Quantum Chemistry of Atoms and Molecules
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Lecture-7
Particle in a Box: Part II

We are discussing particle in a 1D box and we have succeeded in so far learning about the wave functions of a quantum particle in a one dimensional box and the wave functions had turned out to be sine waves.

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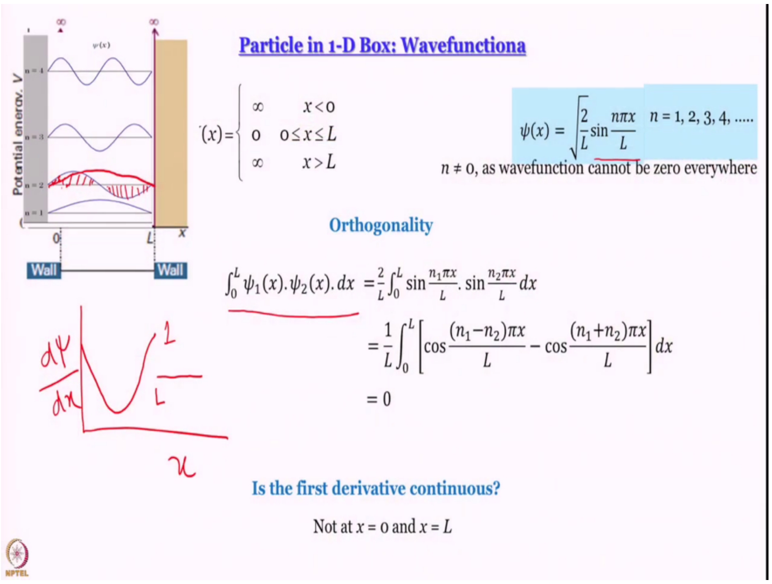

Particle in 1-D Box: Wavefunctiona

$$(x)=\begin{cases}\infty & x<0\\ 0 & 0\le x\le L\\ \infty & x>L\end{cases}$$

$$\psi(x)=\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \quad n=1,2,3,4,\ldots..$$

$n \neq 0$, as wavefunction cannot be zero everywhere

Orthogonality

$$\int_0^L \psi_1(x).\psi_2(x).dx = \frac{2}{L}\int_0^L \sin\frac{n_1\pi x}{L}.\sin\frac{n_2\pi x}{L}dx$$

$$= \frac{1}{L}\int_0^L\left[\cos\frac{(n_1-n_2)\pi x}{L}-\cos\frac{(n_1+n_2)\pi x}{L}\right]dx$$

$$= 0$$

Is the first derivative continuous?

Not at $x = 0$ and $x = L$

And we have seen that only some will be allowed. The wave function that we have established so far our Psi at a Psi of x is equal to root over 2 by L sine n PI x by L where n equal to 1 2 3 4 so on and so forth positive integer and we have established that this set of wave functions well we have normalized that is how we got root 2 by L. We have also established that they are orthogonal to each other that is where we stopped in the last module.

And we have also shown that the first derivative is not continuous at x equal to 0 and x equal to L. So, that really is not such a stringent condition on a wave function. The next step is to understand what are the energies? Since only certain wave lengths are only certain wave functions are allowed only certain energies will be allowed as well let us see how we get to that.

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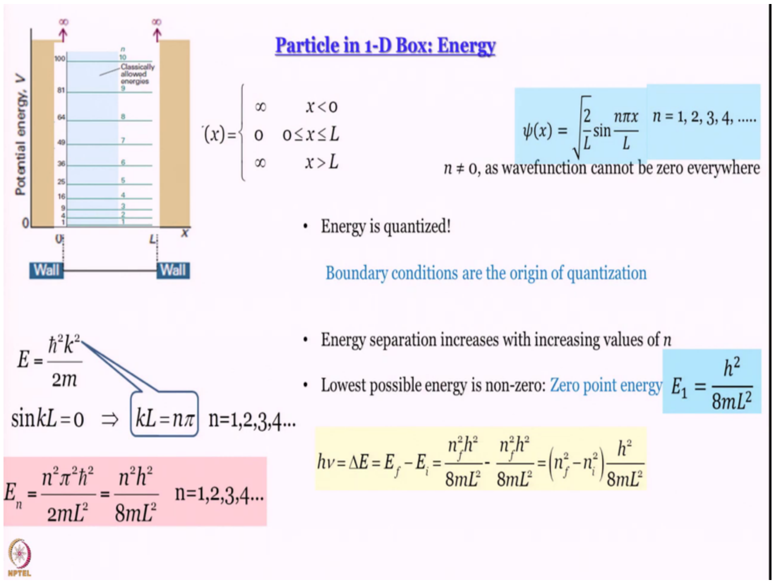

