

Biophotonics
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Lecture - 6
Nature of Matter - Part 1

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Hello, and welcome. So, we shall continue our discussion on biophotonics and this time, we are going to discuss about the nature of matter. Light and matter interacting, interaction between them is all about biophotonics; biophotonics deals with this, specifically, biological matter. So, it makes sense that we understand a little bit of the nature of matter per se.

So, this is also pretty basic high-school level. Anyone who has been to high school should be actually knowing it. So, if you think that you are too good to know about the basic of matter, I ask you to skip this part, we shall see you when the actual hardcore biophotonics starts.

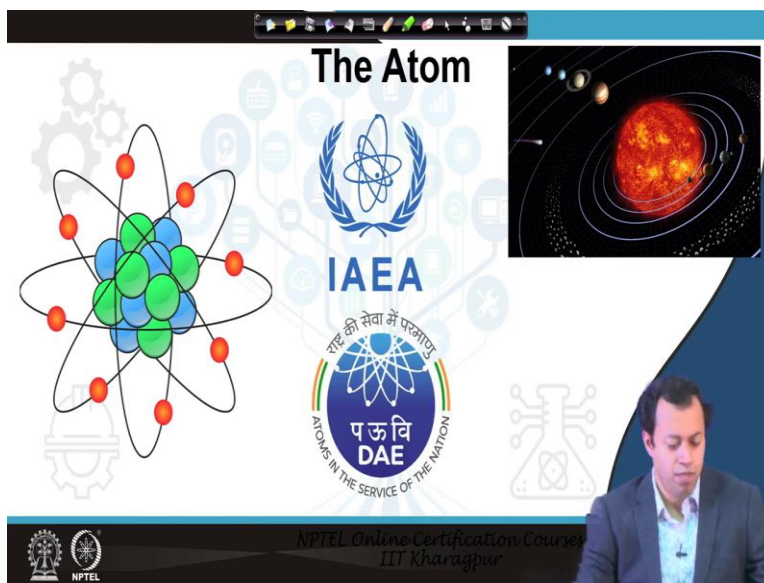
This is merely a revision and a refreshment of something that I assume you already know but might have forgotten with a long practice of something else. For example, if you are electronics engineer at final year or third year perhaps you are too busy writing codes as such; if you are a doctor, you have been dealing with patients; if you are a life-science person from a non-medical background, probably you are involved in cell culture.

So, it is my way of refreshing what you already know plus in my experience, basic concepts are something which everyone thinks that they already know but once you start probing them, you

find out that perhaps they have memorized the concepts in school and with dis-usage have completely forgotten it.

So here we go. Today, we are going to discuss about the nature of matter and every single person who have been to school knows that matter is made up of atom.

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Atoms are these indivisibles, that is what atom stands for; indivisible particle which cannot be divided. However, later it was found that it can actually be divided. It contains this nucleus which contains the nucleus contains positively charged protons and neutral charge neutrons and it has negatively charged electrons running in this specific circular or elliptical path. I consider them as train tracks.

You have train tracks around the nucleus of an atom just like your rail moves in the rail line in a specific path, a specific path has been fixed. According to this particular image, atoms have exactly same thing. You have these paths like orbits, rail lines, or train tracks around the nucleus through which the electrons move very much like a rail carriage or a train.

