DOING PHYSICS WITH PYTHON

QUANTUM MECHANICS

PARTICLES IN BOXES
[1D] SQUARE WELLS

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qm040.py **finite square well**

qm043.py **infinite square well**

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

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)

INTRODUCTION

A particle in a box refers to a system where the particle is confined to a limited region of space. Technological devices mainly made from semiconducting materials such as silicon and gallium that exploit the quantum behaviour of particles in boxes are becoming increasingly important. At the heart of many such devices is a tiny structure called a **quantum dot** that consists of a speck (~ 1 nm across and contain ~100 atoms) of one semiconductor embedded in a larger sample of another semiconductor material. The trapped electrons have wave like properties and occupy energy levels, just as electrons in atoms. Light emitting properties of quantum dots are used in solid state lasers (CD and DVD players), solar cells and as fluorescent markers used in biomedical applications are such a few applications.

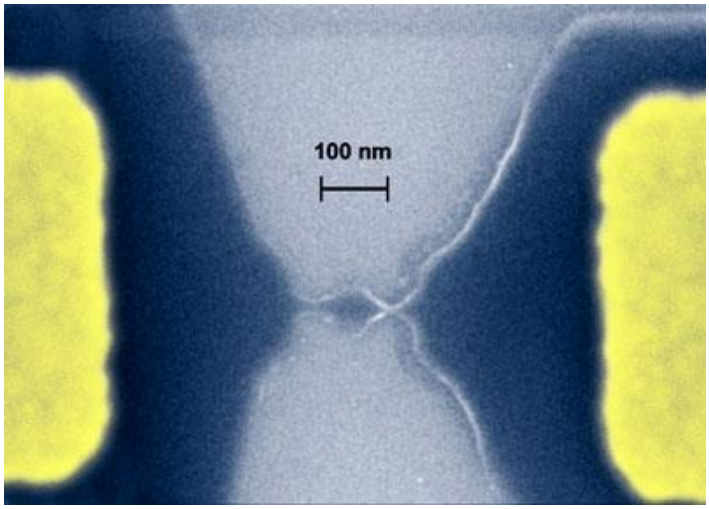

Fig. 1. Quantum dot carved from a graphene sheet

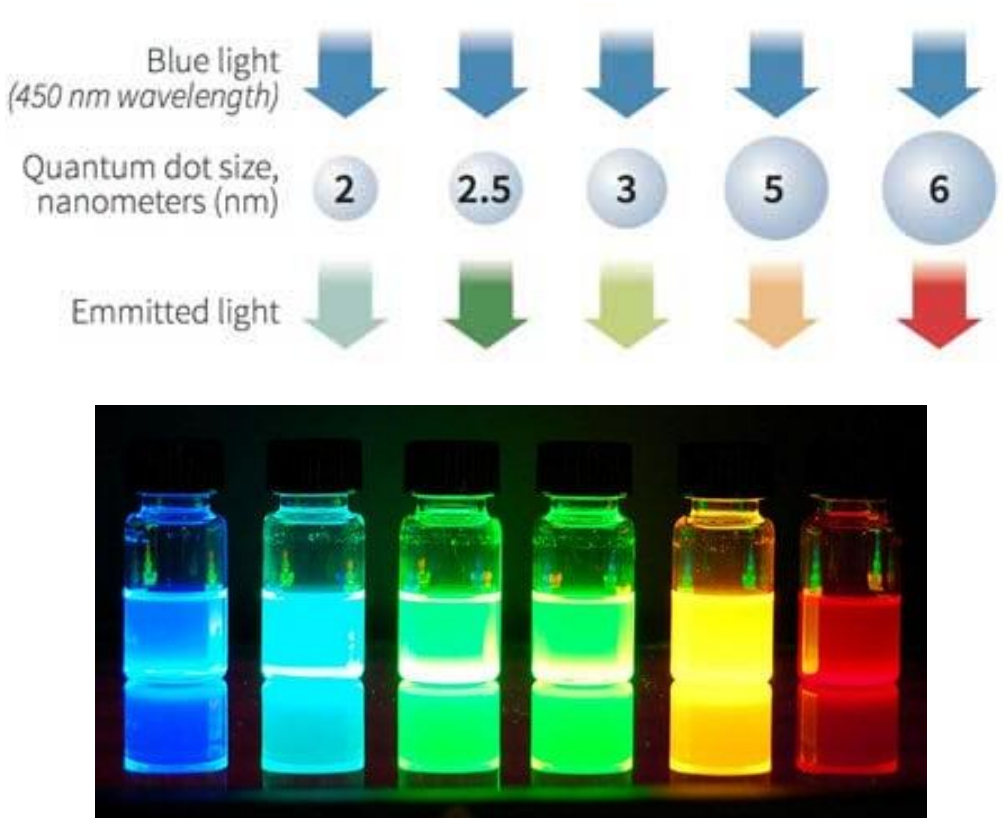

Fig. 2. Photoluminescence of alloyed CdS*x*Se1-*x*/ZnS quantum dots of 6 nm diameter. The material emits different colour of light by tuning the composition and the quantum dot size.

When a particle is confined in a limited region, quantum mechanics yields the predictions that:

- Only certain energy levels are possible.
- There is a zero-point energy, the lowest energy eigenstate. The particle can not have zero total energy.
- There is a finite probability that the particle can be found after a measurement of its position in a classical forbidden region where its kinetic energy is negative.
- The eigenfunctions are standing waves like the vibrations of a guitar string (same vibrations throughout the wave).
- The physical quantities of position and velocity are not defined. You can no longer refer to a moving particle when the particle is confined..

[1D] INFINITE SQUARE WELL

Our first well we will consider is the **infinite square well** of width L. The potential energy well responsible for trapping the electron has abrupt, infinitely high walls, but between the walls, the electron feels a zero-force acting on it. The potential energy function is

$$U(x) = 0 \qquad 0 \le x \le L$$
$$U(x) = \infty \qquad x < 0 \quad x > L$$

According to classical physics, the total energy of a trapped particle in a [1D] square infinite square well can have any positive constant value. Since the potential energy within the well is zero, the total energy is equal to the kinetic energy of the particle ($E = K + U$). Therefore, a non-zero kinetic energy means that the particle would be bouncing back and forth between the impenetrable walls. The region outside the well would never be penetrated by the particle. This region outside the well is called the **forbidden classical region**.

