Statistical Mechanics

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Lecture – 27
Qunatum Statistical Mechanics

Good morning students, today we will start the 3rd chapter on Quantum Statistics.

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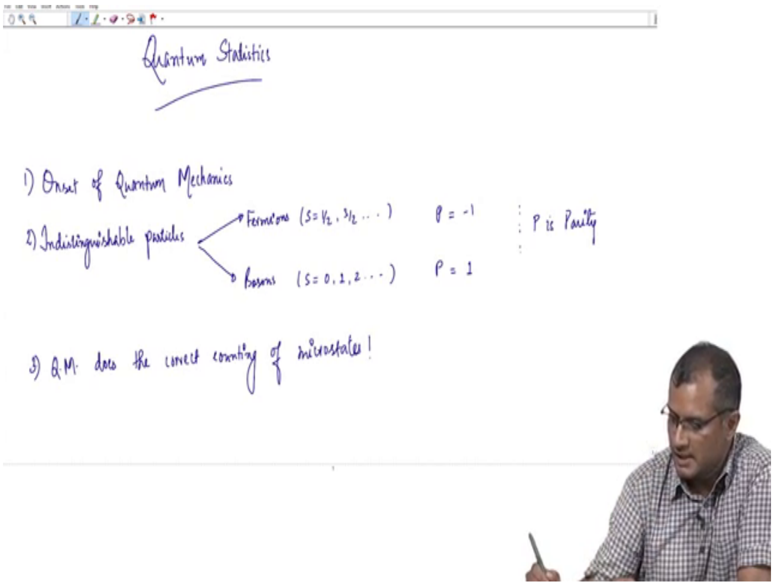

Quantum Statistics

1) Onset of Quantum Mechanics

2) Indistinguishable particles → Fermions ($s = 1/2, 3/2 \ldots$) $P = -1$ → Bosons ($s = 0, 1, 2 \ldots$) $P = 1$

P is Parity

3) Q.M. does the correct counting of microstates!

And I would like to highlight a few points that we are going to discuss in this particular lecture, that will pave the way for more intense and deep discussions in the coming lectures. So, this is the first introduction to Statistical Mechanics of Quantum Systems. Now, the first question that arises in our mind is that why do we need a different level of statistics for quantum systems?

Now, to understand that we must first identify what is the quantum limit of any classical system or what is the classical limit of any quantum system. That being said we are looking at the same system, the system does not change, but it may so happen that for a combination of temperature and density, the system at our disposal may behave quantum mechanically; meaning that it is no longer representable by a deterministic set of rules. Which means at some sufficiently high density or sufficiently low temperature, I will discuss in a short while what do we mean by sufficiently high or low.

So, at high density on low temperature, you would replace classical mechanics with quantum mechanics and we have already seen some kind of a discussion on the onset of quantum mechanics in classical systems. So, we will start off with a small recollection of the fact that. So, first before we recollect anything I would like to put down the points in some order just figuratively to basically decide what we are going to discuss ok.

So, the first thing on the cards is basically onset of quantum mechanics. So, when should I be worrying about quantum mechanical effects that is the first thing to ask, because otherwise after chapter 1 and chapter 2 I know exactly what to do when somebody asks me to compute the heat capacity of a material or susceptibility of a magnetic system. All these questions can be answered using tools of classical statistical mechanics.

But the same system at my hand for example, electrons in a metal or spins on a lattice will classical theories suffice will they give me the right answer. The answer to this question relies on the parameters of the system the physical parameters of the system which are the density on the temperature and that should decide whether I am in the quantum regime or classical regime. We will discuss those parameters very shortly.

The second point in this chapter would be basically a machinery or a theoretical set of tools that appropriately handles the system of indistinguishable particles. Now you have seen in classical statistical mechanics, we do not know how to handle these indistinguishable particles except for the fact that. Once you complete a calculation, you account for the fact that microstates which are only different from each other in only permutation of identical particles are to be seen as just one entity.

And so, you in some sense plug the n factorial pre factor after you have completed your calculation, there is no inbuilt machinery in classical mechanics which handles indistinguishability of particles. So, we will see how quantum mechanically you know starts off with this correct formalism as if its embedded in its DNA ok. So, the n-factorial is not going to be missed it fact in fact, it will be plugged into your calculations from the beginning itself that is number 1.

So, in the context of indistinguishable particles we will be discussing two types of particles which are fermions and bosons. So, basically these are particles with some half integer spins ok. So, you can take spins and so on and so forth and for bosons we will have you know integer spins. So, the fundamental particles are the fundamental indistinguishable particles are classified into fermions and bosons in the quantum mechanics.

And they are basically different from each other in the sense that one corresponds to the parity operator having eigenvalue plus 1 and the other corresponds to the parity operator having eigenvalue minus 1 ok. So, P here is the parity operator and I will talk into some detail about this operator. And we will also basically see that quantum mechanics does the correct counting or correct enumeration of states naturally ok, this correct counting of the macro-states sorry micro-states is natural in the quantum mechanical formulation.

Basically, what is meant here is that when you have an n-particle system you do not start your calculation by just you know doing any deterministic calculation. What you do is write down an in particle wave function and the properties of this n-particle wave function by property I mean whether the wave function is symmetric under permutation of n-particles or not decides whether it is a bosonic wave function or a fermionic wave function. And this symmetry of the wave function in terms of permutation of particles demands that the fermions obey exclusion principle,

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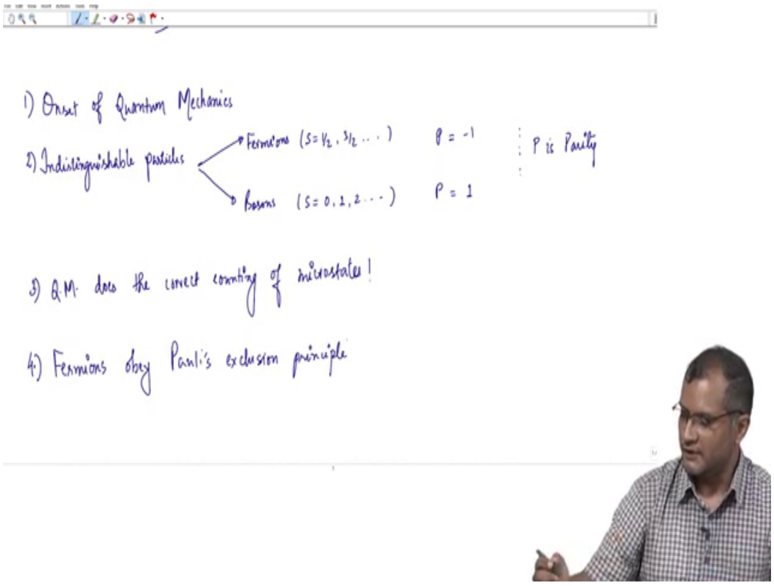

1) Onset of Quantum Mechanics

2) Indistinguishable particles $\rightarrow$ Fermions $(S = 1/2, 3/2 \ldots)$ $P = -1$ ⋮ P is Parity

$\rightarrow$ Bosons $(S = 0, 1, 2 \ldots)$ $P = 1$

3) Q.M. does the correct counting of microstates!

4) Fermions obey Pauli's exclusion principle

So, the last point that I would like to mention here is that a consequence of the symmetrization of the wave function or the anti-symmetrization of the wave function, fermions obey Pauli's exclusion principle and no such restriction is there on bosons ok. So, a couple of things that we should; so, this is basically our menu of topics that we would be covering and if you are doing quantum statistics I believe there should be a nice understanding of; first of all why we need quantum mechanics, where is it that we are lacking in terms of you know a classical understanding of the system.

Then once we present the case for quantum mechanics, we must allow for you know discussion on various types of particles which are the fermions and bosons. We will discover that these two types of particles are nothing but you know the consequences of your wave function over all wave function being symmetric or anti symmetric in terms of a parity operator ok. That is why we call them fermions and bosons; it is just a definition ok.

