ENGINEERING PHYSICS

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Concept of degeneracy

Class #31

- We will first discuss the case of a 3D infinite potential well and then take the 2D well
- The well we have is a cubical well. We will later see what will happen if we destroy the cubical symmetry

Infinite potential well, 3D

Let us look at the eigen energies, $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$

Remember that n_x, n_y, and n_z can take values 1,2,3,….

The lowest energy is given by $E_{111} = \frac{3h^2}{8ma^2}$

The next energy is $E_{211} = \frac{6h^2}{8ma^2}$*. We also have* $E_{121} = \frac{6h^2}{8ma^2}$ *and* $E_{112} = \frac{6h^2}{8ma^2}$

Now we need to know that (211), (121) and (112) do not represent the same state.

*However, their energy values are same. This in quantum mechanics is referred to as **DEGENERACY** .*

Infinite potential well, 3D

How do we know that (2,1,1), (1,2,1) and (1,1,2) represent different states. One way is to write the eigen functions (taking limits of the well as $-\frac{a}{2} < x < \frac{a}{2}, -\frac{a}{2} < y < \frac{a}{2}$ *and* $-\frac{a}{2} < z < \frac{a}{2}$ *:* $\psi_{211} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)\cos\left(\frac{\pi}{a}z\right)$

$$\psi_{121} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \cos\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}y\right)\cos\left(\frac{\pi}{a}z\right)$$

$$\psi_{112} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \cos\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right)$$

They are different

Infinite potential well, 3D

We could also take the limits as : 0 < x < a, 0 < y < a and 0 < z < a. The eigen functions then are

:

$$\psi_{211} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)\sin\left(\frac{\pi}{a}z\right)$$

$$\psi_{121} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}y\right)\sin\left(\frac{\pi}{a}z\right)$$

$$\psi_{112} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)\sin\left(\frac{\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right)$$

They are different again

Infinite potential well, 3D

We recognize a pattern here. Refer to the expression: $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$

If $n_x = n_y = n_z$ then corresponding to the energy, we have only 1 state – NO DEGENERACY

If $n_x = n_y \neq n_z$ or $n_x \neq n_y = n_z$ or $n_x = n_z \neq n_y$ then we have 3 states for the given energy – TRIPLY DEGENERATE

If $n_x \neq n_y \neq n_z$ then we have 6 states corresponding to the given energy – SIX FOLD DEGENERATE

The number of degenerate states for the given energy is referred to as the degree of degeneracy

Infinite potential well, 2D

Now let us go to the 2D infinite potential well and look at the eigen energies.

We have $E_{n_x n_y} = \frac{(n_x^2+n_y^2)h^2}{8ma^2}$

As before the energy is quantized. The lowest energy is given by $E_{11} = \frac{2h^2}{8ma^2}$

The next energy is $E_{21} = \frac{5h^2}{8ma^2}$*. We also have* $E_{12} = \frac{5h^2}{8ma^2}$

The DEGENERACY aspect shows up as well.

Are (2,1) and (1,2) the same state? Let us look at the eigen functions

Infinite potential well, 2D

For the well defined by $-\frac{a}{2} < x < \frac{a}{2}, and\ -\frac{a}{2} < y < \frac{a}{2}$

$$\psi_{21} = \sqrt{\frac{2}{a}} sin\left(\frac{2\pi}{a}x\right)\sqrt{\frac{2}{a}} cos\left(\frac{\pi}{a}y\right)$$

$$\psi_{12} = \sqrt{\frac{2}{a}} cos\left(\frac{\pi}{a}x\right)\sqrt{\frac{2}{a}} sin\left(\frac{2\pi}{a}y\right).$$

Different again

Quiz: Kindly prove it for the well defined by 0 < x < a and 0 < y < a

Infinite potential well, 2D

Now to get the degree of DEGENERACY we note the following:

If $n_x = n_y$, we have only one state for a given energy

If $n_x \neq n_y$ we have two states for a given energy

Therefore, we see whether we take the 3D or 2D well DEGENERACY is definitely present.

Can we destroy degeneracy? Well yes and one of the ways you could do it is make the dimensions of the well slightly different. How will this affect the energy levels?

Infinite potential well, 3D

$$E_{n_x n_y n_z} = \frac{(n_x^2 + n_y^2 + n_z^2)h^2}{8ma^2}$$

How will the expression change if the dimensions are different. Taking the dimensions as a_x, a_y and a_z we have

$$E_{n_x n_y n_z} = \left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right)\frac{h^2}{8m}$$

Now let us see what happens to the states (2,1,1), (1,2,1) and (1,1,2)

$E_{211} = \left(\frac{4}{a_x^2} + \frac{1}{a_y^2} + \frac{1}{a_z^2}\right)\frac{h^2}{8m}$, $E_{121} = \left(\frac{1}{a_x^2} + \frac{4}{a_y^2} + \frac{1}{a_z^2}\right)\frac{h^2}{8m}$ and $E_{112} = \left(\frac{1}{a_x^2} + \frac{1}{a_y^2} + \frac{4}{a_z^2}\right)\frac{h^2}{8m}$

Are they the same?