We will take an electron as the particle and consider its wave properties. The eigenvalues and eigenfunctions for the system of an electron trapped in the [1D] infinite potential well are determined by solving the Schrodinger equation with the boundary conditions that each eigenfunction must vanish at the boundaries (impenetrable well walls).

The energy eigenvalues are given by

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2 m_e L^2} = \frac{n^2 h^2}{8 m_e L^2} \qquad n = 1, 2, 3, \ldots$$

and the corresponding normalized eigenfunctions by

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n x \pi}{L}\right) \qquad 0 \le x \le L$$

$$\psi_n(x) = 0 \qquad \text{else where}$$

The eigenfunction is always zero at the boundaries of the box, and is also zero at *n*-1 points (nodes) inside the box. The de Broglie wavelengths for the particle in the box only depend upon the width of the box

$$\lambda = \frac{2L}{n}$$

and the spacing between adjacent nodes or between adjacent antinodes is $\lambda / 2$.

The stationary-state wave function for the eigenstate *n* is

$$\Psi_n(x,t) = \sqrt{\frac{2}{L}} \sin\left(\frac{n x \pi}{L}\right) \exp\left(\frac{-i E_n t}{\hbar}\right) \quad 0 \le x \le L$$

$$\Psi_n(x,t) = 0 \qquad \text{elsewhere}$$

Each eigenstate describes a **complex standing wave** (a wave that oscillates without propagating through space). The angular frequency ω_n, frequency f_n and period T_n of oscillation are

$$\omega_n = E_n / \hbar \quad f_n = E_n / h \quad T_n = h / E_n$$

The eigenfunctions are thus time dependent. However, the probability density function does not depend upon time

$$\left|\Psi_n(x,t)\right|^2 = \frac{2}{L} \sin^2\left(\frac{n x \pi}{L}\right)$$

where

$$\int_{-L/2}^{L/2} \left|\Psi_n(x,t)\right|^2 = 1$$

The eigenfunctions are orthogonal to each other

$$\int_0^L \Psi_{n_1}^{*} \Psi_{n_2} dx = 0 \qquad n_1 \neq n_2$$

Any wavefunction that satisfies the Schrodinger equation and the boundary conditions can be expressed as linear combination of the eigenfunctions

$$\psi = \sum_n a_n \psi_n \qquad \sum_a a_n^{\,2} = 1$$

Our classical particle with non-zero kinetic energy would just bounce back and forth between the impenetrable walls. But a “real” particle such as an electron does not behave as a classical particle when confined to volumes of atomic dimensions. One can no longer think about the particle as a moving particle since at nodal points there is zero probability of finding the particle. So, how can the particle travel through a node? The particle has no position or velocity before a measurement is made on the system, we only know the probability of locating the particle after the measurement is performed. Before the measurement is made, a particle in a state is described by its wavefunction. This wavefunction gives the most complete description that is possible of the system and it does not assign definite values to either position or velocity.