Then after introducing this definition we will show how it does the correct counting of microstates which is natural or in some sense I keep saying that quantum can axis. Sort of on the start on the word go does the correct counting of microstates, I will explain why is it so.

And as a by-product of this correct counting it also basically shows why fermions will obey Pauli's exclusion principle, that is know to fermions can exist in the same single particle quantum state ok. Because, if you try to force two fermions in the same single particle quantum state then the entire wave function of n-particle system will collapse to 0. When you say that the wave function is collapsed to 0, you mean to; you are saying that explicitly that microstate has 0 probability. So, you will never see this. So, that is the sort of a sketch or the bird's eye view of what I am going to present in today's lecture.

So, let us start with the first point on the menu which is the onset of quantum mechanics. Now, we have seen in the second chapter that we had a length scale which was called as the thermal De Broglie length scale.

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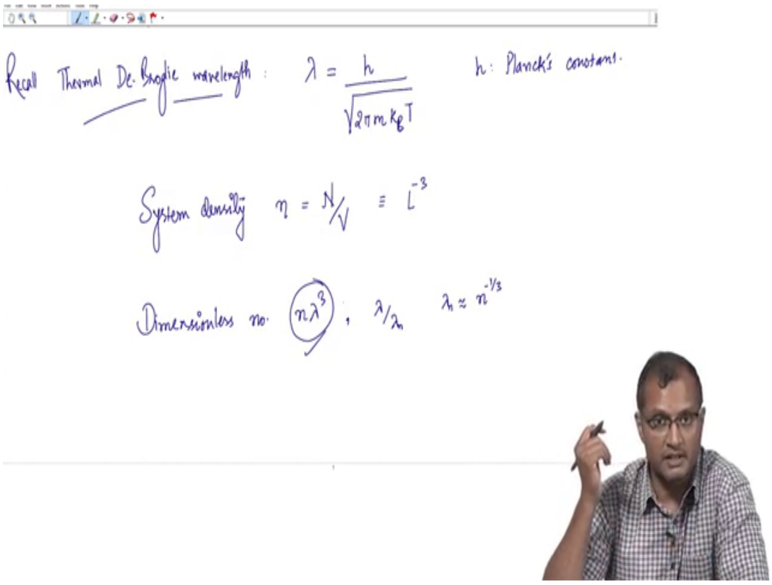

Recall Thermal De Broglie wavelength : $\lambda = \frac{h}{\sqrt{2\pi m k_B T}}$ h : Planck's constant.

System density $n = N/V \equiv L^{-3}$

Dimensionless no. $\boxed{n\lambda^3}$, λ/λ_n $\lambda_n \approx n^{-1/3}$

So, recall that there was a thermal De Broglie length scale, now I call it as a length scale and I am calling it as a thermal length scale because it is associated with the temperature of the system and depending upon how large or how low the temperature is the length scale will vary. We can call it De Broglie wavelength or De Broglie length scale whatever comes to your mind that is not necessary. But its form was we had discovered that this length scale is the Planck's constant h over 2 pi m k B T, where k B is the Boltzmann constant and T is the temperature of h system; h being the Planck's constant ok.

Now, I had said that every system that you study, let us say n-particles in a box or electrons in a metal or gas in this room, you have a certain container or you have a certain box where your particles are you know they exist. So, I know that my system has a density, I call it as small n number density which is the number of particles in the system over the systems volume ok.

So, now you can see that this density has the units of you know it has the units of just l to the power minus 3 because of volume. Now, like I said in the beginning few lectures ago that if you want to see the nature of the system, we can always construct a few interesting dimensionless numbers that will tell us how my system will behave. So, with one length scale lambda, I am going to construct another length scale for my density and compare these two length scales by constructing a dimensionless number.

So, straightforwardly I can construct one dimensionless number construct a dimensionless number ok, you are free to construct other numbers also by the way you can also construct another. So, you can take lambda as one length scale our De Broglie length scale, you divided by some density dependent length scale this is another dimensionless number. Now, how do I construct this lambda n? This lambda n is you know it can be taken as sum n to the power minus 1 by 3, but since we normally work with density which is known to us.

For example for copper, I know that the number of electrons in the metal free electrons is of the order of 10 to the power 28 per meter cube; I know the densities, I know the density of hydrogen in this room. So, I would like to work with this combination of you know this dimensionless number where I know n I know from handbook of materials or by previous laboratory experience or whatever and I know to very good extent what is my De Broglie wavelength.

So, I can choose to work with this dimensionless number ok; purely for convenience sake. So, let us pick up this dimensionless number and see whether we can distinguish the two world's quantum and classical. So, clearly I know that the limit of high density and low temperature is the quantum mechanical world. Because this is where when you take when you look at the expression for the De Broglie wavelength, this wavelength will be very large at very low temperatures as the temperature goes to 0 lambda goes to infinity. So, the wave nature of the particles becomes to dominate, it becomes essentially more and more delocalized.

So, I know that for low temperature is the quantum regime, I also know that if I for any temperature I can increase my density thereby making the inter particle separation smaller and smaller. In such a way that this separation can be made smaller than the De Broglie wavelength that is also a quantum limit for my system.

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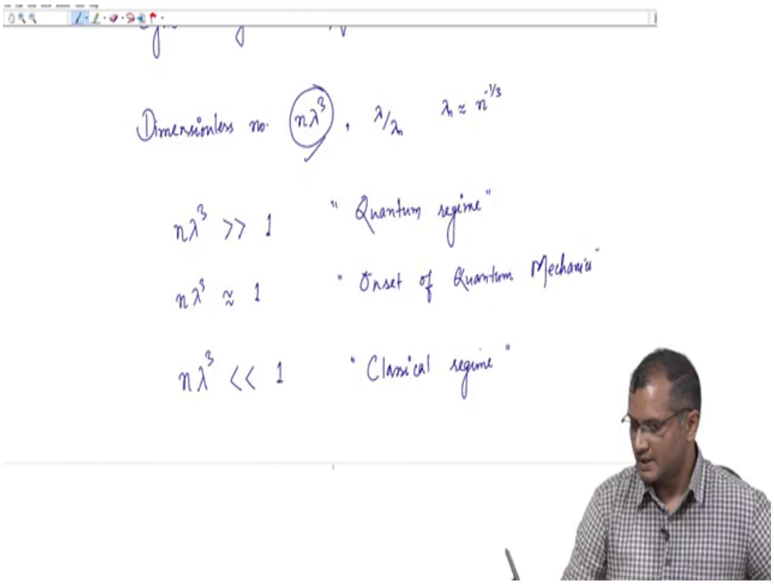

Dimensionless no. $\boxed{n\lambda^3}$, λ/λ_n $\lambda_n \simeq n^{-1/3}$

$n\lambda^3 >> 1$ "Quantum regime"

$n\lambda^3 \approx 1$ "Onset of Quantum Mechanics"

$n\lambda^3 << 1$ "Classical regime"

So, one thing is clear that the dimensionless number n lambda cube being much larger than 1 is the quantum regime. The regime where I make both n and lambda larger and larger ok, because lambda is large means my wavelength is getting large, my wave nature of the particles becomes more and more predominant and density being large means my inter particle separation is also much smaller than the De Broglie wavelength. So, this is definitely a quantum regime and we will I show by calculating numbers this is definitely quantum regime.

I also know that well, just by the preceding argument we can push this limit to the other side. So, I can say that if this dimensionless number it is much smaller than 1 then I am in a classical regime. Of course, because I can push n lambda cube to be much less than 1 by making n very small thereby increasing the separation between particles, such that the particle separation far exceeds the De Broglie wavelength ok.

And lambda is also being very vary you know it is made very small which is like increasing temperature because lambda is proportional to 1 upon square root T. So, both n and lambda are increased that increases n lambda cube and both n and lambda reduced, that reduces n lambda cube is very simple to see why one leads to a quantum effect, the other leads to a classical behavior.