You could do the same exercise with a 2D well.

electrons in a 3D Infinite potential well

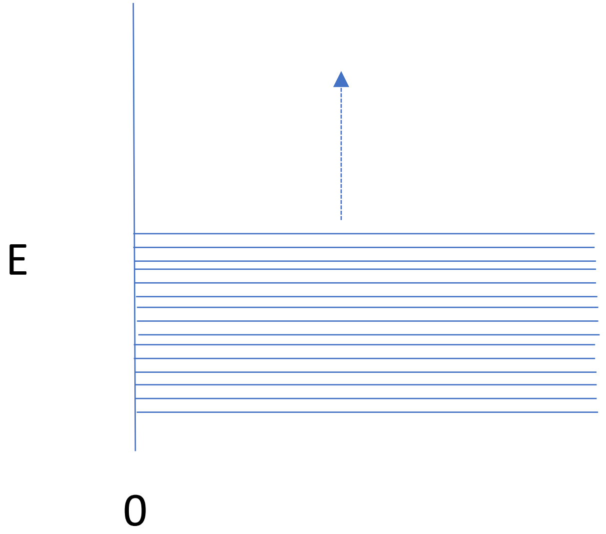
So far, we described the 3D infinite potential well without any reference to which particles being present in the well. In fact, the energy expression $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$ **is really the energy of the entities present in the well**

Now let us put electrons inside the well (these electrons are "free")and then describe the system

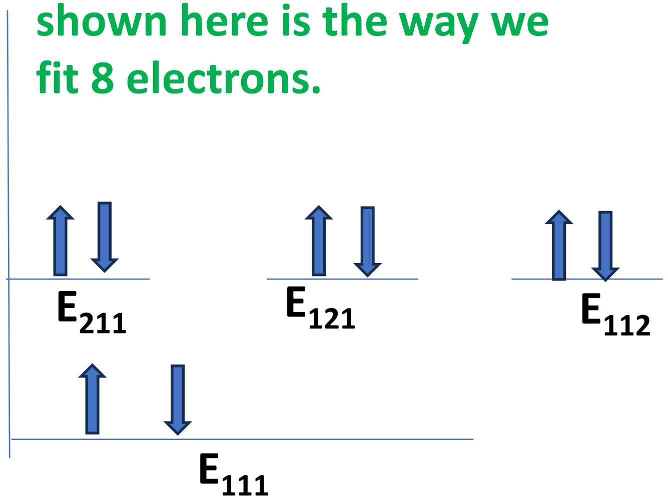
First we represent the energy levels using a simple diagram

electrons in a 3D Infinite potential well

Energy levels for electrons



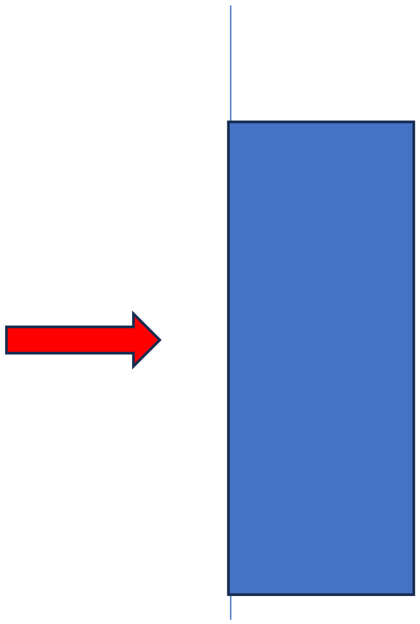
Showing first two energy levels for electrons. For a given level 2 electrons with opposite spins can fit in. shown here is the way we fit 8 electrons.



electrons in a 3D Infinite potential well

If the dimensions of the well increase, then two things happen

- *The energy levels shift to lower values*
- *The separation between the energy levels reduce*
- *Thus, what appears is the set of energy levels very close to each other as if they are continuously distributed. This may be considered as a band of energies.*



electrons in a 3D Infinite potential well

We are interested in knowing the energies of all the electrons as the behaviour of the system depends on this.

How do we do this?

First let us imagine that the 3D infinite potential (we will call this 3D box) well is empty. We then start filling it in till the last electron occupies an energy level.

This is similar to arranging students in classroom where we consider the benches as energy levels.

electrons in a 3D Infinite potential well

If you are given the task of arranging students in a classroom and you do not have access to information about how the classroom looks inside, the questions that will come to your mind are :-

1. How many benches are present in the classroom?
2. How many students can be present per bench?

If this concept is now applied to our 3D well, we need information about the number of available energy levels and the rules for placing electrons in them.

In the next class this will be discussed in detail

Class #31 …….. Quiz….

An electron is placed in a cubical 3D box and we have the degenerate states (2,1,1), (1,2,1) and (3,1,1). Which of the following is a reason as why the (2,1,1), (1,2,1) and (1,1,2) are different states of the electron?

- ❑ The integers refer to the linear momentum of the electron
- ❑ The integers refer to the spin of an electron
- ❑ The integers refer to the angular momentum of the electron
- ❑ The integers do not refer to anything else apart from the energy.

THANK YOU