[1D] INFINITE AND FINITE SQUARE WELLS

reference finite square well

We will compare the eigenstates for an electron confined by finite square well potential where the top of the well corresponds to the zero of the potential energy function and the bottom of well has a negative energy value and the electron confined by an infinite square well.

We can make a comparison of the eigenvalues and eigenfunctions for the infinite square potential well and the finite square potential well by shifting the bottom of the infinite well is to -1000 eV. The width of both wells is $L = w =$ **0.100 nm**.

Energy spectrum: eigenvalues

eV	E_1	E_2	E_3	E_4	E_5	$E6$
infinite	37.6	150	338	602	940	1353
infinite	-962	-850	-662	-398	-59.9	+353
finite	-970	-881	-733	-530	-282	-19.6

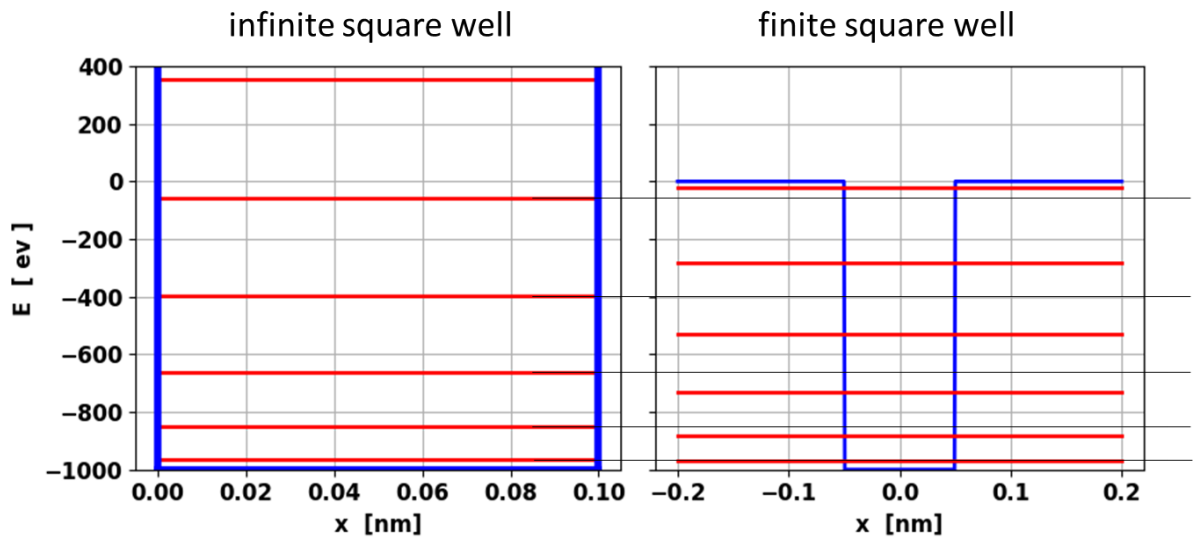

Fig. 3. Energy spectrum for the infinite and finite square wells for the first sixth states. The zero-point energy (lowest possible energy – **ground state**) is the eigenstate ***n* = 1**. The wavelength of an eigenfunction for the finite square well is somewhat larger than those of the infinite well. A longer wavelength corresponds to lower momentum and lower energy. Deep inside the wells, the eigenvalues for both wells are similar but there is increasing divergence towards the top of the finite well. When $E > 0$, the electron is no longer confined to the well, but acts as a free electron which can have a continuous range of total energy E. Thus, the number of bound states is finite, in this case there are only 6 eigenstates. The eigenstates where $n > 1$ are called **excited states**.