Naturally, there is a boundary that separates these two and the boundary is not sharp, the boundary is fuzzy ok. And I will say that n lambda cube of the order 1 is the onset of quantum mechanics ok, this is where you will sort of say that I am not very clear which theory will work. But I am sure that the quantum effects are not ignorable and n lambda cube is of the order 1 its tricky it is not easy. It is very safe to handle the two extreme regimes where the regime n lambda cube being much smaller than 1 almost guarantees that your classical calculations will work with you know they will come out with flying colors.

In the regime n lambda cube greater than 1, classical theories will fail miserably and this is the regime where you have you know electrons in a metal you must invoke a quantum calculation ok. For electrons in a metal at room temperature 300 Kelvin, you will very soon calculate that n lambda cube is much less than 1. So, you must invoke a quantum calculation all your d by your Dulong-Petit law will fail miserably for heat capacity of a metal due to electrons.

And when this dimensionless number is of the order 1, you know that you have to be careful because this is the regime when quantum mechanics begins to show its presence. So, then you can actually construct some sort of a parameter space diagram where at least figuratively you can say whether quantum mechanics applies or quantum mechanics or classical mechanics applies.

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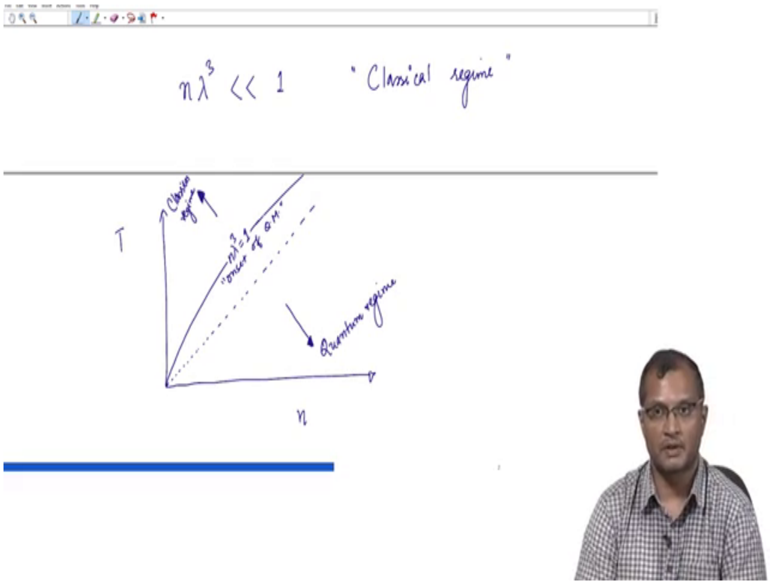

$n\lambda^3 << 1$ "Classical regime"

So, you can say that I will construct a Tn diagram; number density versus temperature and so, in which you know the region of applicability of classical or quantum mechanics. Clearly there is a line of 45 degree slope which is the T equal to n curve.

And my curve n lambda cube equals to 1 would be somewhere like this. So, this is my curve ok; so, deep inside this phase so, this curve that I have computed the solid line is the line of n lambda cube is equal to 1 ok. And the deep inside this phase you will say that your system has quantum effects because that is their region when you have high density and low temperature and deep above this solid line you will say that I have a classical regime.

And somewhere close to the n lambda cube equal to 1 line, you have a you know onset of quantum mechanics. So, I will say I am going to remove the T equal to n line because its making the figure very busy just maybe very faintly I will show. So, this is where I have the one set of quantum mechanics near the solid line is to give you a feeling in terms of numbers.

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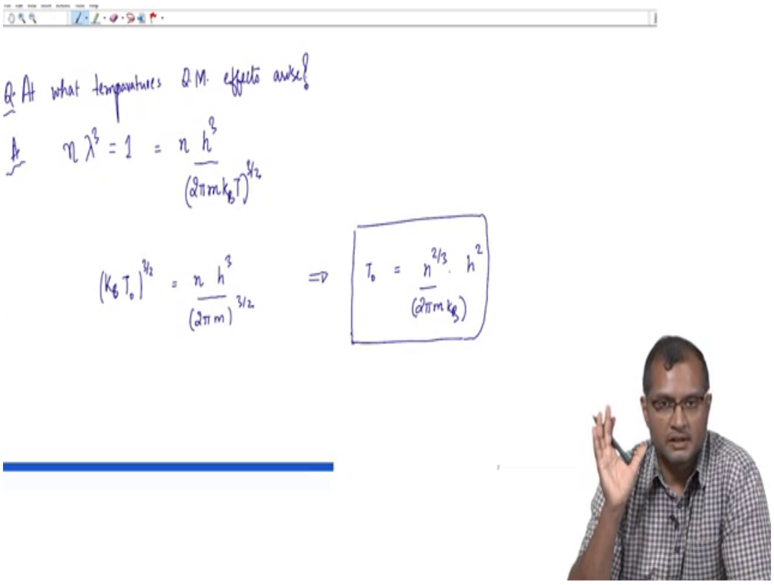

Q. At what temperatures Q.M. effects arise?

A. $n\lambda^3 = 1 = \frac{n h^3}{(2\pi m k_B T)^{3/2}}$

$$(k_B T_0)^{3/2} = \frac{n h^3}{(2\pi m)^{3/2}} \Rightarrow \boxed{T_0 = \frac{n^{2/3} \cdot h^2}{(2\pi m k_B)}}$$

So, if I compute the I will say that; so, at what temperatures do I see quantum mechanics, if that is the question at what temperature is the quantum mechanics begins to take over well you have this relationship. So, that is your question, you can answer this by saying this is the fuzzy boundary n lambda cube equals to 1 this will give me the temperature when quantum effects will begin to you know take effects and I know this is nothing but n times h cube over 2 pi m k B T to the power three half because that is the definition of lambda.

So, now you can compute the temperature from here. So, you can say that my k B T and this is nothing but the in some sense the degeneracy temperature where this particular T is when n lambda cube is 1; so, I am just calling it as T naught. So if I take k T on the other side I will get k T to the power 3 half as n times h cube over 2 pi m to the power 3 half fine, just multiplied both sides with k T to the power three half.

And this gives me k t as nothing but n to the power 2 by 3 into h square over 2 pi m ok. And naturally, if you compute so, if you just you can write down this you can divide it by k B on both sides. So, this is the basically the temperature that corresponds to your n lambda cube equal to 1. So, this is the temperature at which quantum mechanics will begin to take effect.

Let us compute these temperatures for some of the systems that we routinely encounter in our everyday lives. It will give you an idea you will appreciate the fact why should I learn quantum mechanics ok.

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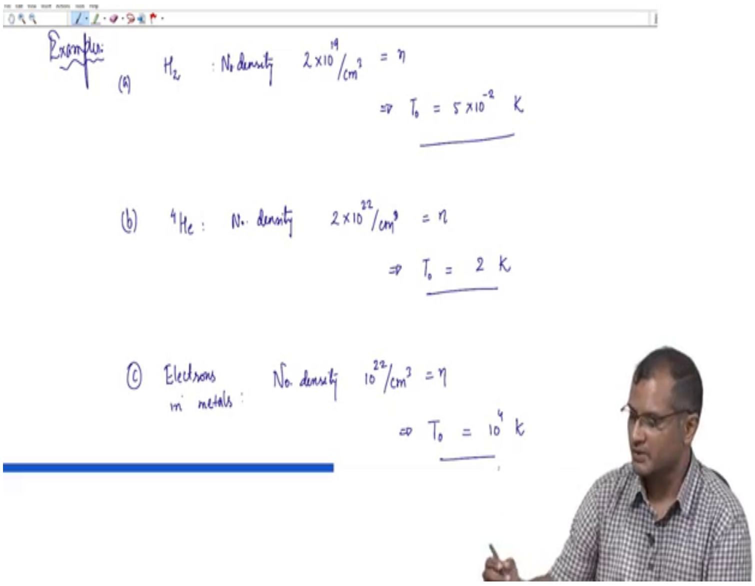

Examples:

(a) H_2 : No. density $2 \times 10^{19}/cm^3 = n$

$\Rightarrow T_0 = 5 \times 10^{-2}$ K

(b) ^4He : No. density $2 \times 10^{22}/cm^3 = n$

$\Rightarrow T_0 = 2$ K

(c) Electrons in metals : No. density $10^{22}/cm^3 = n$

$\Rightarrow T_0 = 10^4$ K

So, I am going to take some examples; the first example that I am going to take is that of you know hydrogen. So, hydrogen for instance as a density and has its written it down here has a number density of 2 into 10 to the power 19 per centimeter cube. So, this is the number density for nitrogen so, this is the n for nitrogen.

