DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

PARTICLE IN A BOX
[1D] SQUARE POTENTIAL WELL WITH A STEP

Ian Cooper

matlabvisualphysics@gmail.com

DOWNLOAD DIRECTORY FOR PYTHON SCRIPTS

qm040S.py **finite square well**

Solution of the [1D] Schrodinger equation by finding the eigenvalues and eigenvectors for an electron confined to a region of space by a finite square potential well with a step.

GitHub

Google Drive

References

Operators, expectation values, Heisenberg Uncertainty Principle

Transverse standing waves

First and Second derivative operators

Bound particle: Eigenstates of a particle confined by a potential well (eigenvalues and eigenvectors)

Bound particle: Square potential wells: finite and infinite

[1D] FINITE SQUARE WELL POTENTIAL WITH STEP

In this article we will consider a finite potential well with a step and is defined by

$$
\begin{aligned}
U(x) &= 0 \quad x_{\min} \le x \le -w/2 \\
U(x) &= U_0 \quad -w/2 < x < 0 \\
U(x) &= U_1 \quad 0 \le x \le +w/2 \\
U(x) &= 0 \quad +w/2 < x \le x_{\max}
\end{aligned}
$$

The well parameters were selected to give six eigenstates as shown in figure 1.

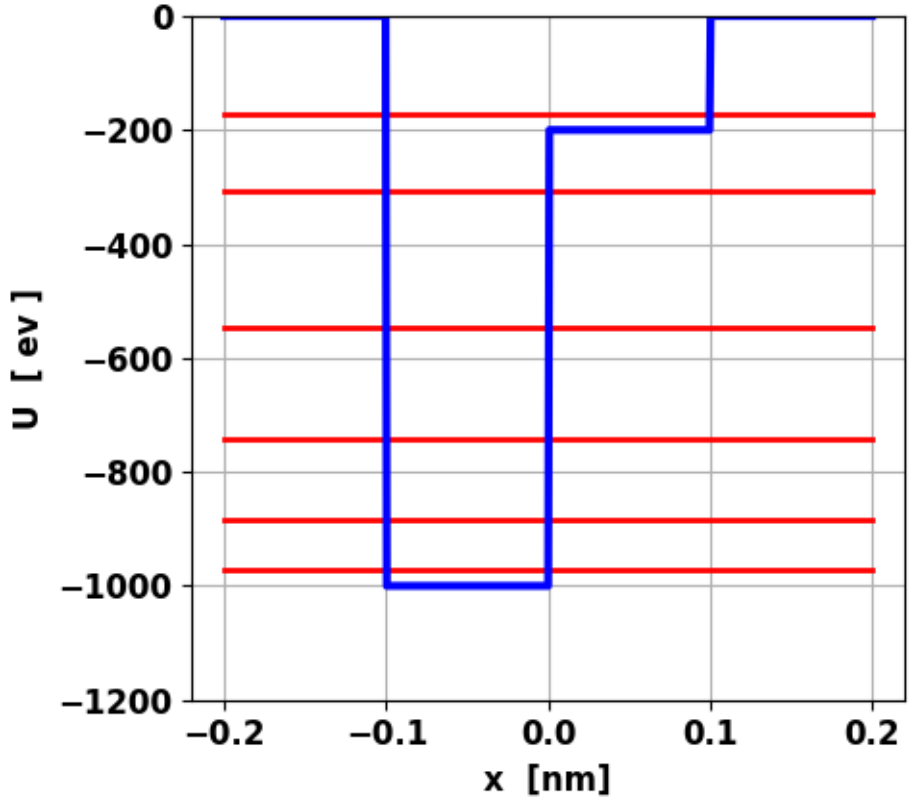

Fig. 1. Energy spectrum and square potential well with a step. The well parameters are: width w = 0.200 nm with depths U_0 = -1000 eV and U_1 = -200 eV.