Eigenfunctions (eigenvectors)

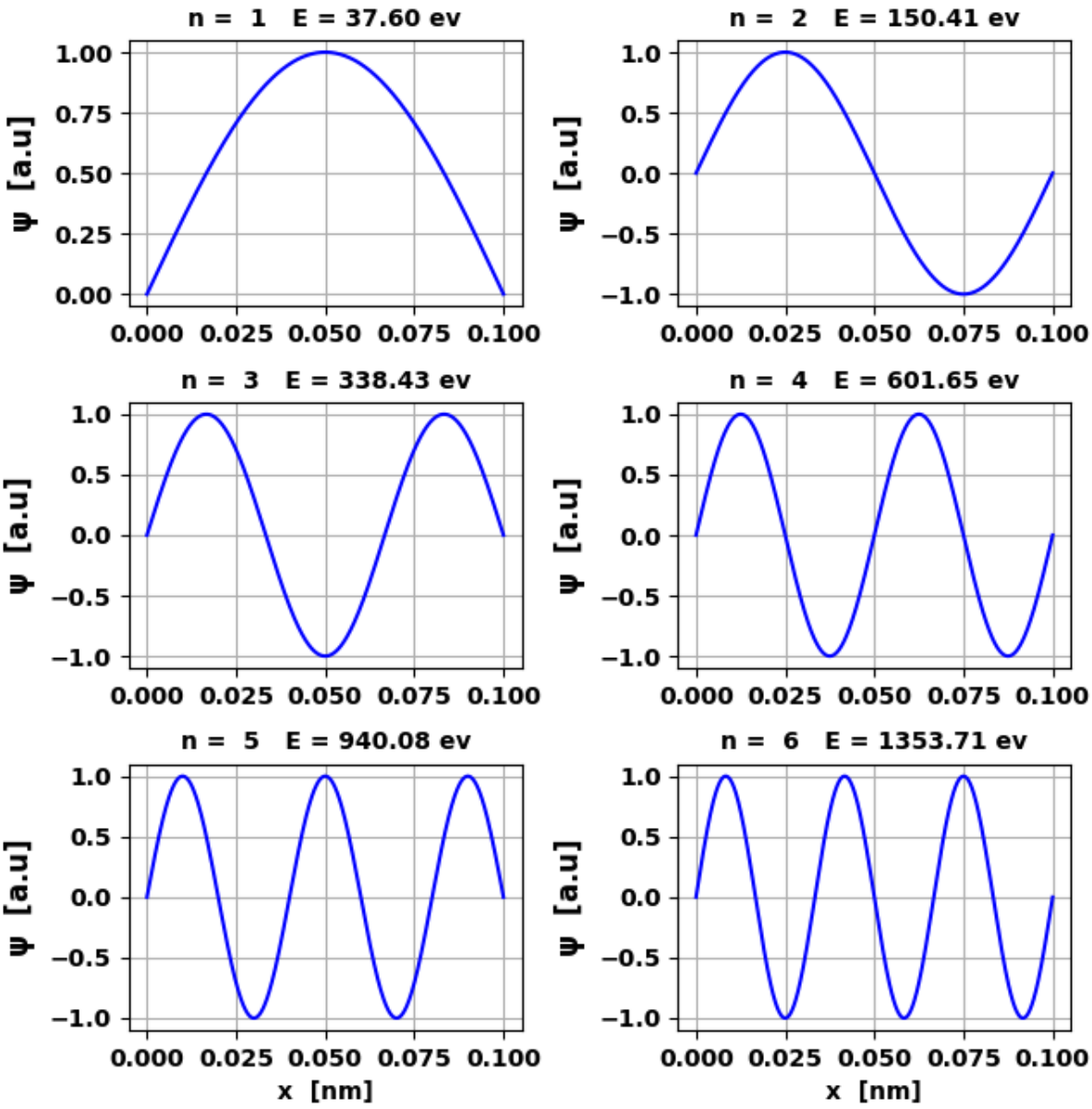

Fig. 4. Eigenfunctions for the **infinite square well** at time t = 0. For each eigenstate the maximum value of the eigenvalue is set to 1. The eigenfunction are sine functions with a value of zero at the boundaries $\psi(0) = 0 \quad \psi(L) = 0$. The eigenfunctions correspond to those of a vibrating string of length L with fixed ends.