Now, if I want to compute the degeneracy temperature; so, this gives me the degeneracy temperature if I compute this it comes out to be around 5 into 10 to the power minus 2 Kelvin. So, somewhere around 0.05 Kelvin for hydrogen, you must invoke quantum mechanics or you must invoke quantum statistical mechanics. So, classical calculation is perfectly valid at room temperature ok, only a thus this low temperature your n lambda cube is of the order 1 that is the meaning of this calculation ok.

Let us take another is there a question; which tells you what? See, I computed this temperature by equating n lambda cube as 1 which is the onset of quantum mechanics. But this temperature you will see quantum mechanical effects, higher temperatures definitely I will be classical ok. So, unless you push your temperatures down to 5 into 10 to power minus 2 Kelvin which is like 0.05 Kelvin, you can treat hydrogen in the air classically.

Let us take another system which is helium-4 liquid helium ok. So, this has a number density of liquid helium has a number density of 2 into 10 to the power 22 per centimeter cube; now this is a higher density. So, I can expect that the degeneracy temperature will be higher, because now I should see quantum mechanics effects with even higher temperature, but this guy is already sitting at a higher density ok.

So, this is the n for it and you plug this number density in this expression like we have you know computed, put the value of Boltzmann constant and Planck's constant. You will find that the degeneracy temperature for liquid helium is of the order of 2 Kelvin's which is in some sense 100 times higher than the previous guy; previous guy was of the order of 0.01, this guy is if the order 1. So, already by boosting density I have actually made quantum mechanical effects come sooner; so, I do not have to go all the way to 0.01 Kelvin now.

Going by this logic, you can expect trouble to come if you go to electrons in a metal; now, why these heat capacity expressions given by Dulong and Petit do not work for metals even at room temperature. So, because of this let us do this calculation also. Now you take typical copper for example, copper which is a perfect you know perfectly good example of a metal and each copper donates one valence electron to the matrix. So, a number density of typical copper block is of the order of 10 to the power 22 per centimeter cube which is my density.

Student: (Refer Time: 30:01).

That is per meter cube ok. So, if you take this number density and do this calculation you will get well as expected because now I will get degeneracy temperature much higher. This degeneracy temperature comes out to be 10 to the power 4 Kelvin. Reason why the two degeneracy temperatures for liquid helium and electrons in the metals are so different; the electrons in the metals having such higher degeneracy temperature. In spite of the fact that both had the same number densities because helium-4 has a much higher mass roughly 8000 times heavier than electron because it has 4 nucleons.

And so, that is the reason why you have such different degeneracy temperatures, but the thing to see here is that for electrons in the metal, the degeneracy temperature; that is the temperature where quantum effects will arise is 10 to the power 4 Kelvin. This tells us that at room temperature which is much below 10 to the power 4 Kelvin, we must invoke quantum mechanical theory to correctly understand heat capacity of solids due to these free electrons.

So, any theory that we invoke on electrons in metals has to be quantum mechanical, these electrons are heavily quantum mechanical at room temperature in the solid metals ok. So, that is the you know that is this basically gives you an filling of the numbers right I must invoke quantum mechanics when I am dealing with electrons in metals because that is a degeneracy temperature; 300 Kelvin is for sure much much lower than 10 to the power 4 Kelvin ok.

So, only when temperatures are much higher than 10 to power 4 you can include you can use a classical theory of electrons in metals, but then at those temperatures you do not have a metal you will probably be you know making a gas out of a metal right. So, now let us proceed with the second topic in the agenda which is if you go back the statistics of indistinguishable particles.

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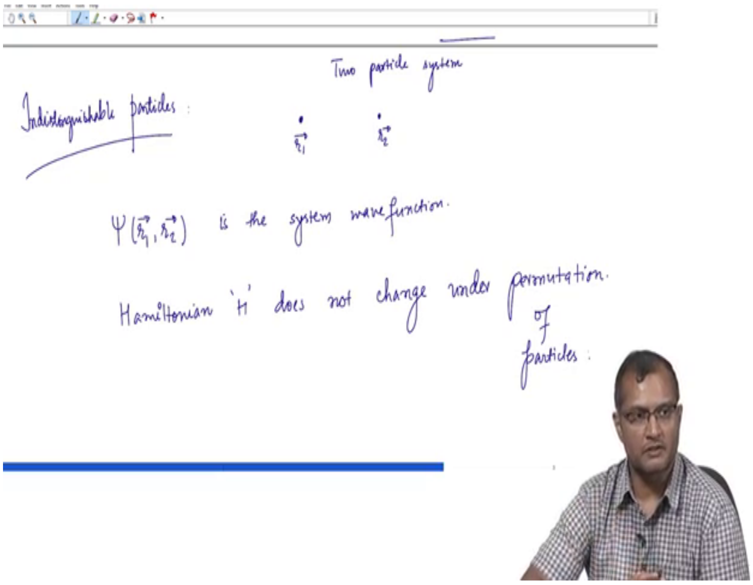

Two particle system

Indistinguishable particles :

$\vec{r}_1$ $\vec{r}_2$

$\Psi(\vec{r}_1, \vec{r}_2)$ is the system wave function.

Hamiltonian 'H' does not change under permutation of particles.

So, indistinguishable particles are handled very carefully in quantum mechanics. For example if I take just the two particle system; one sitting at somewhere location r 1 and another sitting at location r 2 let us take the two particle system ok. So, I am just taking a two particle system. Then I can write down the wave function of my system as the of the two particle system as psi of r 1 r 2 and is the system wave function; I will show how to write down psi which is the overall wave function in terms of single particle wave function and short while.

But I know for sure that if I permeate these two particles that if I make you know r 2 the second particle go and sit on r 1 and the first part it will go and sit at r 2. The Hamiltonian of the system does not change ok, because the Hamiltonian of the system is a function of potential energy and kinetic energy. And clearly if the particles are indistinguishable I am not affecting their potential energy in any way because they are the same particles.

So, permutation of 1 on 2 does not change the potential energy and it clearly does not change energy ok, because I am just putting one particle having some kinetic energy location which is different kinetic energy remains the same. So, Hamiltonian does not change under permutation of particles ok; meaning what? The energy of the system remains the same under permutation of particles.

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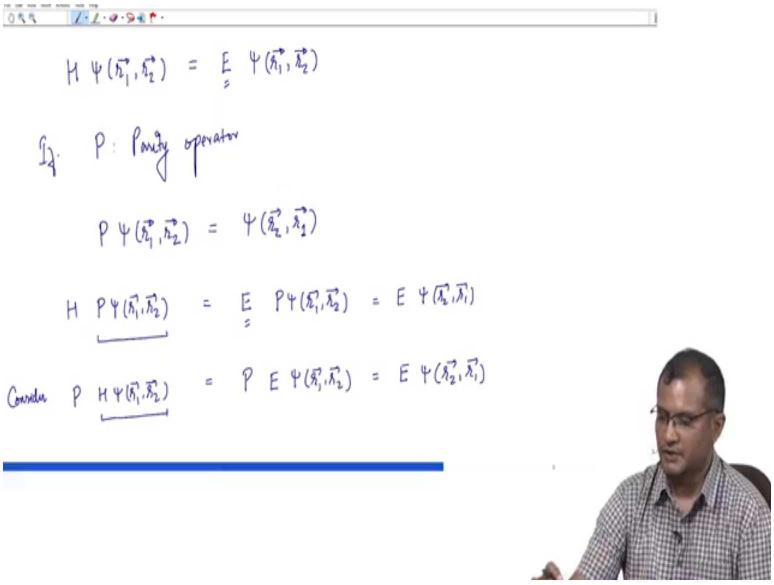

$$H\,\psi(\vec{r}_1,\vec{r}_2) = E\,\psi(\vec{r}_1,\vec{r}_2)$$

Eg. P : Parity operator

$$P\,\psi(\vec{r}_1,\vec{r}_2) = \psi(\vec{r}_2,\vec{r}_1)$$

$$H\,\underline{P\psi(\vec{r}_1,\vec{r}_2)} = E\,P\psi(\vec{r}_1,\vec{r}_2) = E\,\psi(\vec{r}_2,\vec{r}_1)$$

Consider $P\,\underline{H\psi(\vec{r}_1,\vec{r}_2)} = P\,E\,\psi(\vec{r}_1,\vec{r}_2) = E\,\psi(\vec{r}_2,\vec{r}_1)$

This essentially means that if I take the Hamiltonian operator and this an operates on the particle two particle wave function, the eigenvalue which is a total energy of the system does not change if the particles are permuted ok. That is the meaning of the Hamiltonian operator; which means if I think of a parity operator P being the parity operator whose action is to just permute the particles ok. Then I do not expect to see any change in energy which means the parity operator when it acts on the system makes the wave function basically psi of r 2 r 1 simply swaps the two particles at the effect of the parity operator.

