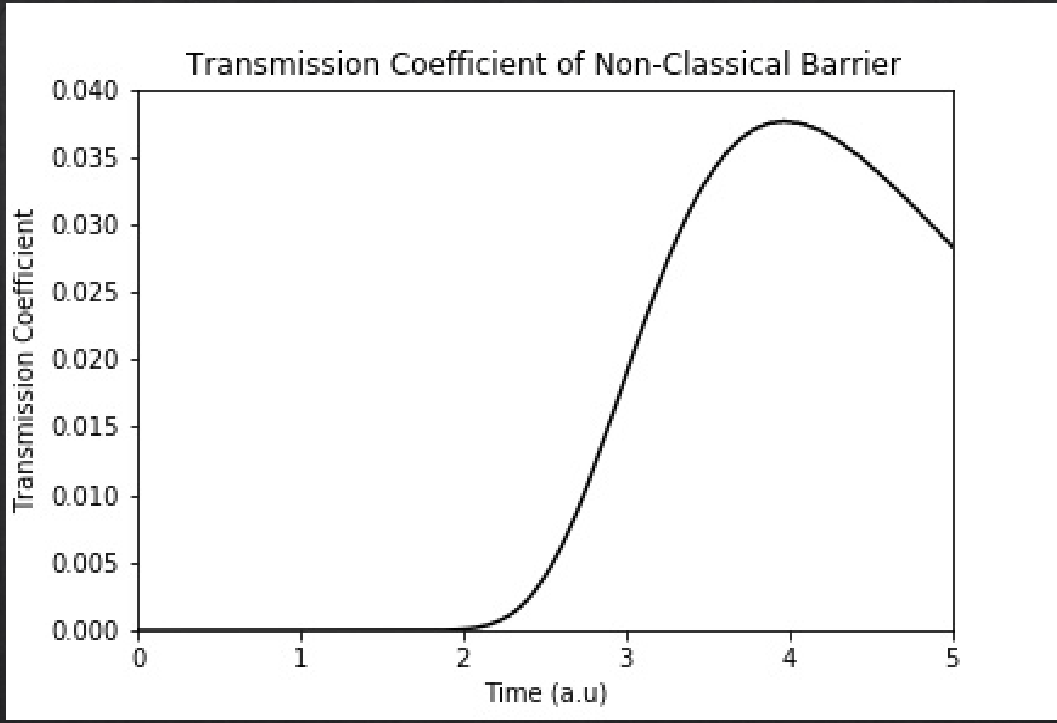
Results IV: Tunneling

Maximum Probability Flux:



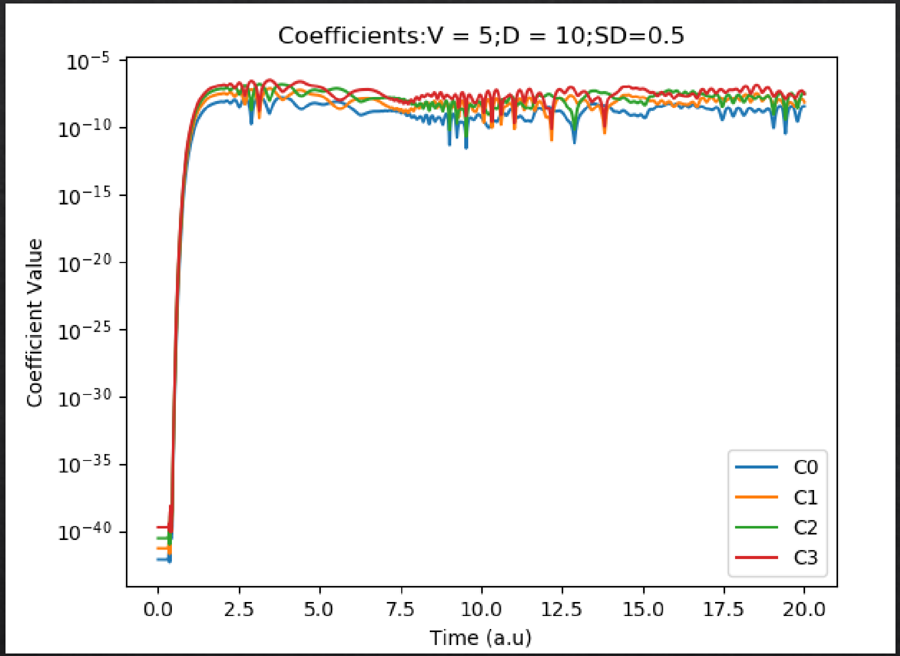
Gaussian packet with central velocity 5 a.u. This displays the time of maximum transmission coefficient.