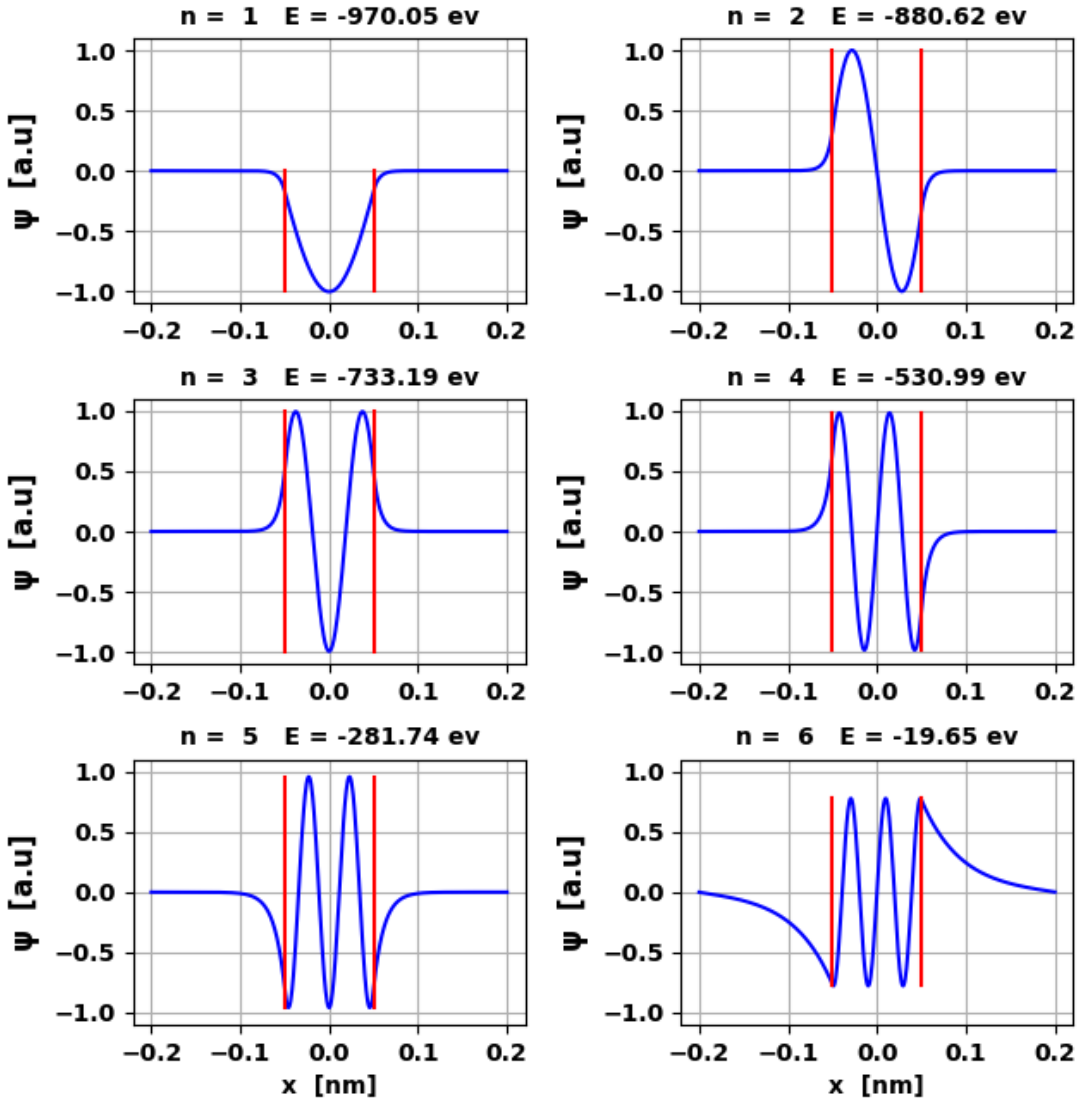

Fig. 5. Eigenfunctions for the **finite square well** at time $t = 0$. For each eigenstate the maximum value of the eigenvalue is set to 1. The eigenfunctions are not zero at the boundaries of the well. Inside the well, the eigenfunctions are sinusoidal but outside, the eigenfunctions are decreasing exponential functions. The eigenfunctions for the finite square well bear close resemblance to those of the finite square well, except that there is a small exponential tail outside the well, showing some penetration of the electron into the classically forbidden regions of negative kinetic energy.