And I know from what I have written here that the Hamiltonian of the system must not change which means the energy of the system should not change, which means if I apply the Hamiltonian operator on this new wave function P of psi r 1 r 2 considering this as my new wave function then I must get the same energy because the energy has not changed ok. So, the same wave function comes back without any change in the energy, this E is the same as this E, but I can also write this as you know I can also consider P app operating on H psi ok.

So, this is my new function this is nothing but P H on psi simply gives me E times and that is the eigenvalue psi r 1 r 2 hmm, but E is just a number this is the eigenvalue. So, I can write this as E times P operating on psi r 1 r 2 which is nothing but psi r 2 r 1 ok. You can compare the previous equation this is also E of multiply to psi of r 2 r 1.

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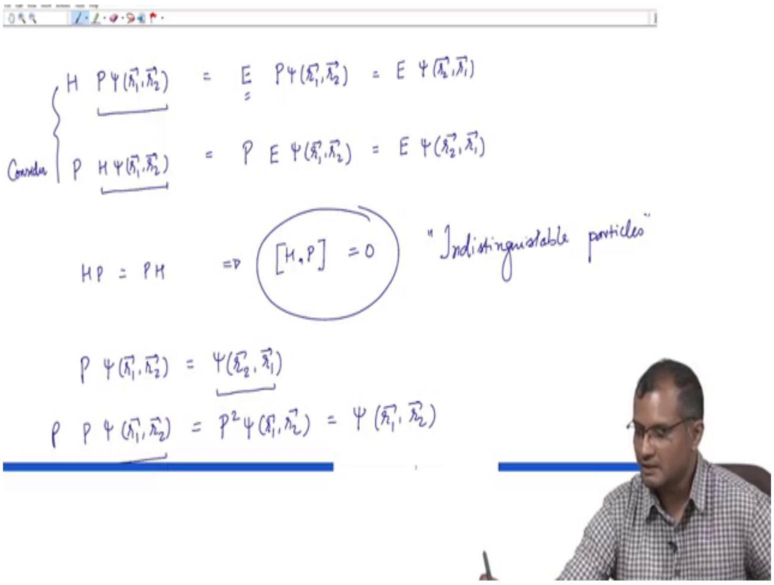

Consider

$$H\,\underline{P\Psi(\vec{r}_1,\vec{r}_2)} = \underset{=}{E}\;P\Psi(\vec{r}_1,\vec{r}_2) = E\,\Psi(\vec{r}_2,\vec{r}_1)$$

$$P\,\underline{H\Psi(\vec{r}_1,\vec{r}_2)} = P\,E\,\Psi(\vec{r}_1,\vec{r}_2) = E\,\Psi(\vec{r}_2,\vec{r}_1)$$

$$HP = PH \Rightarrow [H,P] = 0$$

"Indistinguishable particles"

$$P\,\Psi(\vec{r}_1,\vec{r}_2) = \underline{\Psi(\vec{r}_2,\vec{r}_1)}$$

$$P\,\underline{P\,\Psi(\vec{r}_1,\vec{r}_2)} = P^2\Psi(\vec{r}_1,\vec{r}_2) = \Psi(\vec{r}_1,\vec{r}_2)$$

So, if these two are same I can say that by looking at these two the left hand sides, that my Hamiltonian operator commutes with the parity operator. I can say that the product of these two operators is the same as product of P and H implying that the Hamiltonian commutes with the parity operator for our identical particle system or indistinguishable particles.

And this has very important consequences this is why quantum mechanics does calculations correctly ok, this is the birth of the correct enumeration of states. In a very logical sequence of steps I showed that the Hamiltonian of the system commuted the parity operator, this brings us to the stage that I can write down now the effect of my parity operation done twice.

I already know that P simply swaps the positions; so, P operation on psi r 1 r 2 simply gives me the same wave function now, but the particles permuted. If I do not know what is this new psi, I can compute this new psi by operating P again which is nothing but P square operating on psi r 1 r 2 ok, but I already know what is P operating on psi which is my psi r 2 r 1. So, one more operation of P on this will give me back the old function it will bring the system back to the old state. You made to go and sit in 1, do one more permutation you get back the same old wave function.

So, definitely my P square as an eigenvalue which is 1 and the fact that permutation you know you have seen the here that the Hamiltonian permutes with the parity operator.

Tells me that a permuted wave function has the same energy and hence it is the same state as the previous state if there is no degeneracies ok.

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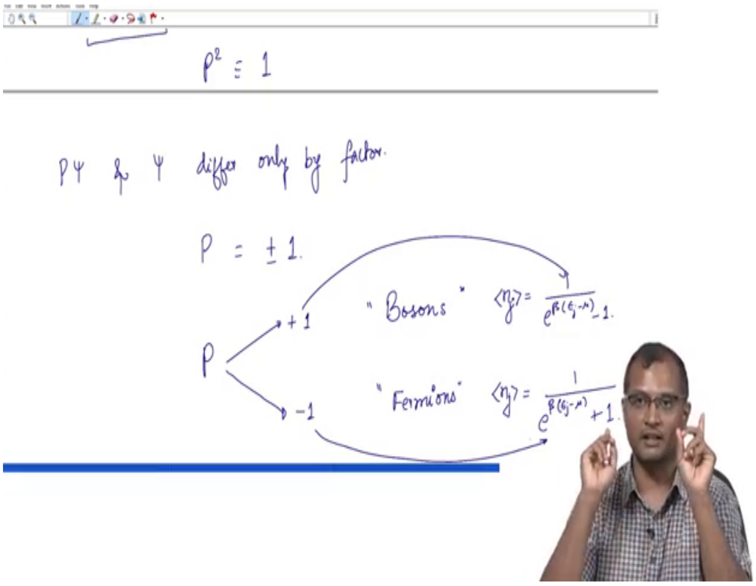

$P^2 = 1$

$P\psi$ & ψ differ only by factor.

$P = \pm 1.$

$P \to +1$ "Bosons" $\langle n_j \rangle = \frac{1}{e^{\beta(\epsilon_j-\mu)}-1}$

$P \to -1$ "Fermions" $\langle n_j \rangle = \frac{1}{e^{\beta(\epsilon_j-\mu)}+1}$

Then there are this is the same state because it has the same energy same Hamiltonian, which means P psi and psi differ only by some constant pre factor ok. It is just the same because if I take P psi and psi they should be differing only by a constant pre factor.

So, the eigenvalue equation is not moved you have the same pre-factor on both sides H operating on P psi will giving me some E operated on P psi. They are the same you know if psi differs from psi by just a factor, you are looking at nothing but h psi equals to E psi ok. You can knock off the constantly factor both sides which tells me that my operator P should have the eigenvalues plus or minus 1, there that is the only way I can make P square 1 ok.