Energy spectrum: eigenvalues

eV	E_1	E_2	E_3	E_4	E_5	$E6$
	-970	-884	-741	-545	-308	-172

Eigenfunctions (eigenvectors)

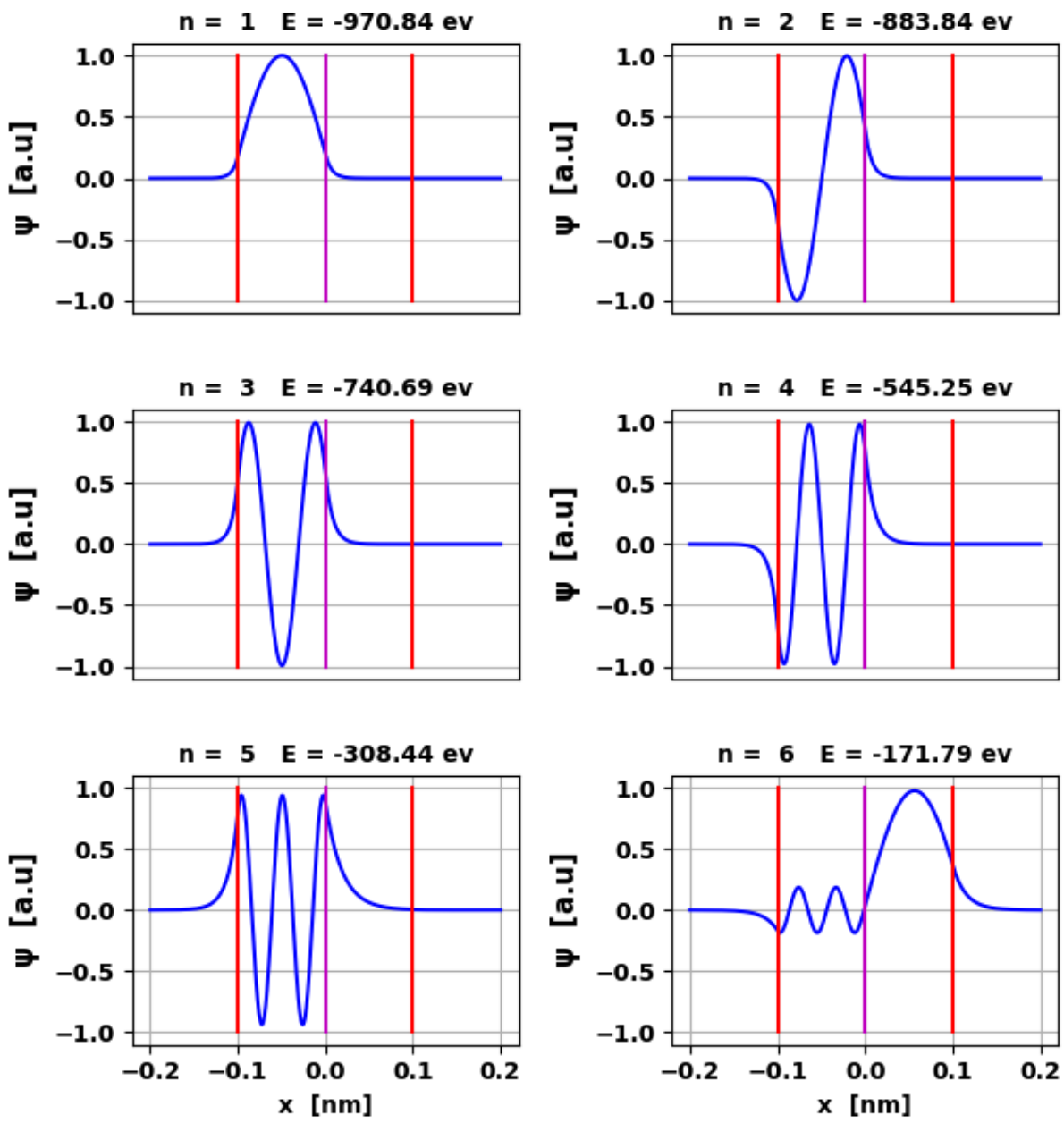

Fig. 2. Eigenfunctions for the **finite square well with a step** at time $t = 0$. For each eigenstate the maximum value of the eigenvalue is set to one.