Probability density functions

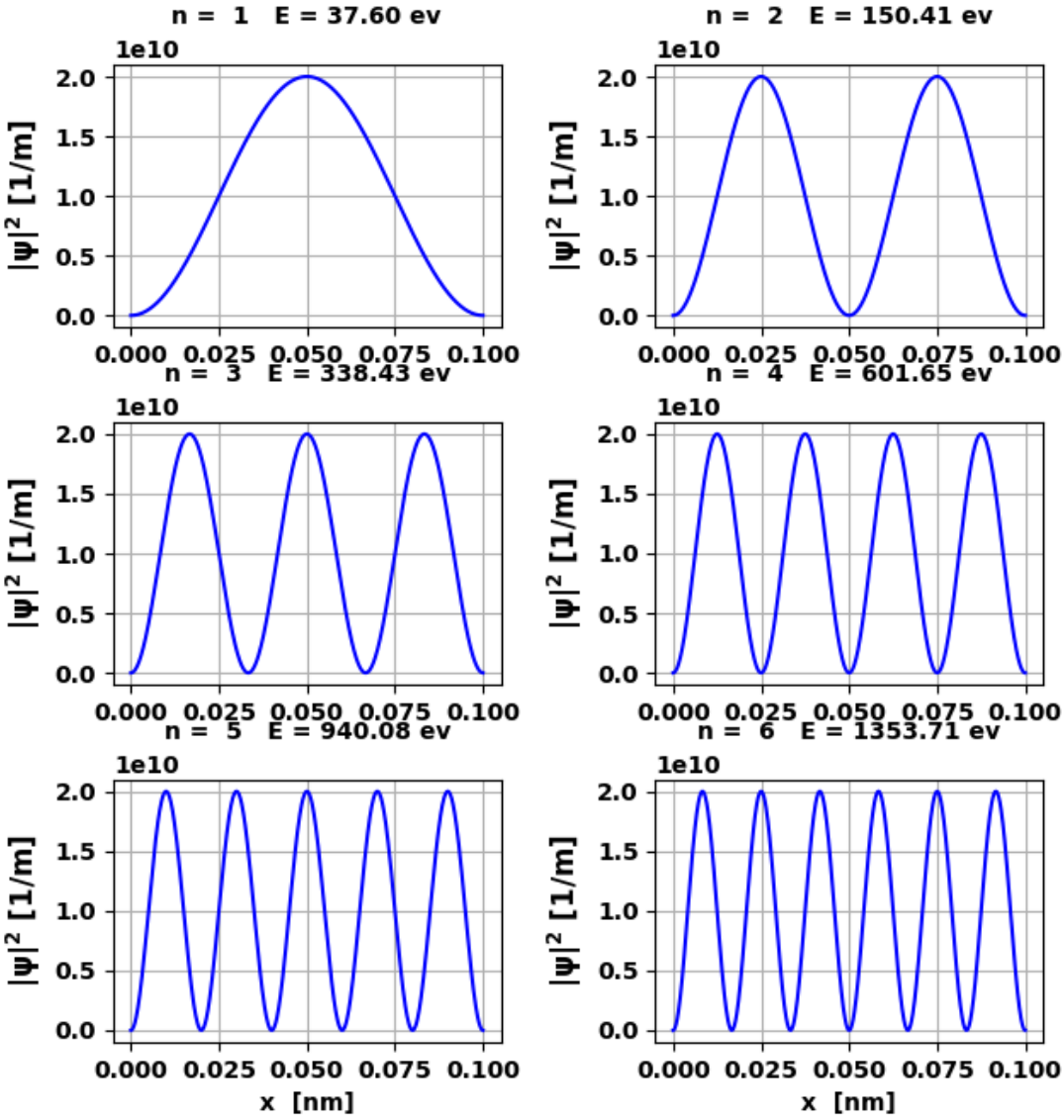

Fig. 6. Probability density function for the **infinite square well**. Area under curves is one since each eigenfunction has been normalized.