Now, this basically leads to two definitions; so, if you have you can define particles or system of particles which have the property of the action of parity operator on the whole system giving an overall positive sign which means is not affecting the system as a system of bosons. And define the other type of there is only two possibility plus and minus 1 as system of fermions. And this is only a definition by the way you can slap the definition you can call P plus 1 as fermions and P minus 1 as bosons.

And everywhere your fermions will obey the Bose statistics and bosons will obey the Fermi statistics. So, what is in a name what is basically to be realized that these types of particles in the due course will be shown to obey a statistics of average number density going as 1 upon e to the power beta some j th level is e j minus mu minus 1 and these guys will be shown to have statistics which is 1 upon e raised to beta e j minus mu plus 1.

What is essentially it is that this should match with this and this should match with this, you can call bosons and fermions either way I do not care. But guys that commute with the parity operator the wave function of the guys which commute with the parity operator and for which the parity operator has an eigenvalue plus 1, I will call them as bosons for historical reasons.

And they will be shown to have statistics which go like this and the other guys will have statistics written below you can call whichever what you want, but historically we call them the first class as bosons and the second class as fermions. So, it is important that this map is between the values of the parity operator and the current statistics.

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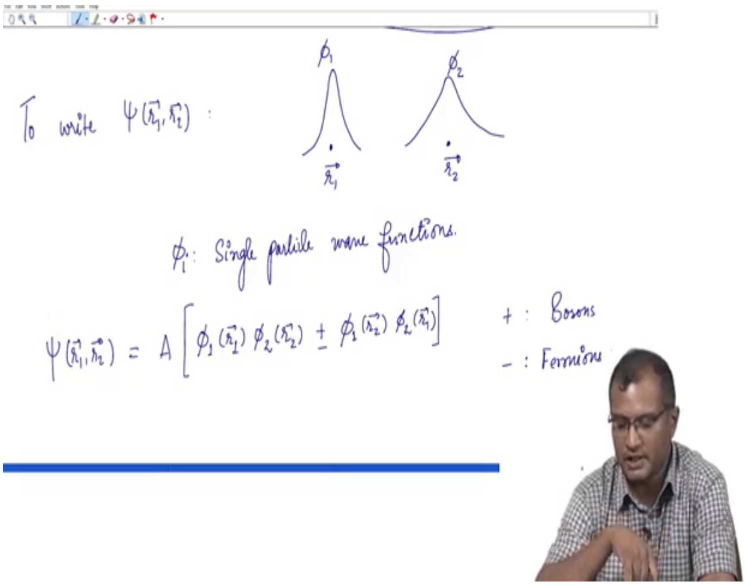

To write $\psi(\vec{r}_1, \vec{r}_2)$:

ϕ_i : Single particle wave functions.

$$\psi(\vec{r}_1, \vec{r}_2) = A\left[\phi_1(\vec{r}_1)\,\phi_2(\vec{r}_2) \pm \phi_1(\vec{r}_2)\,\phi_2(\vec{r}_1)\right]$$

+ : Bosons

− : Fermions

Now, we can write down the wave function of the system this two particle system as some kind of a linear combination of a single particle states so, I will take; now what do I mean by single particle states is the following. So, let me first write down the single particle so, draw a figure. So, to write a psi we consider two single particle states. So, I have 1 particle at location r 1 and another particle at location r 2 meaning of single particle state is that I can consider two localized wave functions at the location of r 1 and r 2. So, maybe you have another wave function which is localized r 2 call the first one as phi 1 call the second one has phi 2.

Classically, you have a particle there at r 1 and r 2, quantum mechanically it is represented by a wave function which is localized around r 1 and r 2 ok. So, it is on non-deterministic quantum mechanics so, I must if there are n particles in this room, I have n single particle wave functions each one of them localized around the particle physical location of that particle.

So, you can write down psi in terms of this phi so, these phi is are basically the single particle wave functions. As simply some normalization constant into you know the only linear combinations that you can construct basically our products of phi 1 and phi 2. So, I will take phi 1 r 1 this is like first particle sitting at location r 1 into phi 2 because this is the joint probability.

So, the fact that my system has two particles at r 1 and r 2 is the given by the joint product of phi localized at r 1 and phi 2 localized at r 2 is that it. For two particles I have one more possibility, that the second particle can sit at r 1 and the first particle can sit at r 2 so, that is given as phi 1 r 2 into phi 2 r 1. See phi 1 and phi 2 are localized wave functions one localized at r 1 the other localized at r 2, we have simply swap the particles ok.

This is for bosons, if I were to write down this wave function for fermions I have to take a negative sign here. Why? Because if I take a positive sign then that would mean that under permutation of the particle, the wave function is not incurring any overall negative sign which means plus sign has to be for the bosons and if these two particles are fermions where under permutation of the two particles. The overall wave function should incur a negative sign and that is only possible if I write down the second product with a negative sign.

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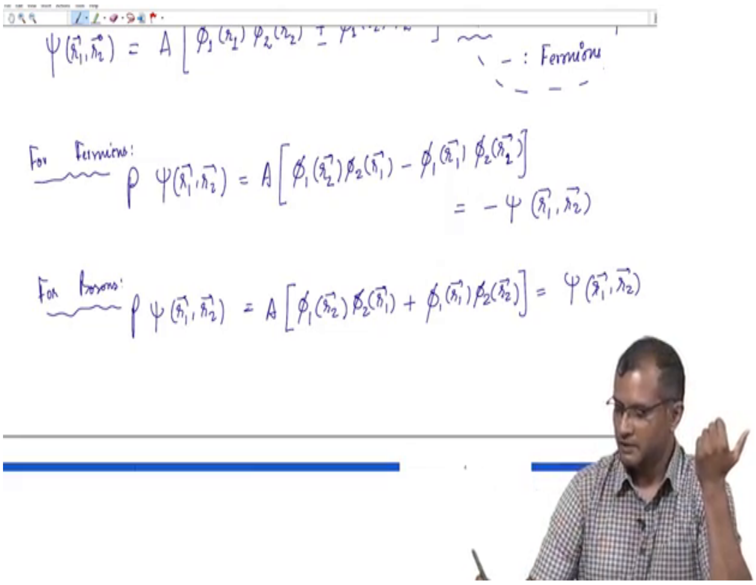

$\psi(\vec{r}_1,\vec{r}_2) = A\left[\phi_1(r_1)\phi_2(r_2) \pm\right.$

$- :$ Fermions

For Fermions:

$$P\,\psi(\vec{r}_1,\vec{r}_2) = A\left[\phi_1(\vec{r}_2)\phi_2(\vec{r}_1) - \phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\right]$$
$$= -\psi(\vec{r}_1,\vec{r}_2)$$

For bosons:

$$P\,\psi(\vec{r}_1,\vec{r}_2) = A\left[\phi_1(\vec{r}_2)\phi_2(\vec{r}_1) + \phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\right] = \psi(\vec{r}_1,\vec{r}_2)$$

So, now you can see the fermions if I swap r 2 with r 1 so, for fermions; so if I apply the parity operator on r 1 r 2 this will give me A times phi 1 r 2 phi 2 r 1. And I have to take the minus sign minus phi 1 r 1 into phi 2 r 2, but this is nothing, but minus of my original fermionic wave function. So, this is what I expect.

Similarly, for bosons if I apply the parity operator then I get back the same function phi 1 r 2 phi 2 r 1 plus because I have a plus sign for bosons already given here, hmm plus phi 1 r 1 into phi 2 r 2, but this is nothing but the old wave function. So, that is why for fermions I had to take a negative sign.

Now, it you can generalize this for three particle system, four particle system, n particle system. So, you can always write down the n-particle wave function by choosing one product and simply doing permutations of these products. And this way you can write down it in the determinant form which is called as the stator determinant form. For the two particles I can thus write down what I have written for the fermions only, for bosons you do not need you cannot write using the determinant form. So, bosons you just have to use a plus sign throat.

