Write a Fortran90 program to solve the TDSE for processes like electron scattering off a barrier in one dimension and tunneling through a barrier using following type of solution:

$$\boxed{\psi(x_i, t_{j+1}) = \psi(x_i, t_{j-1}) - \frac{2i\Delta t}{\hbar}\hat{H}\psi(x_i, t_j)}. \tag{1}$$

The wavepacket at the first step (time t=1) is accomplished by the Euler method

$$\psi(x_m, t_1) \approx \psi(x_m, t_0) + i\Delta t \left[\frac{\hbar}{2m}\frac{d^2\psi(x_m, t_0)}{dx^2} - \frac{1}{\hbar}V(x_m)\psi(x_m, t_0)\right] \tag{2}$$

The potential in atomic unit is $V(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0. \end{cases}$ The initial wave packet is given some initial momentum, k_0, to start with and hence, looks as follows

$$\psi(x) = \left(\frac{2\alpha}{\pi}\right)^{1/4} e^{ik_0(x-x_0)}\ e^{-\alpha(x-x_0)^2}, \tag{3}$$

where k_0 is the initial wave vector and $k_0 = p_0/\hbar$. The other parameters are as follows:

- Gaussian wave packet exponent, α= 20 au
- Gaussian wavepacket initial position, x_0 = -0.5 au
- initial momentum of the particle, p_0 = 20.0 au
- mass of the particle = 14500 au
- starting point of the grid, xmin=-2.0 au
- δx, step size in x= 0.02 au
- δt, time step size= 0.1 au

- total number of time steps = 5000

The operation of the potential energy operator involves only the multiplication of the wave function by the potential energy at the grid points. For the application of $\hat{T}$ of ψ, as we decided in the class, we will use two different schemes

- finite-difference scheme
- Fourier-transformation scheme

As shown the class, the finite-difference is simple, in the sense that the derivative is approximated by a finite-difference. In case of FT, a forward FT of the wave function is performed to get $\phi(k)$ and then this $\phi(k)$ is multiplied by -k^2. The resulting function is then Fourier transformed back to the coordinate space which yields the second derivative. In the present problem, we will use the discrete Fourier transform (FT) method for the purpose. Since we are working on a grid, the discretized version of Fourier transform will look as $\phi(k_m) = \frac{1}{\sqrt{N}} \sum_j \psi(x_j)\ exp(-i\ k_m\ x_j)$. Similarly, an inverse Fourier transformation will look as $\psi(x_j) = \frac{1}{\sqrt{N}} \sum_m \phi(k_m)\ exp(i\ k_m\ x_j)$.

Computation of k and k^2

The maximum length of the grid (L = N Δx) along the spatial coordinate x, determines (Δk) the spacing between two successive points in the momentum space: $\Delta k = \frac{2\pi}{\lambda_{max}} = \frac{2\pi}{N\Delta x}$. In the momentum space (k), the grid is centered at zero and all other points are distributed symmetrically on either side of it. If the maximum momentum represented in the k space is p_{max} (= k_{max} as $\hbar$=1 in au), then the momentum ranges from -p_{max} to +p_{max}. Remember

that p_{max}=$\frac{\pi}{\Delta x}$. k is calculated and stored as follows:

$$k_m = \frac{2\pi m}{L}, (m = 0, 1, 2, ...N/2 - 1) \quad (4)$$

$$k_m = \frac{2\pi(m - N)}{L}, (m = N/2, N/2 + 1, ...N - 1). \quad (5)$$

Writing out the results for movies

Write a short code to print out the x and absolute square of the wavepacket at each 100th time step. The outputs will be in different files. These files can be plotted using any graphics software for visualization, e.g. Gnuplot. Once you have the data files at different times, make a movie using any free software in your Operating System. The movie will show the translation of the wavepacket with time. Each frame should have a label showing the "timestep".