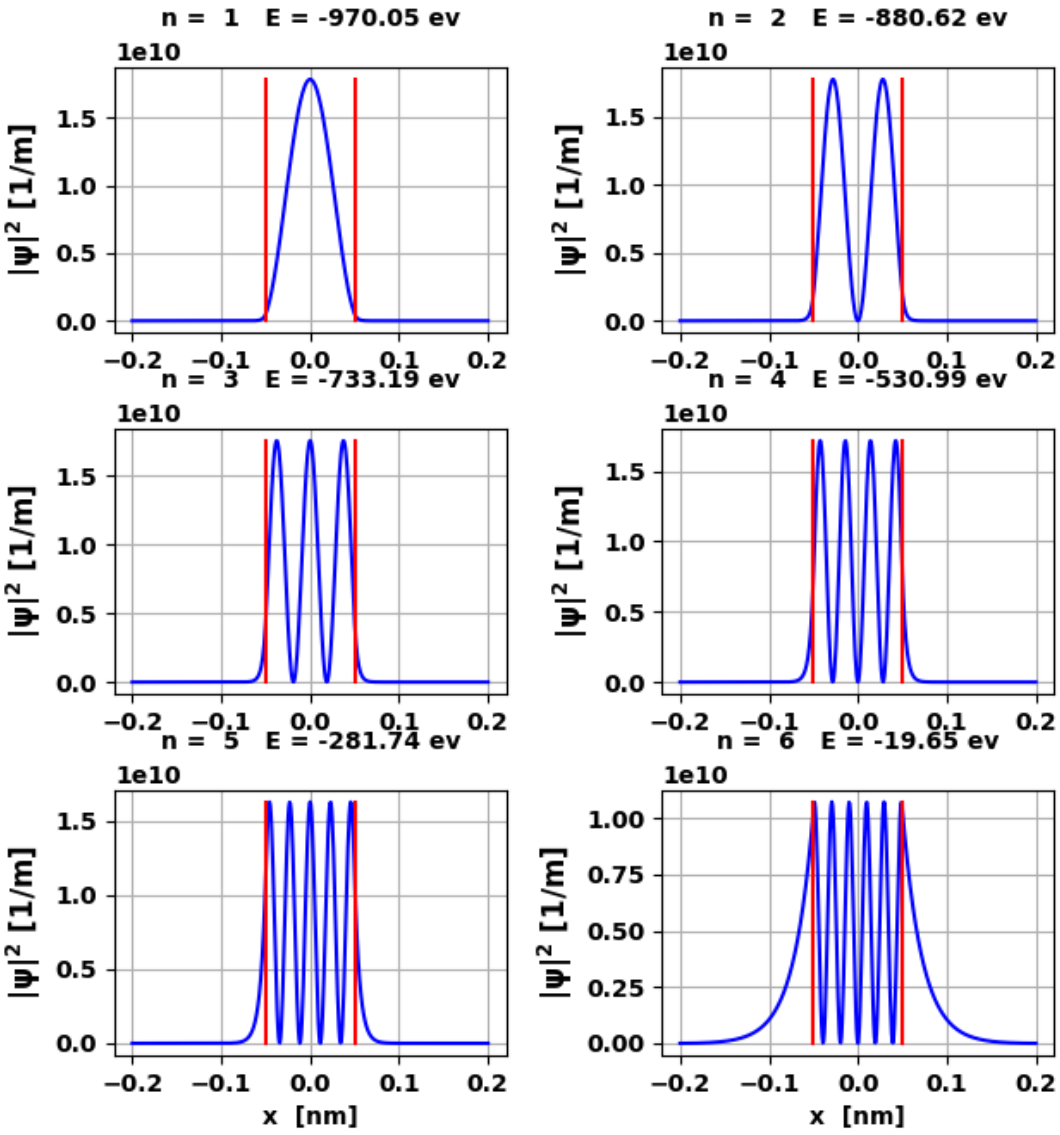

Fig. 7. Probability density function for the **finite square well**. Area under curves is one since each eigenfunction has been normalized. For the eigenstate $n = 1$ (ground state), the highest probability of finding the electron is at the centre of the well. This is in sharp contrast to classical physics which prediction gives the highest probability of finding the electron would be at the edges. In this instance, it is surprising that the electron "avoids" the edges.

We have not yet addressed the question about how our single electron emits a photon (electromagnetic) radiation. This will be discussed in another article.

Transitions between states

You can also model nuclear systems where the width of a well is in the order of femtometres and depths in the order of 50 MeV. For example, a proton is bound to the neutron by the strong nuclear force. Although this is a [3D] system, it is possible to model the deuteron involving a finite square well of depth 38.5 MeV occupying a spherical region of radius 1.63×10^{-15} m. One energy level is found (ground state) with this model, so there are no excited states. In this ground state, the eigenfunction extends far beyond the confines of the well giving a 50% change of finding a particle in a classically forbidden region and the expectation value for the separation of the two particles is 4×10^{-15} m.

I tried modifying Code **qm040.py** *to model the deuteron, but it did not work?*