Particle in 1-D Box: Energy

$$(x)=\begin{cases}\infty & x<0\\ 0 & 0\le x\le L\\ \infty & x>L\end{cases}$$

$$\psi(x)=\sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \quad n=1,2,3,4,\ldots..$$

$n \neq 0$, as wavefunction cannot be zero everywhere

- Energy is quantized!

Boundary conditions are the origin of quantization

$$E=\frac{\hbar^2k^2}{2m}$$

$$\sin kL=0 \;\Rightarrow\; \boxed{kL=n\pi} \quad n=1,2,3,4\ldots$$

$$E_n=\frac{n^2\pi^2\hbar^2}{2mL^2}=\frac{n^2h^2}{8mL^2} \quad n=1,2,3,4\ldots$$

- Energy separation increases with increasing values of n
- Lowest possible energy is non-zero: Zero point energy $E_1=\frac{h^2}{8mL^2}$

$$h\nu=\Delta E=E_f-E_i=\frac{n_f^2h^2}{8mL^2}-\frac{n_i^2h^2}{8mL^2}=\left(n_f^2-n_i^2\right)\frac{h^2}{8mL^2}$$

This here is the expression for energy for a free particle if you remember and this is the energy that our particle would have as long as it is inside the box and it can be only inside the box E equal to h cross square k square by 2m. But then we have also learned from the boundary condition that Psi must vanish at x equal to L that kL is equal to n PI and n is a positive integer. So, the obvious next step is to take this scale in equal to n PI expression and plug it in to the energy expression of a free particle.

The moment we do that the energy expression becomes E of n is equal to n square h square by 8 mL square where n is a positive integer. What just happened? Well quantization of energy happened. Now we are saying that only certain values are allowed and now we should say something that we deliberately did not say while discussing the wave functions in the last module. What is n? n turns out to be a quantum number for the particle in a box.

And this is the beauty of Schrodinger's treatment unlike Bohr's treatment where the quantum numbers fell from the sky quantum numbers arise naturally simply from the probabilistic interpretation of the wave function provided by Max Born. Here we are seen an example of energy like energy other quantities like momentum angular momentum these are also quantized and everything arises from the imposition of some boundary condition or the other so now we learn a very, very important lesson in quantum mechanics.

We learn that quantization finds its origin in the boundary conditions which we know arise out of Born interpretation this is very important to understand I have seen many students who have got any say in chemistry good mark and all but and they can do the math associated with quantum mechanics. But this very fundamental concept has sometimes not sunk in. Let us all be very clear about this, this is a one of the founding tenets of founding principles of quantum mechanics that quantization really arises out of boundary conditions.

The moment that happens we can breathe easy now our conscience is clear we have not imported a quantum number from anywhere just to satisfy some experimental observation somewhere. It has arisen naturally out of boundary condition. This is a great revelation but that is not all. What we see in particle in a box is that look at the energy ladder the separation in energies increases as you go higher and higher up.

That is one thing. The second thing is another important observation zero energy is not possible because the smallest value of n the quantum number is one and for that energy has a value of h square divided by 8 mL square which is nonzero this brings us to the concept of zero-point energy and this is something that becomes a governing factor when we discuss simple harmonic oscillator. We find that a free particle a quantum free particle can never be at rest.

And it can never be at rest because if it is at rest is going to violate uncertainty principle. Let us see it comes to rest it would have come to rest at some position. So, x is defined precisely delta x is 0 and since it has come to rest completely the momentum is also 0 plus minus 0, so Delta x into Delta px is 0 that violates uncertainty principle. Uncertainty principle we are going to talk a little more about uncertainty principle later on when we take a break from these quantum mechanical systems and discuss the operators and demonstrate uncertainty principle nicely using the position and momentum operators.