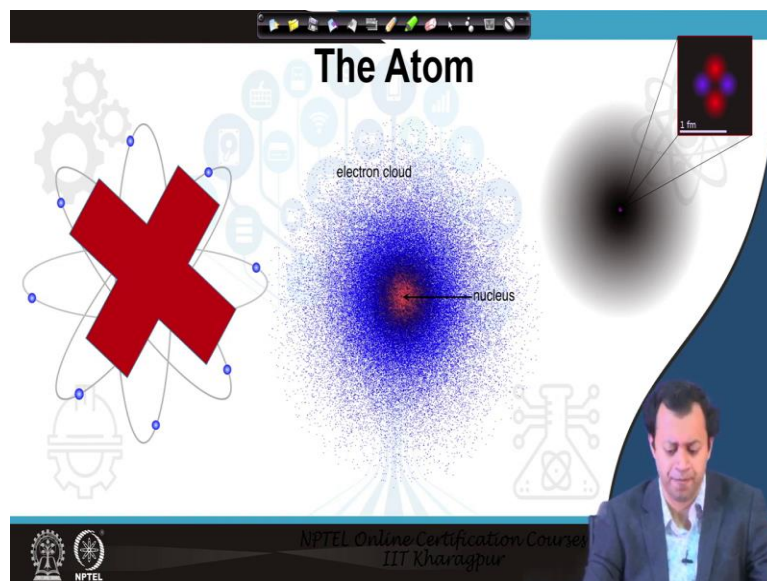
And this image is embedded in our head. We all have it everywhere, anybody who kind of thinks of atom, this is the image that usually pops up in their mind. And you have seen this image being represented in very, very prestigious agencies.

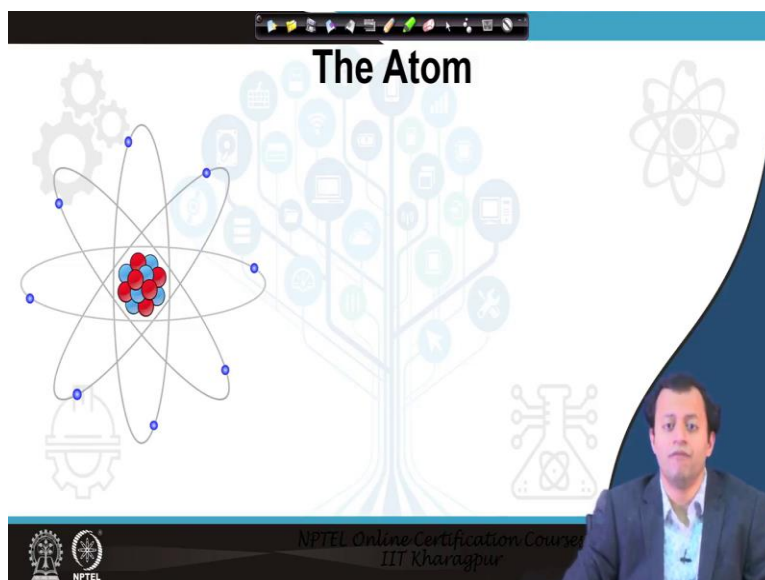
For example, these two agencies; International Agency of Atomic Energy, which is part of United Nation, they also do this train-tracked like things where you have the nucleus and the electrons are moving around.

This is the Indian Department of Atomic Energy and you see these kinds of train-tracks type things, a fixed path, through which electrons around the nucleus move and the entire system, entire system forms the atom very, very much like our solar system.

You have the sun and you have fixed path through which different planet mercury, Venus, earth, Mars, Jupiter, Saturn, they move and life is good.

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Well, there is a small problem and that is it is completely wrong. It is completely, totally, absolutely wrong. Atoms are not like this. The electrons around the nucleus does not move in a fixed path, it moves in orbitals. Though the term sounds similar to orbit, but orbitals and orbit are completely different thing. This image is so, so very, very wrong. Therefore, we are going to reject this all total.

Except for the part where nucleus is made up of protons and neutrons and some other fundamental particles, the electrons do not move in a fixed path around the nucleus. More or less, the schematic diagram, of the atom, could be considered like this where at the center there is a nucleus granted, nucleus is made up of the same thing as I discussed previously, and then there is a probability distribution, there is an electron cloud around it.

Now, understand what I am going to say very, very carefully. There is a probability distribution of electrons around the nucleus. There is uncertainty in its position. So, I will give you couple of analogies so that this gets embedded in your head, you are never going to forget it.

Suppose, I have a nucleus containing neutrons and protons and I have put a CCD camera near it. The CCD camera is monitoring this nucleus 24/7 and every time there is a movement of an electron around it, it takes picture. Well, it takes picture anyways even if there is no electron movement but it takes picture through a large period of time.

After gathering all the pictures for a large period of time, say, for example, 10 years, 20 years, 30 years, 40 years, we come to some kind of a probability distribution that the electron mostly stays

in this, this, this area and as we move around from the nucleus, as we move away from the nucleus, there is less chance of finding an electron.

