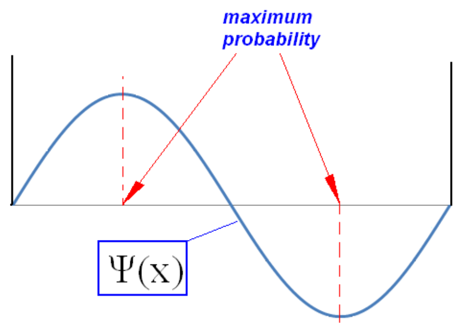
Modern Physics

Particle in a box

Problem 1.- Consider an electron confined to an infinite square wave potential. Assuming it is in the first excited state: sketch its wave function and indicate the places where it has the maximum probability of being found.

Solution:



Problem 2.- Consider a simple model of a quantum dot as a cubic box of side *L=15nm*. Suppose you trap 6 electrons in the dot that occupy the lowest possible energies. Ignoring all electron-electron interactions, but the Pauli Exclusion Principle, how much kinetic energy is stored in the dot?

Solution: You can place two electrons in the state that corresponds to $n_x = 1, n_y = 1, n_z = 1$ but the other 4 will have to go to the first excited state that has quantum numbers $n_x = 1, n_y = 1, n_z = 2$ or $n_x = 1, n_y = 2, n_z = 1$ or $n_x = 2, n_y = 1, n_z = 1$, since the energy is: $E = \frac{h^2}{8mL^2}(n_x{}^2 + n_y{}^2 + n_z{}^2)$ the total energy for the 6 electrons is:

$$Total\ E = \frac{h^2}{8mL^2}\left[2(1^2+1^2+1^2)+4(1^2+1^2+2^2)\right] = \frac{30h^2}{8mL^2}$$

In joules: $Total\ E = \frac{30h^2}{8mL^2} = \frac{30\times(6.62\times10^{-34}Js)^2}{8\times9.1\times10^{-31}kg\times(15\times10^{-9}m)^2} = 8.0\times10^{-21}J$

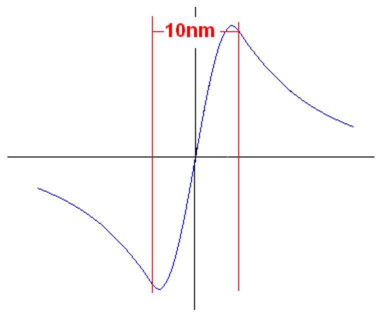
In eVs: $Total\ E = \frac{30h^2}{8mL^2} = \frac{30\times(4.14\times10^{-15}eVs)^2}{8\times511{,}000eV/c^2\times(15\times10^{-9}m)^2}$

$$Total\ E = \frac{30h^2}{8mL^2} = \frac{30\times(4.14\times10^{-15}eVs)^2\times(3\times10^8 m/s)^2}{8\times511{,}000eV\times(15\times10^{-9}m)^2} = 0.05eV$$

Problem 3.- The first excited state of an electron confined in a 1 dimensional box has energy of 3eV higher than the ground state. How much is the energy of the second excited state?

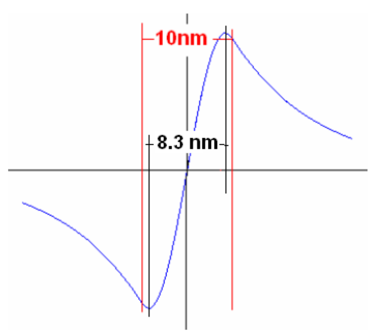
Solution: Particles in a one dimensional box have energies given by $E_n = n^2 E_1$, where $E_1 = \frac{h^2}{8mL^2}$, so the energy of the first excited state, which corresponds to *n=2* is $E_2 = 4E_1$, and the difference with the ground state energy is $E_2 - E_1 = 3E_1$.
The problem states that this difference is 3eV, so the energy of the ground state is 1 eV, then the second excited state that corresponds to *n=3* has an energy of **9eV.**

Problem 4.- An electron is confined in a square wave potential of length 10nm. Estimate the depth of the potential (in eV) to bind the electron in its first excited state as shown in the figure.



[Suggestion: you can estimate the de Broglie wavelength from the figure and then calculate the kinetic energy. To bind the electron the total energy will have to be negative.]

Solution: We can use a ruler to measure the wavelength of the function inside the trap. For example, measure the distance between the two peaks of the function (one negative the other positive) and use the width of the trap as your scale, the distance between the peaks is 8.3nm and that means that the wavelength is 16.5nm. $\lambda \approx 16.5nm$



Knowing the de Broglie wavelength allows us to calculate the kinetic energy of the particle, since:

$$K.E. = \frac{p^2}{2m} = \frac{\left(\frac{h}{\lambda}\right)^2}{2m} = \frac{h^2}{2m\lambda^2} = \frac{(4.135\times10^{-15}eVs)^2(3\times10^8 m/s)^2}{2(0.511\times10^6 eV)(16.5\times10^{-9}m)^2} = \textbf{5.53 meV}$$

To trap the electron, the total energy needs to be negative, which means that the depth of the trap needs to be at least 5.53 meV.