But then the thing is uncertainty principle is a law of nature it is a boundary beyond which one cannot probe nature. So, it is not a question of making a better equipment that will let us see something you cannot see today we can never do it as far as the current understanding of quantum mechanics is you cannot do better than the best. You cannot violate uncertainty principle and that is why a free particle can never be at rest because that would violate uncertainty principle since it would be associated with zero uncertainties of conjugate properties that is an another important revelation from particle in a box.

Now let us talk about the energy gaps between successive levels, what about that? If you take any energy gap well right now it is E f - E i so n f square – n i square let us say I take n f Square to be n i square + 1 we can work out what the gap will be let us take it keep it simple. Let us say n equal to 1, n equal to 2, 2 square is 4, 1 square is 1 whatever it is no matter which pair of quantum numbers you take you get a constant.

For that constant what is the value of h square by 8 mL square if I change L. If L is increased since your L square is in the denominator energy gap between the two chosen energy levels is going to decrease. Larger the box smaller is the energy gap actually I should not have written h square here that would should come after another piece of discussion that we have coming up but well bear with me until then.

We are really talking about the energy gaps. So, if L is small then energy gaps are larger if L is large then energy gaps are small what does that mean if you keep on increasing the size of the box the energy levels keep coming closer and closer and closer so beyond a certain value the energy levels will come so close to each other that you cannot tell between this energy level and the next one. So, you do not have discrete energy levels anymore rather you have a band that would be the classical limit.

So this is another beautiful thing that comes out of our discussion just wise changing the dimension of the box one can go from quantum world to classical world and back and it makes perfect sense in both the worlds. This is another point of strength another reason why we gain confidence in this treatment. Now comes, the discussion that should have come before I could write h nu.

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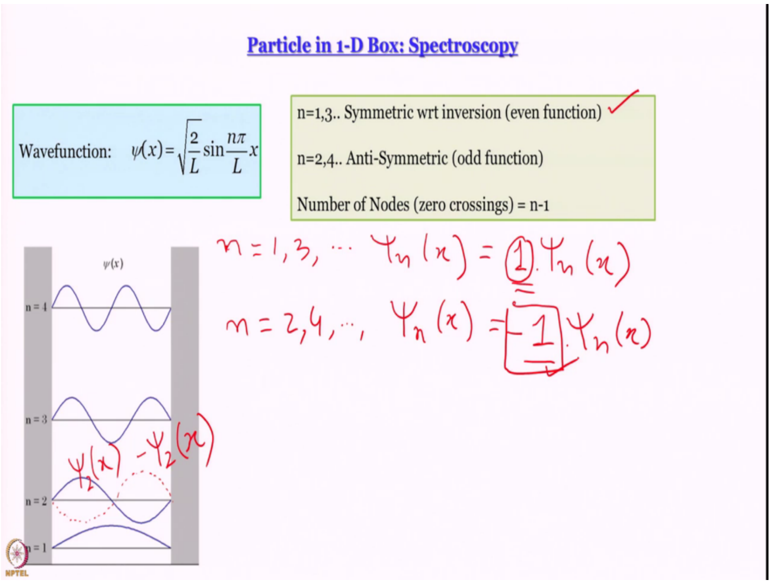

Particle in 1-D Box: Spectroscopy

Wavefunction: $\psi(x)=\sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x$

n=1,3.. Symmetric wrt inversion (even function) ✓

n=2,4.. Anti-Symmetric (odd function)

Number of Nodes (zero crossings) = n-1

$n=1,3,\cdots\ \psi_n(-x)=\underline{\textcircled{1}}\cdot\psi_n(x)$

$n=2,4,\cdots,\ \psi_n(-x)=\boxed{\underline{-1}}\cdot\psi_n(x)$

Let us talk a little bit about the spectroscopy of particle in 1D box what is spectroscopy? Spectroscopy is a study of interaction of radiation with matter I think we all know that. Why do you want to talk about spectroscopy all of a sudden we are talking about quantum mechanics quantum chemistry because well I ended up saying this for some excuse or the other in every course that I teach because I really like it.

One of my esteemed colleagues told me long ago that spectroscopy is just quantum mechanics in action. You do a theoretical treatment it is quantum mechanics you try to do an experiment that will manifest quantum mechanical principles you have to use spectroscopy. So, what you see in the spectrum is what you work out in quantum mechanics and remember of the origins of spectroscopy several most where sorry of the origins of quantum mechanics several where spectroscopic in nature.