So, there is no specific fixed path like the train tracks, the rail lines that you saw in previous pictures, the rail lines that you saw in previous pictures. Remember, Heisenberg's uncertainty principle you cannot actually have position and speed together.

If you have a rail track like this, if you have a rail track like this, then it is very easy to pinpoint the location of an electron. You know the speed, you know the time, you know the distance, you figure out the position no problem.

However, here it is merely a probability distribution, a prediction, or a forecast that it might be present in this particular place. I will give you an analogy. Suppose, I have fixed a camera in my backyard. I have fixed a camera in my backyard and it is taking picture of the weather, it is taking picture of the outside world, it is taking picture of the sky and everything around it for continuously.

For 10 years, every single day, this camera has monitored my backyard. And when I have compiled the overall data for 10 years, say, starting from the year 2010 to 2020, I have compiled the data of every day, how my backyard looks like or how the weather in my backyard looks like, I have seen 7 out of 10 years, there was rain at 10 a.m. on July the 10th.

Understand what I am saying. I have compiled the data from the camera that has continuously clicked images for 10 years from the year 2010 to 2020, and I have seen that 7 out of 10 years, not consecutively, randomly distributed 7 out of 10 years, there was rain at 10 a.m. on 10th July.

Now, I am being asked will in the year 2021 or 2022, will there be rain on 10th July at 10 a.m. What will be your answer? Can you say 100 percent yes? You will say chances are. There is a probability for all those data that I have collected, all those data that I have collected for the past 10 years not more than that, it says, 7 out of 10 times it has happened.

Does it mean that there is a guarantee that it is going to happen in the next year? There have been three instances where it has not. What outcome is going to happen in the coming year depends on so many different factors but at the same time, we need to accept that there is an uncertainty associated with it.

There is an uncertainty associated with it, we cannot with 100 percent guarantee predict that there will be rain at that specific time, specific location in that specific year. We have to have some kind of uncertainty associated with it. So, the distribution of the electrons around a nucleus in an atom has uncertainty associated with it. We can make only predictions just like weather forecast.

Ask yourself this question, how many times you have listened in the news that next day there is going to be a 90 percent chance of rain, and next day when you have gone out with an umbrella in your hand, you have seen there is no rain.

So, what happened, what exactly happened? It was a forecast, it was uncertainty that was associated with; 90 percent possibility, there is a high chance of rain but maybe, just maybe there is not going to be any rain that specific day.

I am emphasizing on this so that it becomes absolutely clear that whenever we talking about atoms or electrons or sub-atomic particles as such, you cannot, cannot guarantee. You can have, you can make some kind of bold prediction that in the month of July sometime from 10 a.m. to 10 p.m., there could be rain; the probability of that happening is quite high.

But when you are actually fixing it, actually pinpointing it, 10 a.m., 10th July will there be rain? Your probability distribution or your uncertainty increases significantly. And that is what the essence of atom is.

We know electron is present, we know the electron will be near about somewhere in this area just like in the month of July, sometime there will be rain. But predicting the exact time, exact position, exact location, exact speed is near impossible.

In fact, these are even better images of atoms where you will see that this is the nucleus which contains, this is schematic basically, your protons and neutrons around and there is this electron cloud surrounding it. There is this electron cloud surrounding it and nowhere any of this looks like this train track, rail line orbit type things moving around.

This has to be made absolutely clear. If you have understood this, it will be very easy in the coming sense. Several of you already know it, I understand but I am just, as I said, refreshing it.

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The Schrödinger Equation

"I don't like it, and I'm sorry I ever had anything to do with it."
Erwin Schrödinger on probability interpretation of quantum mechanics

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So how exactly are we going to predict? If we are going to predict anyways, there is a 70 percent chance of finding electron, 90 percent chance, 100 percent; 100 percent will not happen, 20 percent, 30 percent; how are we going to predict it? We are going to predict it by this thing called the Schrodinger equation.

