# Particle in a Box - MATLAB exercise

Nikola Zotev (nikola.zotev@ed.ac.uk)

In this exercise, you will have the opportunity to write a short MATLAB script to illustrate some important concepts connected to wavefunctions, and practice your newly acquired programming skills. The task is based on the good old particle in a box model. Do not feel constrained to the steps outlined below - experiment with the code and see what you can learn.

**Task 1:**

- Create a new script file. You may consider starting the file by clearing old variables from the workspace (*clear*), clear the command window (*clc*) and close old figures (*close all*).
- Define variables for the box length (let's say 10 au), $\hbar$ and the mass of the particle (electron). Ideally, you would use atomic units so these are set to unity but it is a good practice to keep them as variables in case you need to change to some other units.
- Define a vector representing your x values.
- Use Eq. 22 in your lecture notes to compute the wavefunctions for state with n=1 and n=2.
- Plot the two wavefunctions on a single plot and label the figure. Compare your results to FIG. 1 in the notes.
- What are the expectational values for the position in the two states? What are the most probable values?

**Task 2:**

- Define a vector to represent the momentum space of the particle. What is the range that you need to use?
- Using Eq. 23 in your lecture notes, calculate the momentum wavefunction for n=10,20. Plot the corresponding probability amplitude, label and compare to FIG. 2.
- Add the mometum function for n=100. What has changed?

**Task 3:**

- Define an empty 2xM matrix (use *zeros()*), where 2 is the number of states and M is the number of points in space. Populate the matrix, using a *for* loop, with the values of the wavefunction for states n=12 and n=13.
- What is the period of oscillation, T, for a wavepacket comprising these states.
- Define a wavepacket, assuming equal probability for the two states, at times t=0, T/4 and T/2.
- Check that the wavepacket is normalised at each timestep.
- Plot the probability amplitude on three sub-figures. Compare with FIG. 4 in the notes.
- If you have time, try making a short animation using timepoints between t=0 and t=2T.
- What is the formula for the flux for this wavepacket? Calculate its values from t=0 to t=T, and plot them.