Blackbody radiation we looked at the spectrum or hydrogen emission spectrum the spectroscopy and quantum mechanics goes hand-in-hand. So, it curious to know what kind of spectroscopy we expect for a particle in a box. We have this energy levels suppose I can I go from any level to any level if I shine light of appropriate energy. Can I go from 1 to 2, can I go from 1 to 3, can I go from 3 to 4 how do we know that?

We know that by considering symmetry of the wave functions to keep things simple you can do it in a more complicated way as well. Today we want to discuss the asymmetry aspect of it because symmetry is another important thing that appears in nature and actually governs many properties of things. For those who are interested in learning symmetry in a better way we did have an NPTEL course a couple of years ago on symmetry in chemistry.

All those lectures are now available on You Tube you can go through them but it will require a little bit of preparation it will use something called group theory. But coming back to this now what we say is something that does not require much preparation what we are saying is look at n equal to 1 wave function it is symmetric with respect to inversion which means if I just interchange 0 and L the wave function remains the same Psi remains Psi.

Look at n equal to 3 it is symmetric, so these symmetric functions with respect to inversion are called even functions. Now look at Psi for n equal to 2 if I interchange 0 and L what will happen will Psi remain Psi or will it become something else I think it is not very difficult to see that Psi is not going to remain Psi for n equal to 2 if I just interchange this what will it become it will become something like this.

So this is Psi 2 of x upon inversion I am going to get – Psi 2 of x so even for this I can write an eigenvalue equation what I can write is for n equal 2 for n equal to 1 3 etcetera Psi n of x is equal to 1 multiplied by Psi n of x so eigen value equation with eigen value of 1 for n equal to 2 4 and so on and so forth Psi n of x forgive my bad hand writing is equal to we said minus Psi n of x so might as well write minus 1 multiplied by Psi n of x.

So the eigen value here is minus 1, so if the eigen value is 1 then we call it a symmetric or an even function. If I eigen value is minus 1 then we call it an anti-symmetric or an odd function okay I hope that is well understood and one more thing number of nodes is n - 1 as you can see here for n equal to 1 number of nodes is 0. For n equal 2 number of nodes is 1 and so on and so forth. Well let me erase what I have just written because I have actually written on top of things are going to actually appear the moment I try to go ahead.

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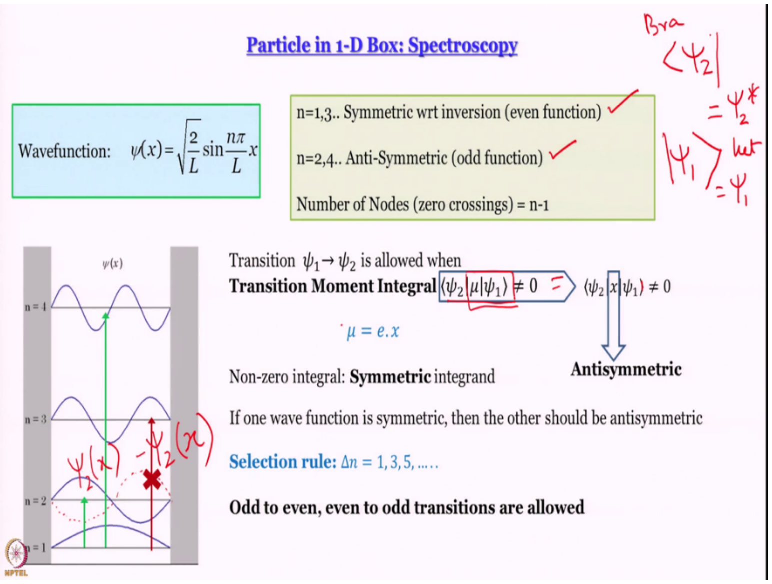

Particle in 1-D Box: Spectroscopy

Wavefunction: $\psi(x)=\sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x$

n=1,3.. Symmetric wrt inversion (even function) ✓

n=2,4.. Anti-Symmetric (odd function) ✓

Number of Nodes (zero crossings) = n-1

Bra $\langle\psi_2| = \psi_2^*$

ket $|\psi_1\rangle = \psi_1$

Transition $\psi_1 \rightarrow \psi_2$ is allowed when

Transition Moment Integral $\langle\psi_2|\mu|\psi_1\rangle \neq 0 \Rightarrow \langle\psi_2|x|\psi_1\rangle \neq 0$

