Exercise 4
Split-operator method and fast Fourier transform

Solve computationally the time-dependent Schrödinger equation for a double potential well using the split-operator method

$$-\frac{1}{2m}\nabla^2\psi(x) + V(x)\psi(x) = E\psi(x), \text{ where} \tag{1}$$

$$V(x) = \frac{C}{2}\left(|x| - x_0\right)^2 \tag{2}$$

with the initial wave function

$$\psi_n(x, t=0) = \left(\frac{m\omega}{\pi}\right)^{1/4} e^{\frac{-m\omega(x-x_0)^2}{2}}, \text{ where} \tag{3}$$

$$\omega = \sqrt{C/m}. \tag{4}$$

The height of the potential in the middle depends on the choice of x_0. Choose x_0 such that the height is higher than about 10 eigenvalues of a harmonic oscillator with the potential $Cx^2/2$.

Plot the density depending on time. If you can make a movie - great! Otherwise, you can put a set of snapshots into a presentation/pdf file. Study, how the time evolution of the density depends on the height of the potential in the middle.

Choice of parameters
Please select C of order ∼500 – 1500 N/m, which is a typical values for force constants of diatomic molecules (transform N/m to the atomic units). Please select the mass of order from 0.5 to 20 Dalton, which corresponds approximately the mass of 900 to 4000 Hartree atomic units. This is a typical reduced mass of light diatomic molecules.

Output of results
All parameters that can be varied must be defined and read from an input file. The output of results - a pdf file/presentation. The calculated energy must be presented in eV. Length must be presented in nm, Ångstrom or Bohr.

Tipp
You can use a library to perform fast Fourier transforms, but be careful and read their manual, because they are designed to output positive frequencies.