Now, for the love of god, medical student or life-science students do not switch off now by hearing the term Schrodinger equation. I am going to derive it, I am just going to mention it and I am going to tell you how it is useful, how you can utilize it in your day-to-day biology. So, do not worry, do not switch it off, this is my request.

First, let me tell you a little bit more about this gentleman called Erwin Schrodinger, the Austrian Irish physicist. He was quite famous, got Nobel prize in Physics in 1933 for writing the Schrodinger equation. And almost all of you must know about the Schrodinger cat experiment, the thought experiment which we wrote to Einstein that quantum superposition unless I open the box, I will not know whether the cat is dead or alive.

So, unless the box is open, the cat is both dead and alive at the same time. It is a thought experiment, he thought it is a ridiculous, you know, thought experiment which he was thinking but actually, it became extremely popular in, you know, popular culture, you see tattoos and t-shirts of Schrodinger wave equation.

He basically tried to derive this probability of finding an electron around the nucleus. He derived several mathematical formulas, several mathematical questions, several mathematical

expressions which gives us the probability distribution which predicts or which forecasts more or less where is the possibility of finding an electron around the nucleus is.

And there is obviously uncertainty associated with it, there is obviously something counter-intuitive associated with it. For example, this concept of something both dead and alive, both on and off, we are utilizing it in quantum computers these days.

But when Erwin Schrodinger was asked what he himself thinks about quantum mechanics this was his answer, I do not like it, and I am sorry I ever had anything to do with it. Read a little bit about Erwin Schrodinger, he had a very, very colorful life, he was working at various different universities.

He was a known opponent of Nazism. Because of that, he was sacked from his job as a physics professor from University of Graz, Austria. He went to various universities in Ireland and maybe a bit in America.

What you probably do not know that while he was sacked from his job and he was put under house arrest and then he fled from Nazi Germany to Italy with his wife, he was actually given the position of a Chair of Physics in University of Allahabad in British India. And he accepted it but to the best of my knowledge, he did not join.

Erwin Schrodinger born as a Lutheran but had huge interest in Vedanta philosophy, he was influenced by Schopenhauer and he wrote a seminal book after getting Nobel prize and after doing all of this Nobel prize on what is life where he dabbled or where he questioned or where he tried to see biology from an engineering or a physics point of view, where he tried to see how genes can pass information from organism to organism.

So anytime, if you yourself question that I am a physics person, why I am studying biology, or if you find yourself asking this question that I am a biologist, why do I need to go for Schrodinger equation, remember these giants, these titans, Schrodinger himself worked on biology, he was interested how information is passed through organism to organism genetically.

The scientists Watson and Crick who developed the, who discovered basically DNA, write how their work was influenced by Erwin Schrodinger's own thought process, Erwin Schrodinger's book. Even Richard Feynman, the father of nanotechnology, while working in Caltech has

worked little bit on genetics. So, every time you find yourself doubting why I should be doing this or should I be doing this, being a physicist, should I be learning about biology or being a biologist, should I dabble in quantum mechanics, remember if you do, if you so choose to do, you will be in great company.

You will be in the company of some of the titans, some of the giants who did not see the difference between physics, maths, and biology and all these boundaries. They basically bridge the boundary to look what is in the other side.

Anyways enough history, let us discuss a little bit about Schrodinger equation. I promise you I will make it as easy as it is possible.

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The slide is titled "The Schrödinger Equation". It features several icons: gears, a lightbulb, a tree, a hard hat, and a circuit board. The main equation is
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x)$$
 labeled "Time independent Schrodinger equation". Below it, text states: "The simplest example is a particle (say electron) in free space so, $V(x) = 0$, Therefore, the time-independent Schrödinger equation is". This is followed by the simplified equation:
$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi(x)$$
. At the bottom left is the NPTEL logo and "Reference 1,2". At the bottom right is a video feed of a man in a suit. The footer text reads "NPTEL Online Certification Courses IIT Kharagpur".

So, Schrodinger equation basically deals with the ψ function. This is a time-independent Schrodinger equation which simply means that the timing part is omitted or removed or we are not considering the time.

What we are considering is the position or the probability distribution of a sub-atomic particle or a very, very small particle having specific amount of potential energy and specific amount of kinetic energy, what are the distribution with it.