$\mu = e.x$

Antisymmetric

Non-zero integral: **Symmetric** integrand

If one wave function is symmetric, then the other should be antisymmetric

Selection rule: $\Delta n = 1, 3, 5, \ldots\ldots$

Odd to even, even to odd transitions are allowed

But what we have done is we have learnt what even and odd functions and as we will see now the symmetry has an important role to play in determining transitions between which pair of levels is going to happen and which pair of levels is not going to happen that is determined by a quantity called transition moment integral. Transition moment integral is integral Psi 2 star mu Psi1 I think we have introduced this bracket notation already just to revise what this means is this if I write integral well not integral.

If I write Psi like this unless we let me write Psi 2 let me write Psi 2 this vector with the arrow pointing towards left this is called a bra vector and Psi 2 in bra vector essentially means Psi 2 star this is another way in which you can write since we have written Psi 1 here let us write Psi 1 and when we write it in this angular brackets like this, this is called the ket vector this simply means we can say Psi 1. When we write them together into something like this bra Psi 2 ket Psi 1 then we together call it bracket and this implies not just Psi 2 star Psi 1 but it is integral over the entire space integral Psi 2 star d tau.

So what we have here is integral Psi 2 star but in this case of course Psi 2 star is same as Psi because our wave functions are all real and this entire thing is the ket vector. So, this second line actually has no meaning it is there only to have symmetry so that it looks good. So, in the second in the ket vector we have mu Psi 1 what it means is that this is integral Psi 2 I will not write Psi 2 star anymore because we know that Psi 2 is a real wave function Psi 2 multiplied by mu multiplied by Psi 1 and here again I will write dx limits will be 0 to L.

Because the limit will be 0 to L essentially because we know that beyond x equal to 0 and x equal to L your wave function does not even exist. So, this is the transition moment integral and that has to be equal to nonzero for a transition to be allowed for a transition to take place. Once again in this course we are not going to going to the detail of where this transition moment integral comes from but there is an earlier NPTEL course that we had offered on molecular spectroscopy there we have a little more discussion on this aspect the videos are available whoever is interested may please have a look.

Now with this background we might as well write mu equal to e into x that is very well known and e is a constant, so we take e out and well I have to erase these as well otherwise you will not be able to see anything I guess so if I take out then the integral has integrals Psi 2 x Psi 1 now that has to be nonzero, for an integral to be nonzero the integrand has to be symmetric what does that mean? What is the integrand? Psi 2 x Psi1.

Suppose the integral is I if the integrand yeah maybe I will call the integrand I and what we raised this later because I am writing on things in a place where things will come, so what we are trying to say is this. Suppose you do an inversion and the integrand becomes minus I, what will happen to the integral? In the integral was integral I dx that will become minus integral of I dx but see just because we have inverted the box cannot change the value of the integral.

So then we have to write integral of I dx is equal to minus integral of I dx when I was told when is x when is q equal to minus q only when q equal to 0. So, what we see is that for an anti-symmetric integrand the integral vanishes it becomes 0 and so the transition is not allowed if the integrand is anti-symmetric. So, what you are saying essentially is that for a transition to take place we want a nonzero integral and to get a nonzero integral the integrand would better be symmetric with respect to inversion.

Now see what is x is it symmetric is it anti-symmetric its anti-symmetric this is brought out even better if you place the origin in between if you say that what is now L by 2 that is 0 then from plus will go to minus x is definitely anti symmetry sorry x in this case is actually symmetric this is a mistake it is symmetric. So, your next time is fine 0 to L right it is not going to change sign. So, if one wave function is symmetric then the other has to be anti symmetric that's the issue.

So now what does that mean that means selection rule is that delta n is 1 3 5 so on and so forth from executed from n equal to 1 level one can go to n equal to 2 level it cannot go to n equal to 3 level right odd to even, even to odd transitions are allowed. So, one can have this transition and this transition 1 to 2 and 1 to 3 one cannot have 1 to 2 transitions.