Probability density functions

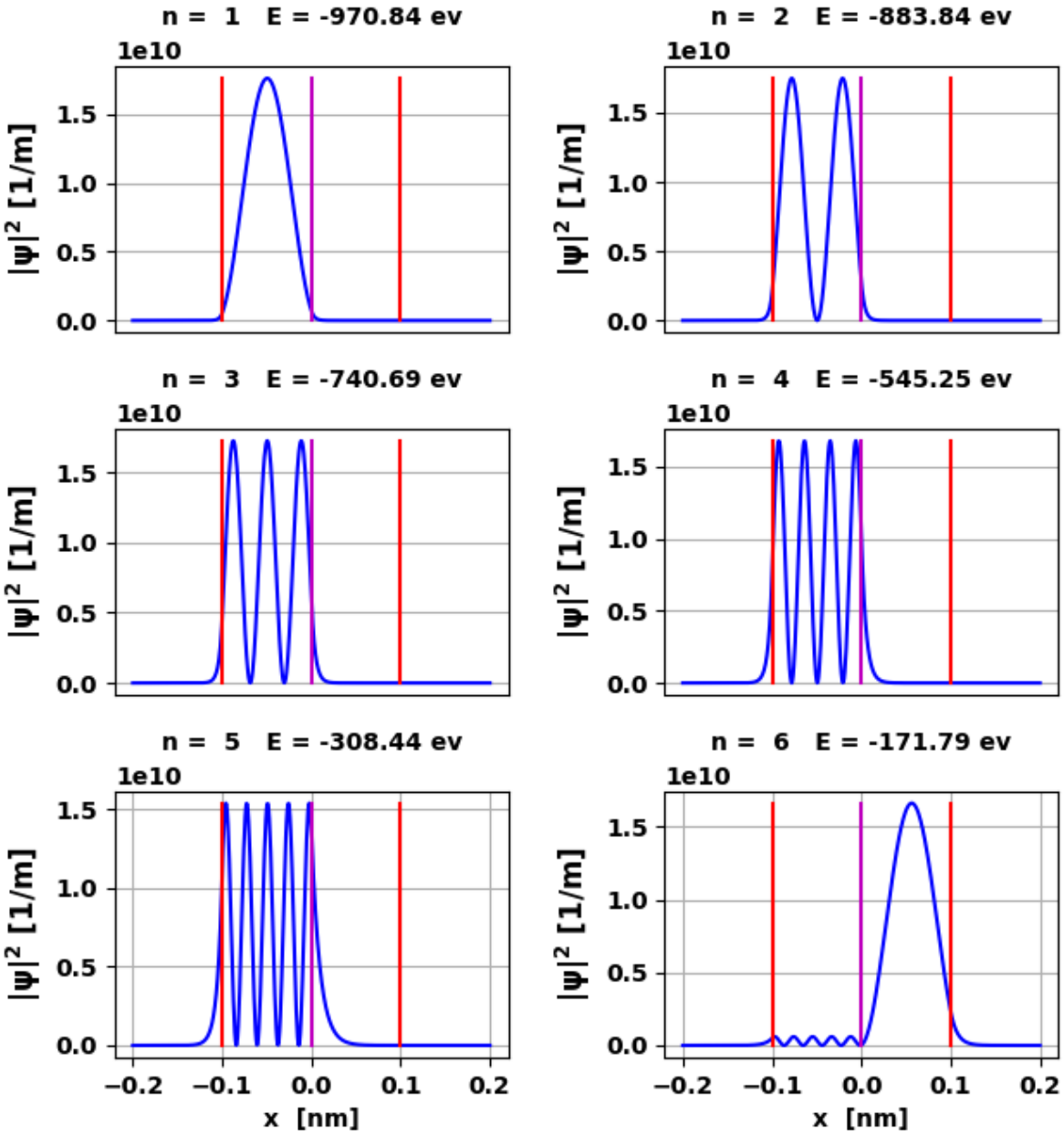

Fig. 3. Probability density function for the **finite square well with a step**. Area under curves is one since each eigenfunction has been normalized.