Now, here if his needs to be told that Schrodinger wave equation is mostly for very small particles, particles which have a dual nature. You all must know by this time light has a dual

characteristic, it is both wave and particle, and subatomic particles like electrons also have a particle and a wave nature.

So, this is mostly to deal with the dual nature particles, particles who have less mass and therefore, their wave nature is prominent do not apply Schrodinger wave equation to me or yourself as what position you will find me by solving the Schrodinger wave equation So, do not worry if you do not fully understand it. This is the time-independent Schrodinger equation, I will tell you what this. So $\psi(x)$ or ψ , as a hardcore physicist would like to say; $\psi(x)$ is the probability distribution of finding a particle at location x . m is the mass, \hbar is the reduced Planck's constant. Planck's constant E is equal to $h \nu$, \hbar is $\hbar/2\pi$ and this is the double differentiation.

$V(x)$ is the potential energy, so a particle, say, an electron moving with a potential energy $V(x)$. The probability distribution is given by this particular function where E is the total energy. E is the total energy of such a particle and this $\psi(x)$ is the overall distribution, the probability, the wave function; the wave function of that particle.

What does wave function mean? Wave function simply means the probability of amplitude. The quantum state of its existence, whether it will be present or not present; the probability, not definite but the probability. The probability of the amplitude, the probability of this happening. So, the probability distribution is given by this formula.

In the simplest example, in the simplest example that we are going to consider now, hydrogen atom, the elementary element, we say that the potential energy is considered 0. This is $V(x)$ term is considered 0, thereby you get the overall distribution, the overall wave function coming up to be very, very simple with this.

Remember, m is mass, \hbar is the reduced Planck's constant, E is energy, and $\psi(x)$ is the probability distribution.

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The Particle in a Box

Inside the box, the Schrodinger equation needs to be solved with the following conditions

$$V(x) = 0$$

$$\psi(x) = 0 \text{ at } x = 0 \text{ and } x = l$$

These condition can be satisfied by choosing

$$\psi(x) = \sin kx, \text{ for any value of } k$$

For $x = l$,

$$\psi(l) = 0 = \sin kl = \sin n\pi$$

Therefore, $kl = n\pi$, or $k = \frac{n\pi}{l}$

Final solution of total energy E in this case turns out to be

$$E_n = \frac{n^2 h^2}{8ml^2} \text{ for } n = 1, 2, 3, 4, \dots$$

Handwritten notes in red:

- $n = 1, 2, 3$
- $E_1 = \frac{1^2 h^2}{8ml^2}$
- $E_2 = \frac{2^2 h^2}{8ml^2}$
- $E_3 = \frac{3^2 h^2}{8ml^2}$
- $E_4 = \frac{4^2 h^2}{8ml^2}$
- $E_5 = \frac{5^2 h^2}{8ml^2}$
- $E_6 = \frac{6^2 h^2}{8ml^2}$
- $E_7 = \frac{7^2 h^2}{8ml^2}$
- $E_8 = \frac{8^2 h^2}{8ml^2}$
- $E_9 = \frac{9^2 h^2}{8ml^2}$
- $E_{10} = \frac{10^2 h^2}{8ml^2}$
- $E_{11} = \frac{11^2 h^2}{8ml^2}$
- $E_{12} = \frac{12^2 h^2}{8ml^2}$
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- $E_{18} = \frac{18^2 h^2}{8ml^2}$
- $E_{19} = \frac{19^2 h^2}{8ml^2}$
- $E_{20} = \frac{20^2 h^2}{8ml^2}$

Reference 1,2

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Now, we consider the very easy. You have learnt it, I know but indulge me, I am going to repeat it again. We are going to consider it that we have restricted the particle, say, an electron in a potential well. What does that mean? So basically, we were trying to create how an electron will behave around a nucleus.

So, if this is the nucleus and there is an electron moving around it in whatsoever manner, there is some amount of conditions that needs to be fulfilled for this electron to keep on moving rather than collapsing into the nucleus or drifting away.