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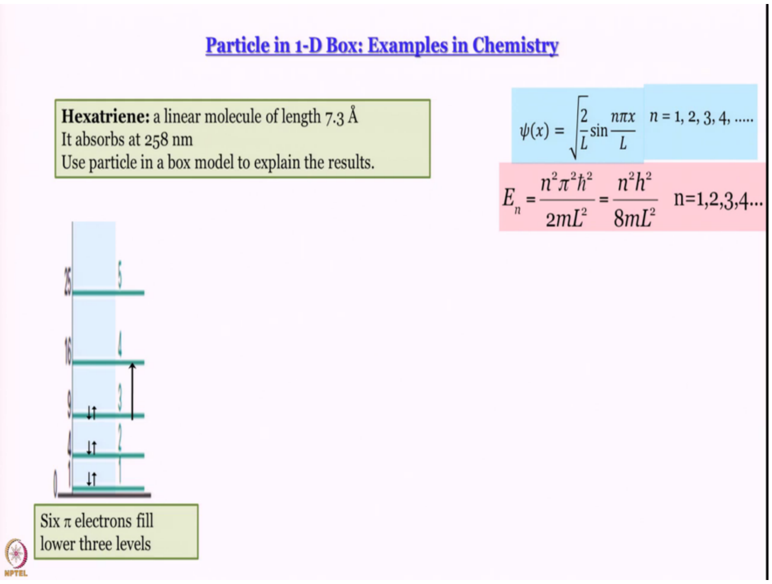

Particle in 1-D Box: Examples in Chemistry

Hexatriene: a linear molecule of length 7.3 Å
It absorbs at 258 nm
Use particle in a box model to explain the results.

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L} \quad n = 1, 2, 3, 4, ...$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2} \quad \text{n=1,2,3,4...}$$

Six π electrons fill
lower three levels

So, all right we have got some insight into quantum mechanics using this particle in a box model. Now the question is does it have any application can this model by itself be applied in some chemical system and the answer is yes that is what will take in the next module. So, what is spectroscopy? Spectroscopy is the interaction of radiation with matter and essentially it involves transition from one energy level to the other.

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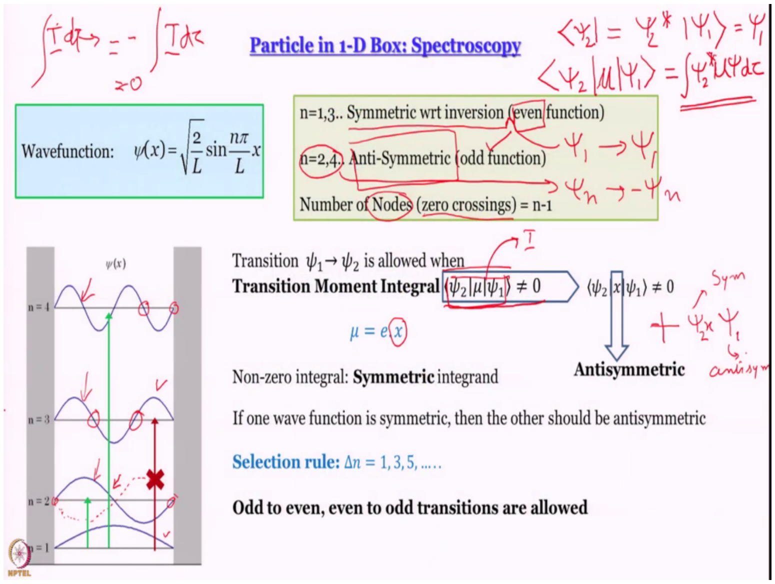

$\int \dot{I} d\tau \to = - \int I d\tau$

$= 0$

Particle in 1-D Box: Spectroscopy

$\langle\psi_2| = \psi_2^* \quad |\psi_1\rangle = \psi_1$

$\langle\psi_2|\mu|\psi_1\rangle = \int \psi_2^* \mu \psi d\tau$

Wavefunction: $\psi(x) = \sqrt{\frac{2}{L}} \sin\frac{n\pi}{L} x$

n=1,3.. Symmetric wrt inversion (even function)

n=2,4.. Anti-Symmetric (odd function)