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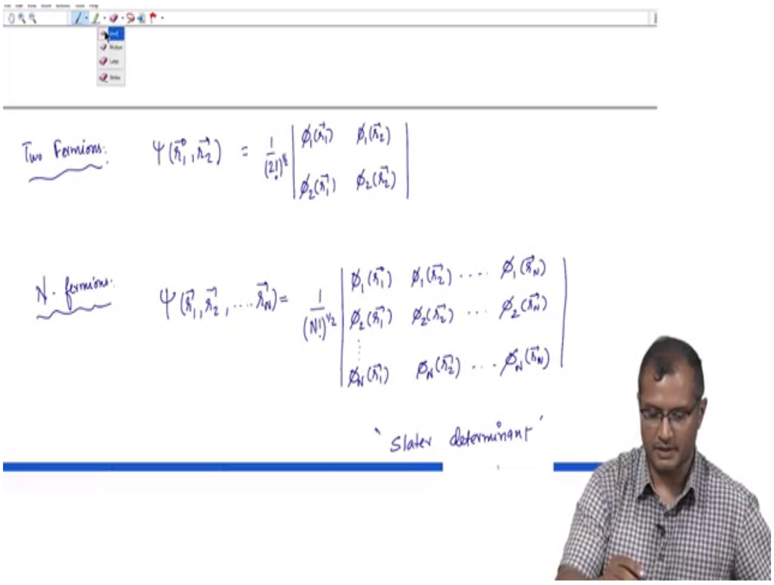

Two Fermions: $\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{(2!)^{1/2}} \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_1(\vec{r}_2) \\ \phi_2(\vec{r}_1) & \phi_2(\vec{r}_2) \end{vmatrix}$

N-fermions: $\Psi(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N) = \frac{1}{(N!)^{1/2}} \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_1(\vec{r}_2) & \cdots & \phi_1(\vec{r}_N) \\ \phi_2(\vec{r}_1) & \phi_2(\vec{r}_2) & \cdots & \phi_2(\vec{r}_N) \\ \vdots & & & \\ \phi_N(\vec{r}_1) & \phi_N(\vec{r}_2) & \cdots & \phi_N(\vec{r}_N) \end{vmatrix}$

'Slater determinant'

So, for two fermions that we have just discussed you can write down these this wave function also in the determinant form what I have written here? This particular this equation A times phi 1 r 1 into phi 2 r 2 minus phi 1 r 2 into phi 2 r 1 in the determinant form, you can write it as a times a determinant phi 1 r 1 ok.

And similarly for three fermions for I would say for N fermions, let us write down for N fermions directly. You can write this N-particle wave function as some normalization constant ok, I will call this as A 2 for two particles normalization. And this I will call for N particle normalization as phi 1 r 1, the last row being phi N. It is called as a stator determinant of form for historical reasons.

Couple of things to be you know sort of kept clear here is what is this normalization constant ok? So, we can work out the normalization constant by and this will give us the N factorial you know logic. You see for two particles, how many combinations could you construct? 2, 1 2 and 2 1 with three particles you had 6 because that is three factorial. So, the N particles I can construct N factorial permutations.

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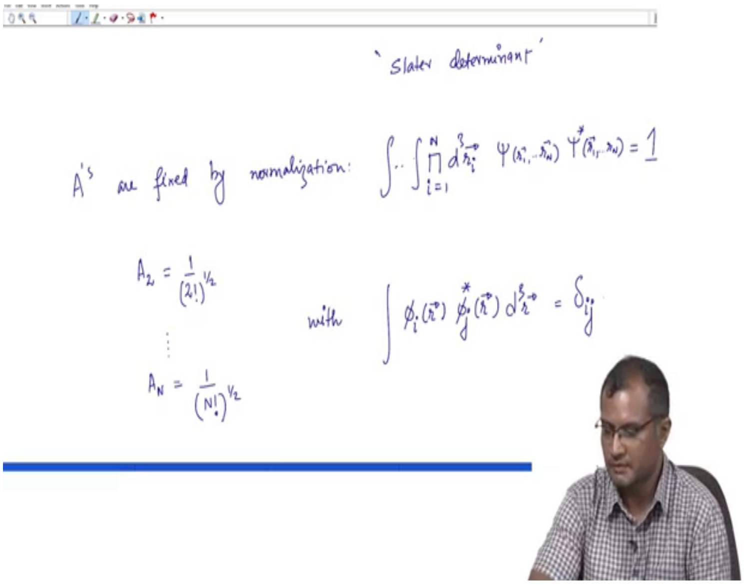

'Slater determinant'

A's are fixed by normalization: $\int \cdots \int \prod_{i=1}^{N} d^3\vec{r}_i \; \Psi(\vec{r}_1, \ldots \vec{r}_N) \, \Psi^*(\vec{r}_1, \ldots \vec{r}_N) = 1$

$A_2 = \frac{1}{(2!)^{1/2}}$

$\vdots$

$A_N = \frac{1}{(N!)^{1/2}}$

with $\int \phi_i(\vec{r}) \, \phi_j^*(\vec{r}) \, d^3\vec{r} = \delta_{ij}$

So, this normalization constant is fixed so, this A s are fixed by the normalization that your integration over the entire volume ok. So, I will take volume I going from 1 to N d cube r i size now N particle wave function ok, psi psi psi star is equal to 1 this is my normalization so, volume integral of psi psi psi star is 1 ok.

So, for example, in 2d I can think of A 2 as just 1 upon factorial 2 to the power half, because when you do a psi star this will become 1 upon factorial 2. And precisely you know the; so, the normalization on single particle wave functions also need to be specified here and I am going to write down. With this single particle normalizations given as and that is very simple to see why you have you know the sort of a orthogonality of these single particle wave functions. So, this is the orthogonal scalar product ok.

So, the orthogonality of the functions are basically represented as this integral phi with its complex conjugate given as the Kronecker delta function alright; that is the meaning of this orthogonality.

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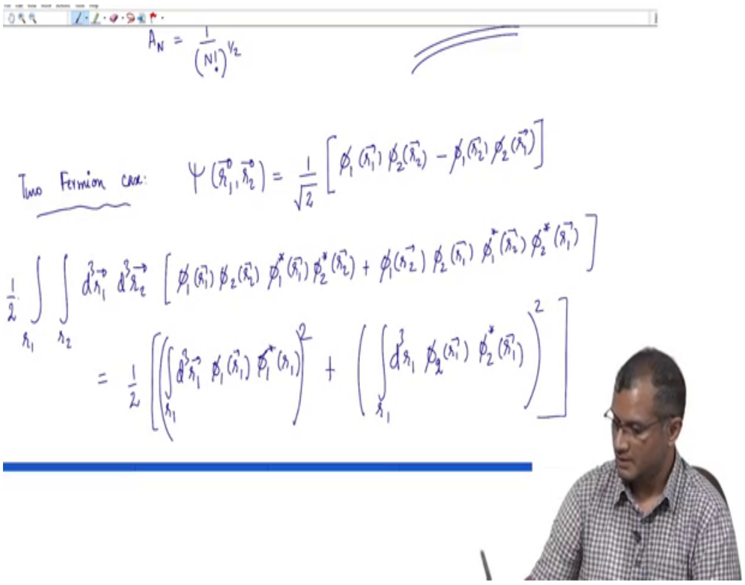

$$A_N = \frac{1}{(N!)^{1/2}}$$

Two Fermion case: $\Psi(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}}\left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2) - \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\right]$

$$\frac{1}{2}\int_{r_1}\int_{r_2} d^3\vec{r}_1\, d^3\vec{r}_2 \left[\phi_1(\vec{r}_1)\phi_2(\vec{r}_2)\phi_1^*(\vec{r}_1)\phi_2^*(\vec{r}_2) + \phi_1(\vec{r}_2)\phi_2(\vec{r}_1)\phi_1^*(\vec{r}_2)\phi_2^*(\vec{r}_1)\right]$$

$$= \frac{1}{2}\left[\left(\int_{r_1} d^3\vec{r}_1\, \phi_1(\vec{r}_1)\phi_1^*(r_1)\right)^2 + \left(\int_{r_1} d^3r_1\, \phi_2(\vec{r}_1)\phi_2^*(\vec{r}_1)\right)^2\right]$$

You can check so far for the simple two particle case, two fermion case you had your psi r 1 r 2 given as phi 1 r 1 phi 2 r 2 minus phi 1 r 2 phi 2 r 1. And I have to take the normalization as 1 upon square root of 2, 2 factorial is 2. It becomes very clear, why? Because of this norm so, I have these orthogonality of the single particle wave function that gives the norm as 1 upon square root n factorial.