There has to be a specific demarcated area, an overall area where there is a chance that the electron will survive either getting drifted away or falling collapsing into the nucleus. Because remember, nucleus is positively charged, the electron is negatively charged. If electron comes too close to the nucleus, obviously, the nucleus will accept it.

The nucleus will attract it and it will fall into the nucleus and it will get destroyed or it will form neutron or whatever. Or if the electron is too far away from the nucleus, there is very little connection, very little force of attraction between these two. And thereby there is no effect, no interaction whatsoever.

So, we need to ensure that the presence of an electron is in a boundary; is in a boundary. If it is going out of the boundary, say, if there is the nucleus here, if it is going close to the nucleus, it will fall into it and we do not know what happens or if it goes away from the boundary, if it gets

away from too much from the nucleus, the nucleus has no effect on it and the electron will simply drift away.

So, we have restricted the movement of the electron in this two-dimensional box which has a length of l , suppose. Suppose these two directions are infinite, is an infinite potential well and you have put a particle, supposedly electron, because we are modeling electron around it.

When you have put conditions such as this that the distribution of electron is 0 at x is equal to 0, there is no electron present here. Probability of electron at the nucleus is 0 and the probability of finding electron outside this particular boundary is also 0, you come to a particular solution.

You come to a particular solution, I am not doing to give you the solution any high-school modern physics books will give you the entire derivation, just go through it and you will know what I am actually talking about.

But when you have inputted these conditions, these boundary conditions, you will find out that the necessary condition for this to satisfy is $\sin kx$ for any value of k which happens to be $\sin n\pi$ where π is radian remember π is 180 degrees where n is any integer number 1, 2, 3, 4, 5 and putting all of this into the equation that you previously saw, gives us the energy, the total energy of an electron existing inside a boundary condition is this.

Now, what does that mean, what exactly is the interpretation? I am giving you certain amount of derivations. So, what does this actually means? What means is since n is equal 1, 2, 3, 4 whole numbers per se; why is my pallet coming as pink?

So, since n is equal to 1, 2, 3, 4, etc., remember this. This n is equal to 1, 2, 3, 4, you have $E_1 = (1)^2(h)^2/8ml^2$. $E_2 = (2)^2(h)^2/8ml^2$ and so on, and so forth which means what again? Which means simply this.

Like I said in the previous lecture, you can only get discrete values of energy since n is 1, 2, 3, 4, there is no correct solution other than this. There is no other solution for Schrodinger wave equation when you have put into this boundary condition. So, therefore, $\omega_1 \omega_2 \omega_3$ or $\nu_1 \nu_2 \nu_3$, etc. There is no $E_{1.25}$ or $E_{2.234}$, this thing does not exist.

Moral of the story. Moral of the story, when you have put electron in a boundary condition, it further restricts itself into allowed and disallowed states; it quantized itself. When electron has put in a specific, specific boundary condition, it restricts itself into discrete levels.

Just like you have a ladder, there is nothing in between a ladder, you have to put your feet either here or here or here or here; when you have put some kind of condition onto an electron, imagine yourself as the electron and the ladder as your path.

You can only stay or you can only put your foot in the steps of the ladder which are specific, which are quantified. There is nothing in between them, there is allowed state, that is the steps and then there is disallowed states that is in between.

This is your E_1 , E_2 , E_3 , and so forth. There is no such thing as $E_{1.5}$, 1.25, 1.18. It is discrete number, it is whole number; n is a whole number. If obviously n is 0, then everything collapses. But it is 1, 2, 3, 4, meaning the energy levels of an electron around a nucleus is most definitely quantized.

So, there are specific energy level, specific distribution that we somewhat understand, somewhat predict but there is still uncertainty associated with it that at a specific time, at a specific location, we understand it should be somewhere at energy level 1 or somewhere at energy level 2 but pinpointing it at this particular position at length x_1 at time t_1 is impossible.