$\psi_1 \to \psi_1$

$\psi_n \to -\psi_n$

Number of Nodes (zero crossings) = n-1

Transition $\psi_1 \to \psi_2$ is allowed when

Transition Moment Integral $\langle\psi_2|\mu|\psi_1\rangle \neq 0$ $\langle\psi_2|x|\psi_1\rangle \neq 0$

I

Sym

$+ \psi_2 x \psi_1$

antisym

$\mu = ex$

Non-zero integral: **Symmetric** integrand

Antisymmetric

If one wave function is symmetric, then the other should be antisymmetric

Selection rule: $\Delta n = 1, 3, 5, \ldots\ldots$

Odd to even, even to odd transitions are allowed

And to be honest we are not spectroscope is something that is not at all new to us because after all quantum mechanics is something there are sort of arisen out of spectroscopy. I am deeply indebted to a colleague who many, many years ago told me that spectroscopy is just quantum mechanics in action. All these calculations that we do in quantum mechanics is manifested in interaction of radiation with matter because as the only way in which you can probe the energetics of a system experimentally and quantum mechanics is all about the energy levels and wave functions and so on and so forth.

Now see just because there are two levels it does not mean that a transition will necessarily take place in spectroscopy something that is very important is selection rule. And selection rule which tells us which transitions are allowed and which transitions are not arises from something called transition moment integral. Transition moment integral is integral Psi 2 mu Psi 1 and the condition is that this transition moment integral must be nonzero. Now I think we might have introduced this nomenclature earlier as well.

But just to make sure in case we have not let me just do it once again what we have written here is this in the Dirac notation this is called ket vector sorry bra vector and when we write a wave functions inside it let us say I write Psi 2 in a ket vector bra vector it essentially means Psi 2 star complex conjugate of Psi 2 of course in our case we do not feel you have to worry about complex conjugates because our wave functions of particle in a box are all real.

This is now a vector, if you write like this so this is Psi 1 in what is called ket vector and what it essentially means is you can just write Psi 1 itself. A lot of complicated discussion becomes simpler if one uses bracket notation in our case it is almost trivial we might as well write the integral but it at least saves us a hassle of writing d tau and all that all the time. So, we will use bracket notation but I should tell you what this means, what we have written here, when you write like that so when you write bra Psi 2 ket Psi1 then it essentially means integral over all space Psi 2 star Psi 1 d tau.

In our case d tau can really should be replaced as dx because we are working in one dimensional space. Now one more thing it is possible that I might want to multiply this Psi one by something or make some operator operate on something what we have done is that we have used the operator dipole moment operator which means basically multiplication of a dipole moment. So, this is what it means but you might notice that there is an additional vertical line after Mu like this that is just to make things look good.

It still means bra Psi 2 ket Psi 1 ket Mu Psi 1 this is what it means this is your transition moment integral. And the condition for transition moment integral is the for transition moment integral to be nonzero is what we have to determine if you want to know which transitions take place and which transitions do not take place. For that purpose we are going to use here the property of symmetry of wave functions.

One can of course plug in the expressions for wave functions and do it the hard way work out the integral and that has to be done many times. But many times you do not have to go through all that hassle symmetry is a fundamental property of systems which determines many of its aspects. So, here we will see how nicely one can use symmetry arguments to determine whether this integral is 0 or not.

Remember we do not really need to know at this point whether what is the value of the integral is, if that is what we require then of course we have to work it out but if you only want to know whether it is 0 or nonzero we will see how we can do it nicely with symmetry. To do that let us first recognize that all these wave functions where n is odd this one or this one n equal to 1 n equal to 3 these are symmetric with respect to inversion.

What is the meaning of symmetric with respect to inversion if I say this is Psi 1 right so I write something like this Psi 1 and then I invert it so I interchange 0 and L in this case let us say then upon inversion it will remove Psi 1 it will remain Psi 1 that is the definition of being symmetric or what is called an even function. However look at this n equal to 2 or this n equal to 4 what happens if I interchange 0 and L the function is going to change shape.

Now this is plus Psi 2 if I interchange 0 and L you are going to have a function that essentially will look like this, so upon inversion what happens for n equal to 2, 4 etcetera where n is even. We get Psi n becomes minus Psi n and that makes it anti symmetric with respect to inversion and such functions are called odd functions. Let me digress a little bit and point out that the number of nodes remember what nodes means nodes node means a point where the wave function go through 0 and change sign.