So, you can write down the normalization condition as now you have two particles, so, you do a double integral. So, you do 1 integral on r 1 second 1 r 2 you can a d cube r 1 d cube r 2 psi psi psi star ok. So, you take 1 psi from the right hand side and the star of it will give you another 1 by 2 factorial so, there is a 1 upon 2 that comes out side. And what you have is basically phi 1 r 1 into phi 2 r 2 multiplied to its own complex conjugate ok.

So, I am going to write down phi 1 star r 1 into phi 2 star r 2 is multiply to its own complex conjugate. And the second term also multiplied to its own complex conjugate. So, that will come with a plus sign now because minus minus plus so, this will be a phi 1 r 2. The cross terms by virtue of this orthogonality will disappear. So, whenever you have a cross multiplication say you have a phi 1 r 1 into phi 2 r 2 multiplied to phi 1 star r 2 and phi 1 star r 1 that will go to 0, because on 1 integration coordinate if the phi i and phi j are not the same in this K delta function will be 0 ok.

So, you have only two terms that will basically contribute and I can write this as now 1 upon 2. The first term can be written as integral on r 1 d cube r 1 phi 1 r 1 into phi 1 star r 1 into integral r 2. I can simply write down this as a square of this because these are independent integrals plus integral on r 1 I can do this integral on r 2 if you want. If I want to do it in r 1 then I have to choose phi 2 here ok.

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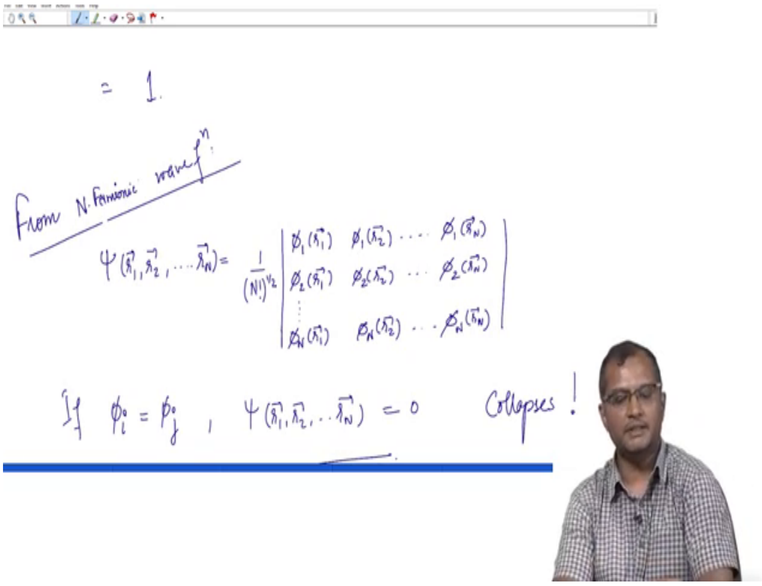

$= 1.$

From N-Fermionic wavef^n:

$$\Psi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_N) = \frac{1}{(N!)^{1/2}} \begin{vmatrix} \phi_1(\vec{r}_1) & \phi_1(\vec{r}_2) & \cdots & \phi_1(\vec{r}_N) \\ \phi_2(\vec{r}_1) & \phi_2(\vec{r}_2) & \cdots & \phi_2(\vec{r}_N) \\ \vdots & & & \\ \phi_N(\vec{r}_1) & \phi_N(\vec{r}_2) & \cdots & \phi_N(\vec{r}_N) \end{vmatrix}$$

If $\phi_i = \phi_j$, $\Psi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_N) = 0$ Collapses!

And the other integral is basically a definite integral the same type so, there is nothing but the square of this integral is it ok. Because r 1 and r 2 are independent I can write a square of that which is nothing but 1 because each one of them is 1 from the orthogonality. So, this is how I am going to write down the normalization pre-factors; so, for these A n I am going to write down 1 upon N factorial square root and for A 2 I am going to write down 1 upon 2 square root 2 factorial ok.

So, now you can see if I just use this N particle wave function, I can see how Pauli's exclusion principle naturally arises, can you see why; can you see why? So, suppose. So, from this N particle wave function which is written in the form of determinant I can simply use a property of determinant. If 2 rows of a determinant becomes same then the determinant collapses, which means if some random i th row becomes the same as the j th row. Let us say phi 2 row becomes the same as the phi 3 row then the determinant will collapse.

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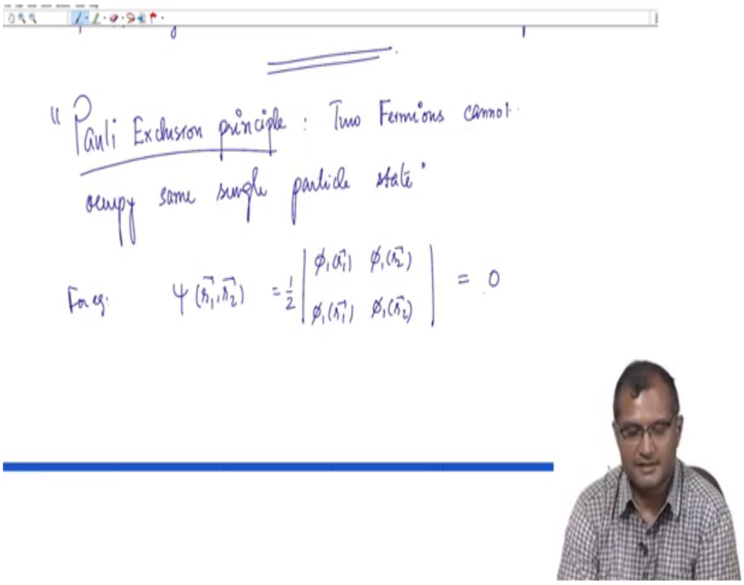

"Pauli Exclusion principle : Two Fermions cannot occupy same single particle state"

For eg: $\Psi(\vec{r}_1,\vec{r}_2) = \frac{1}{2}\begin{vmatrix}\phi_1(\vec{r}_1) & \phi_1(\vec{r}_2)\\ \phi_1(\vec{r}_1) & \phi_1(\vec{r}_2)\end{vmatrix} = 0$

So, the N particle wave function will collapse to 0 which actually is the mathematical statement of the Pauli's exclusion principle for fermions ok. Now I must not write down N particle wave function, I must be very specific that this later determinant is a N fermionic wave function ok. So, that is the region of Pauli's exclusion principle that you cannot force 2 fermions to occupy two identical single particle states.

So, if 2 single particle states i and j; phi i and phi j become the same then the entire wave function the system will collapse and that microstate has 0 weight in your microstate ok. Two fermions cannot occupy the same single particle state because that would simply make two rows of my stator determinant identical ok.

And for example, for a 3 part two particle system its very simple psi psi r 1 r 2 its very simple to see why; it would simply make I have got a 1 upon factorial two outside right which is 1 by 2 and I am going to write down phi r 1 phi 1 r 2 and I made phi 2 as phi 1 so, this becomes phi 1 r 1 and it becomes phi 1 r 2 this is 0 determinant.

So, this is the fact that your system had an odd parity you could write it as a slicker determinant and because you wrote it as a determinant and the fact that you cannot write to you know rows and determinant which are you know identical without making me determinant itself 0 gives this Pauli's exclusion principle that is seen in qunatum mechanics. So, it is an algebraic linear algebraic consequence of you know doing a quantum mechanics on these industry (Refer Time: 05:20) particles.

So, that is the end of our lecture, in the next class we will carry over from here and provide two different statistics for these. So, called different types of identical particles the fermions and the bosons will show how are these statistics derived from first principles in these two systems. In this class we have only discussed why we have two different types of statistics because of the.