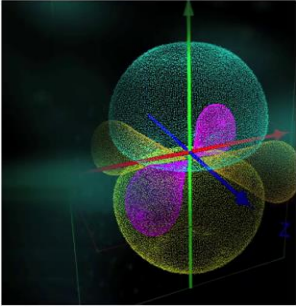
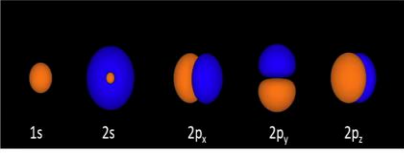
This is something that you have to understand, this is something it is very basic. Several of you already knew it but it is my interpretation or my way of telling you what this has been.

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The gap ΔE between two successive levels E_n and E_{n+1} can be given as

$$\Delta E = (2n + 1) \frac{h^2}{8ml^2}$$

Quantized State of Atoms



So, therefore, when we are looking for gap between two successive levels E_n and E_{n+1} we get this particular value. This is the gap, this is the energy gap between E_1 and E_2 or any successive energy levels.

And when we are actually trying to find out from a complex mathematical calculation how the electron will be distributed, what are its probability function, what would be its energy around a nucleus, we get these orbitals.

Orbitals again are the probable path, the probable volume, the probable area that the electron may take with 90 percent certainty. With 90 percent certainty, there is always going to be an uncertainty level associated and these are the orbitals that you can find 1s, 2s, 2px, 2py, and 2pz.

We are going to discuss little bit more about that because remember, the previous example that we saw, it was a very, very easy example or an idealized case with only length existing and the height is infinite. The particle in a box is a very easy example but an atom is a three-dimensional structure. It is spherical and several different forces are working on it so that probability distribution of the electron around it is also going to be not straight lines but these kinds of circular or dumbbell-shaped or bun-shaped structures.

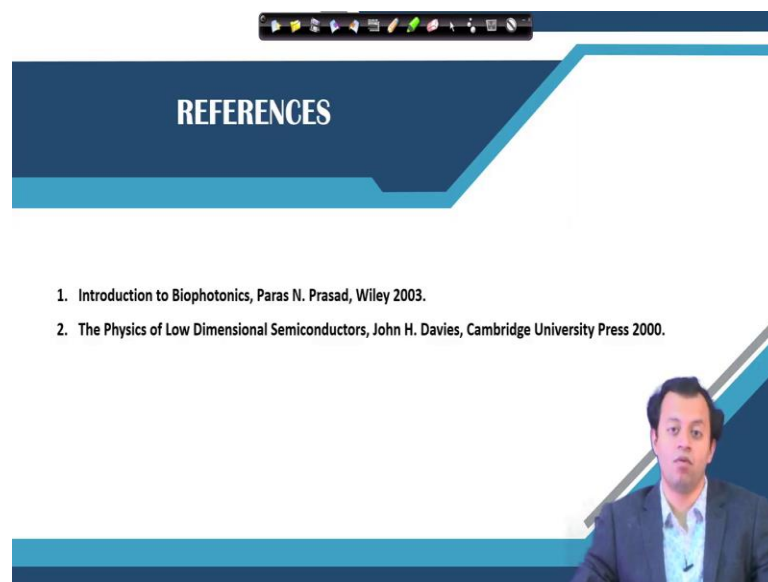
The more you go, the different orbitals, higher orbitals, d-type, f-type they become more and more complicated. And thereby, the quantized state of atoms happens, this is probably the

example, a schematic of some of this probability distribution of electrons around an atom, around a nucleus.

So, at the center, there is the nucleus and this is the probability distribution, this is overall the probability distribution of electrons of different energy levels, different distribution. Now, you know already why this image is not used.

Everybody uses the previous image with the train-tracks type thing running around the nucleus and it is manifested everywhere. That is much more sleek, compact, and a beautiful image as compared to this. But if you are me, every time you see an image of an atom represented like that with train tracks running around, you will scoff off.

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So, we are going to stop here for today and from tomorrow onwards, in the next lecture, I am going to discuss bit more about how atoms form bonds. So, thank you, I hope that it was not very complicated.

I hope it was not extremely easy if you have found it extremely easy and waste of time, then I am sorry, but I have to start from this level and slowly we will go and take a much more complicated and much more complex topic in the coming weeks.

So, do not worry, we are going to discuss a bit more about atoms and quantized state of matter in the latter class. Thank you very much.