So this is not a node this is so number of nodes is n - 1 where n equal to 1 there is no node number of nodes is 0 when n equal to 2 number of nodes is 1 when n equal to 3 number of nodes is 1 here and 1 here. So, that is something that is yes there we should know it. Now coming back to our original discussion what how do we know whether this integral is going to be zero or not well let me write on this side so that I do not have to erase it later on.

See an integral is nonzero when let us call let me call this I the integrand this one is I. So, what happens if I change a sign upon inversion? Let us say upon inversion I becomes minus I what happens to the integral? The integral is I d tau over all space that becomes minus I d tau but the issue is we are talking about a transition between two levels that cannot change depending upon which one we decide to be which point we decide to be zero and which point we decide to be L.

Just upon inversion the sign cannot change right so when will this happen in any case? If this is equal to this, they are saying that the integral cannot change upon changing sign so that means integral I d tau must be equal to minus integral my integral I d tau must be equal to minus integral I d tau when will that happen? When both are equal to zero is not it. Say q equal to -q only when q is equal to 0 otherwise it is impossible.

So what we learn is that this I has to be symmetric and I here is a triple product two wave functions and your dipole moment. Is dipole moments symmetric or is it anti-symmetric? Let us not forget that we can write dipole moment as mu equal to e into x where e is electronic charge x is displacement, x is it symmetric or is it the anti-symmetric? Well we have said this already that a symmetric integrand is required for the integral to be nonzero.

We are now asking the question what about x is it symmetric or is it anti-symmetric? What happens when we invert x becomes minus x naturally so x is definitely anti-symmetric. So, now when will this triple product be symmetric. So, we are doing inversion right we take this and do an inversion. When we do an inversion x changes sign, x becomes minus x. Let us say Psi 2 is symmetric, so Psi 2 will remain Psi 2, now if Psi 1 is also symmetric what will happen? Then this triple product changes sign which means the integral changes sign which means the integral is 0.

How can one avoid it? Only when Psi is anti-symmetric, so if Psi 2 is symmetric Psi 1 would better be anti-symmetric sorry for my horrible handwriting then what will happen is that due to x your minus sign due to Psi 1 also you have another minus sign and the whole thing becomes plus. So, what we are saying is that if one wave function is symmetric the origin or the destination then the other the destination or the origin respectively has to be anti symmetric that is the condition for the transition moment integral to be non zero that is the condition for the transition to be what we call in the language of spectroscopy, allowed.

So the selection rule then is Delta n will be equal to 1, 3, 5 so on and so forth why? Because if you remember the wave functions alternate wave functions are symmetric and anti-symmetric n equal to 1 symmetric n equal to 2 anti-symmetric n equal to 3 symmetric again n equal to 4 anti-symmetric once again. So, Delta n equal to 2 can never happen what happens if I want to go from say Psi 1 to Psi 2, Psi 1 is symmetric, so Psi 1 to Psi 3.

Psi 1 is symmetric x is anti-symmetric Psi 3 is symmetric so Psi 1x Psi 3 the whole thing is anti-symmetric. So, that integral vanishes and that transition is not allowed now if you want to know where this transition moment integral comes from that requires a little more of quantum mechanics. In fact we have discussed it in some detail in an earlier course that we had floated in on NPTEL course on molecular spectroscopy of physical chemists perspective.

So whoever is interested in knowing more about where transition moment integrals come from can go through those videos of that course which are now freely available on YouTube. I believe but for the purpose of this course at least for now we are going to take this transition moment integral business axiomatically and we are going to proceed from here. So, doing that what we have learnt is that for a particle in a box Delta n has to be 1 3 5 odd to even, even to odd transitions are only allowed which means that you can have this transition 1 to 2 you can have this transition 1 to 4.

But you cannot have this transition one two three why not because as we said several times 1 and 3 are both symmetric making the triple product which is the integrand of transition moment integral anti-symmetric. So, this is the discussion we wanted to have on spectroscopy of particle in a box and this is what tells us which transitions take place and which transitions do not with this background we are now prepared to go ahead and talk about color.

And we are ready to talk about whether or not there can be some application of the simple particle in a box in real chemical systems.