Note 1: in the above calculation, I used $m = \frac{0.511\times10^{6} eV}{(3\times10^{8} m/s)^2}$ for convenience, to get the answer directly in eV, but you can use $m = 9.1\times10^{-31} kg$ instead, being careful to use Js for the units of *h*.

Note 2: Notice that 5.53meV is less than $k_B T$ at room temperature ($k_B \times 300K \approx 26meV$).

Problem 5.- Consider a simple model of a quantum dot as a cubic box of side 5nm. Suppose you trap three electrons in the dot. Ignoring all electron-electron interactions but the Pauli Exclusion Principle, how much energy is stored in the dot?

Solution: The minimum energy of the three electrons will happen when two electrons occupy the ground state (two electrons because they can have spin up or down) and one electron occupies the first excited state. So, the quantum numbers would be:

$$Ground \quad state \rightarrow n_x = 1, n_y = 1, n_z = 1 \rightarrow E = (1^2 + 1^2 + 1^2)E_o = 3E_o$$
$$First\ excited \quad state \rightarrow n_x = 2, n_y = 1, n_z = 1 \rightarrow E = (2^2 + 1^2 + 1^2)E_o = 6E_o$$

The total energy for the 3 electrons will be $2\times3E_o + 6E_o = 12E_o$, where $E_o = \frac{h^2}{8mL^2}$, and given the value given in the problem:

$$E_o = \frac{(4.135\times10^{-15} eVs)^2 (3\times10^{8} m/s)^2}{8(0.511\times10^{6} eV)(5\times10^{-9} m)^2} = 0.015 \text{ eV}$$

The total energy is 12×0.015 eV = **0.18 eV**

Problem 7.- Consider a simple model of a quantum dot as a cubic box of side *L*=6nm. Suppose you trap 4 electrons in the dot that occupy the lowest possible energies. Ignoring all electron-electron interactions, but the Pauli Exclusion Principle how much kinetic energy is stored in the dot?

Solution: The minimum energy of the four electrons will happen when two electrons occupy the ground state (two electrons because they can have spin up or down) and two electrons occupy the first excited state (you can put up to 6 electrons in that first excited state due to its degeneracy). The quantum numbers would be:

$$Ground \quad state \rightarrow n_x = 1, n_y = 1, n_z = 1 \rightarrow E = (1^2 + 1^2 + 1^2)E_o = 3E_o$$
$$First\ excited \quad state \rightarrow n_x = 2, n_y = 1, n_z = 1 \rightarrow E = (2^2 + 1^2 + 1^2)E_o = 6E_o$$

The total energy for the 4 electrons will be $2\times 3E_o + 2\times 6E_o = 18E_o$, where $E_o = \frac{h^2}{8mL^2}$,

The total energy is then:

$$E = 18\left(\frac{h^2}{8mL^2}\right) = 18\frac{(6.62\times 10^{-34}\,Js)}{8(9.1\times 10^{-31}\,kg)(6\times 10^{-9}\,m)^2} = \mathbf{3\times 10^{-20} J}$$

Problem 7a.- Consider a simple model of a quantum dot as a cubic box of side *L*. Suppose you trap 4 electrons in the dot that occupy the lowest possible energies. Ignoring all electron-electron interactions, but the Pauli Exclusion Principle how much kinetic energy is stored in the dot?

Solution: The minimum energy of the four electrons will happen when two electrons occupy the ground state (two electrons because they can have spin up or down) and two electrons occupy the first excited state (you can put up to 6 electrons in that first excited state due to its degeneracy). The quantum numbers would be:

$$Ground \quad state \rightarrow n_x = 1, n_y = 1, n_z = 1 \rightarrow E = (1^2 + 1^2 + 1^2)E_o = 3E_o$$
$$First\ excited \quad state \rightarrow n_x = 2, n_y = 1, n_z = 1 \rightarrow E = (2^2 + 1^2 + 1^2)E_o = 6E_o$$

The total energy for the 4 electrons will be $2\times 3E_o + 2\times 6E_o = 18E_o$, where $E_o = \frac{h^2}{8mL^2}$,

The total energy is then **$18E_o$**

Problem 8.- Calculate the ground state and the first excited state kinetic energies of an electron confined to a one-dimensional square well potential of 90nm length.

Solution:

Ground state: $E_1 = 1^2 E_o = \frac{h^2}{8mL^2} = \frac{(6.62\times 10^{-34}\,Js)^2}{8(9.1\times 10^{-31}\,kg)(90\times 10^{-9}\,m)^2} = \mathbf{7.43\times 10^{-24}\ J}$

First excited state: $E_2 = 2^2 E_o = \frac{4h^2}{8mL^2} = \mathbf{2.97\times 10^{-23}\ J}$