Transmission Coefficient:

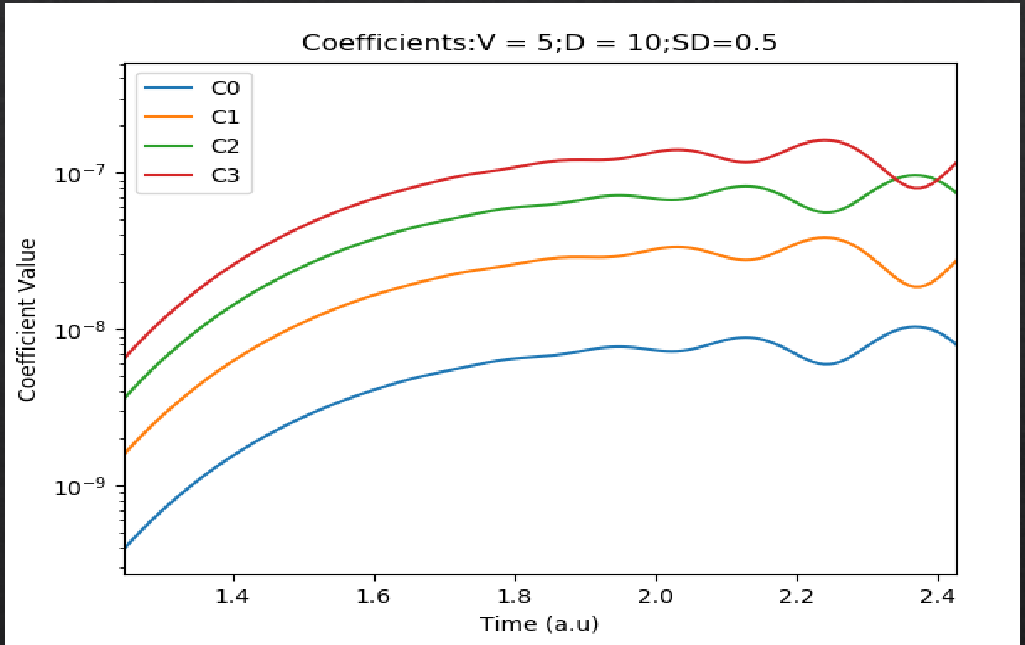


Transmission coefficient as a function on time. This transmission coefficient is probability flux.

Results IV: Capture



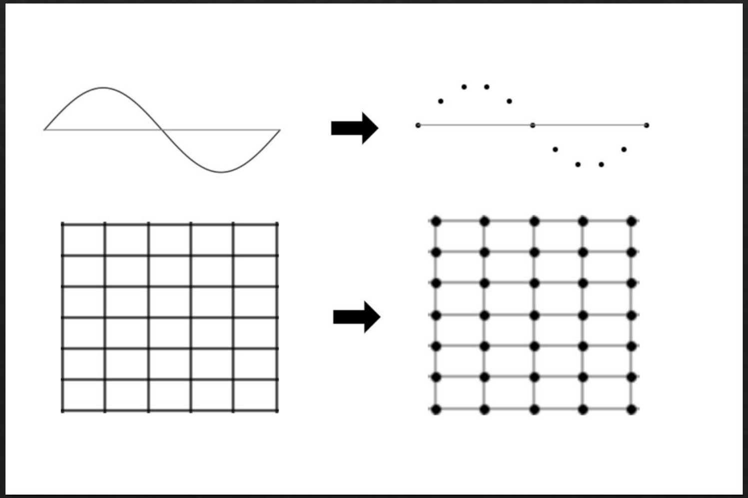
Expansion coefficient of states for a Gaussian packet given a central velocity v=5 and a standard deviation of 0.5.

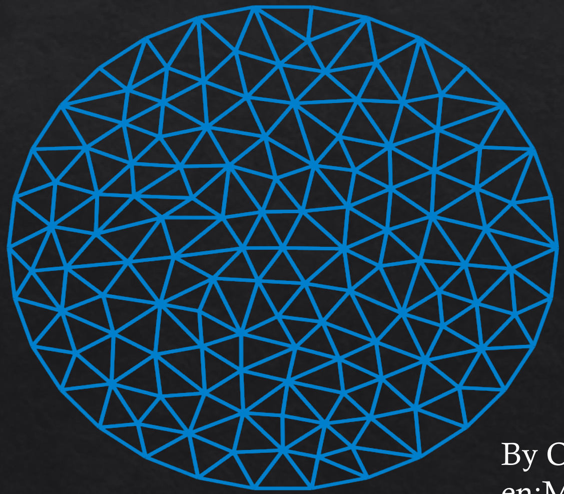


Zoomed view of the increase of occupation probability before it is dominated by interference.

Future Work I

- FDM notoriously has problems with scaling dimensionality. The grid → mesh → lattice.
  - Any type of mesh based scheme has this problem.
- FDM has trouble with domains of arbitrary geometry.
  - If you still want to work with a mesh based model, something like Finite Element Method (FEM) is a fruitful alternative.





By Oleg Alexandrov - self-made, with en:Matlab, Public Domain, https://commons.wikimedia.org/w/index.php?curid=2245302

Future Work II:

- The problem of dimensionality could be fixed with a mesh free scheme which solutions are not reliant on an established grid.
  - An example of this would be Radial Basis Function schemes, which involve interpolation of solutions using specific types of functions that are well localized.
- Beyond method comparisons, a stronger emphasis on scattering experiments is possible to explore.