Quantum Interpretation: Eigenstate $n = 6$

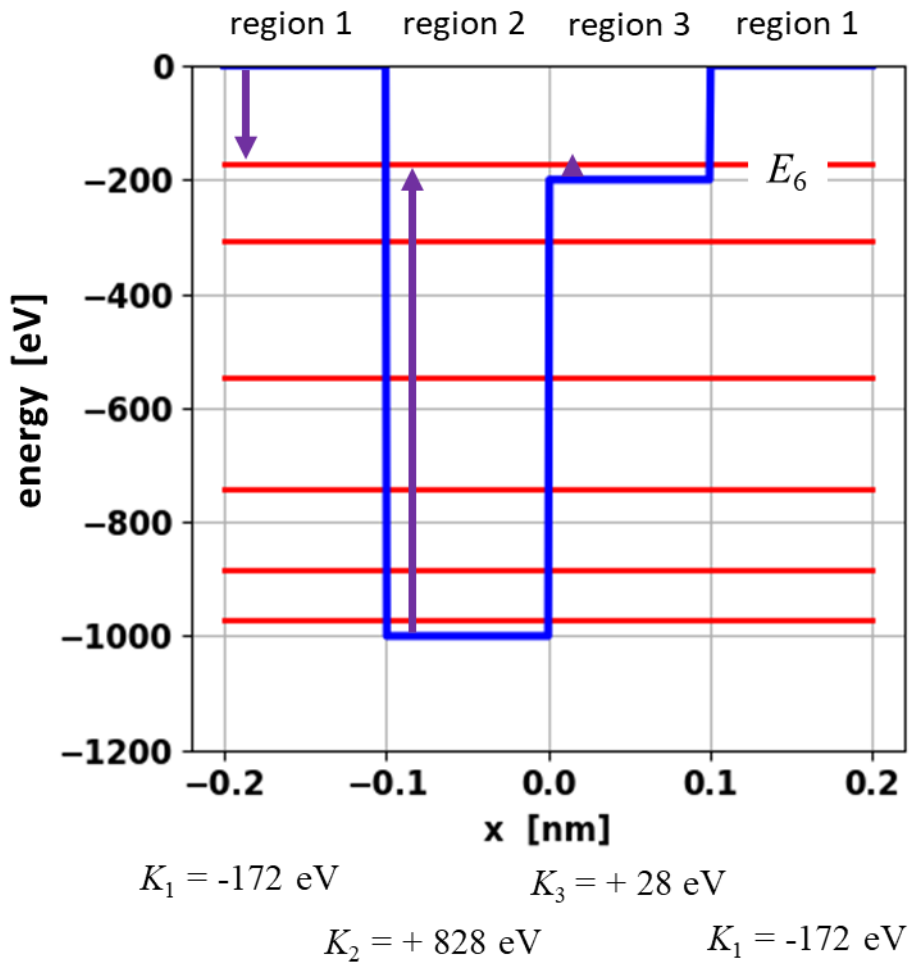

Fig. 4. Energy spectrum diagram and potential well with a step. Kinetic energies are for eigenstate $n = 6$.

In regions 1 the kinetic energy K_1 is negative and this is the classically forbidden region. However, on making a measurement on the system, there is a finite probability of finding the electron in this classically forbidden region due to the wave properties of an electron. The kinetic of the electron in region 2 is much greater than the kinetic energy in region 3 ($K_2 = 828$ eV > $K_3 = 28$ eV). Therefore, the

momentum $p_2 > p_3$, which means that $\lambda_2 < \lambda_3$ as shown in figure 2 for the state $n = 6$. The maximum of the eigenfunction occurs in region 3 and this is the region of the highest probability of finding the electron. This can be shown by considering the eigenfunction and its slope at the boundary between regions 2 and 3. We can consider the eigenfunction to be expressed as a sine function, then

$$\psi = A\sin\left(\frac{2\pi}{\lambda}x + \phi\right) \quad \frac{d\psi}{dx} = \left(\frac{2\pi}{\lambda}\right)A\cos\left(\frac{2\pi}{\lambda}x + \phi\right) = m$$

$$A\sin\left(\frac{2\pi}{\lambda}x + \phi\right) = \psi \quad A\cos\left(\frac{2\pi}{\lambda}x + \phi\right) = \frac{m}{2\pi}\lambda \quad m \neq 0$$

These equations can be squared and added to eliminate the phase ϕ to give the equation for the maximum value of A

$$A = \sqrt{\psi^2 + \frac{m^2}{4\pi^2}\lambda^2}$$

At the boundary, the eigenfunction ψ and its slope $m = d\psi / dx$ must be continuous function of x. So, at infinitesimal distances close to the step, the values of both ψ^2 and m^2 are equal in magnitude on either side, but the value of the wavelength changes discontinuously as the wavelength is greater in region 3 than region 2 $(\lambda_3 > \lambda_2)$. Therefore, the coefficient A increases with increasing wavelength, hence $A_3 > A_2$ as shown in figure 2 for $n = 6$.

This result of greater amplitude with larger wavelength is important because any potential energy function can be approximated by a series of step functions. This implies that for any potential energy function regions of smaller kinetic energy or smaller momentum and larger wavelength have larger maximum value of the amplitude of the eigenfunction than adjacent regions of larger kinetic energy or momentum and smaller wavelength.

In nonuniform potential wells the wavefunctions are not sinusoidal, but over a small part of the cycle, the potential energy does not change much, and so we speak loosely of a local “wavelength”.