

**Quantum Mechanics**  
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**Lecture – 41**  
**Identical Particles & Quantum Computer - II**



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**Multi-particle system**

- Helium atom will have two electrons -
- If we ignore the interactions between the two electrons, then the potential energy of the helium atom will be  
sum of potential energy of each electron with two protons inside the nucleus

Even if the interactions are included, there is a principle called Pauli's exclusion principle which is obeyed by system of electrons.

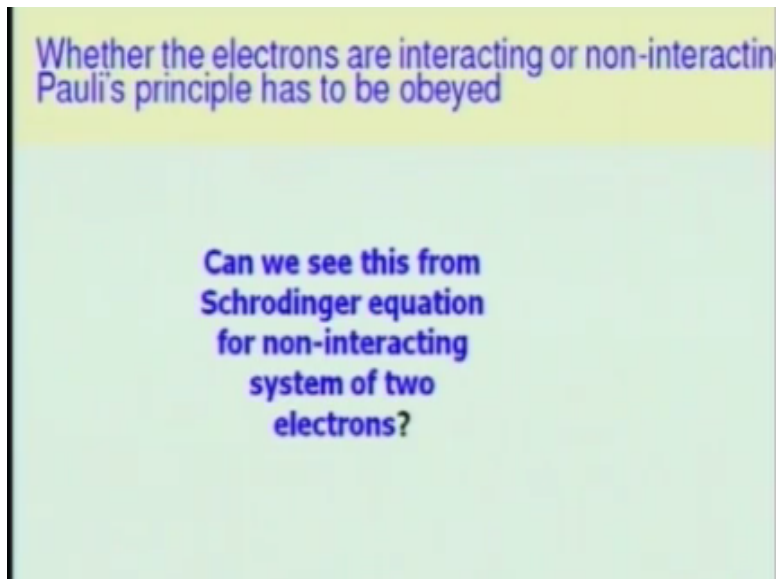
The principle states "no two electrons can share the same set of quantum numbers"

Suppose, you go to a helium atom or something or a multi particle system, helium atom has 2 electrons just to make the system simple, let us take them to be non-interacting, it is not quite correct but whether they are interacting or non-interacting, what has to be obeyed if suppose, I put the first electron in set of quantum numbers let us put the first electron in the ground state which is  $n = 1, l = 0$  and  $s = 1/2$  or  $m_s = +1/2$  suppose, you put the first electron.

Can you put the second electron there? whether it is interacting or non-interacting? This is also an experimental data that is Pauli's exclusion principle, okay the second electron positioning should be such that both the electrons cannot have the same set of all the quantum numbers. So you can try to see even if the interactions are included, Pauli's exclusion principle cannot be violated it has to be obey.

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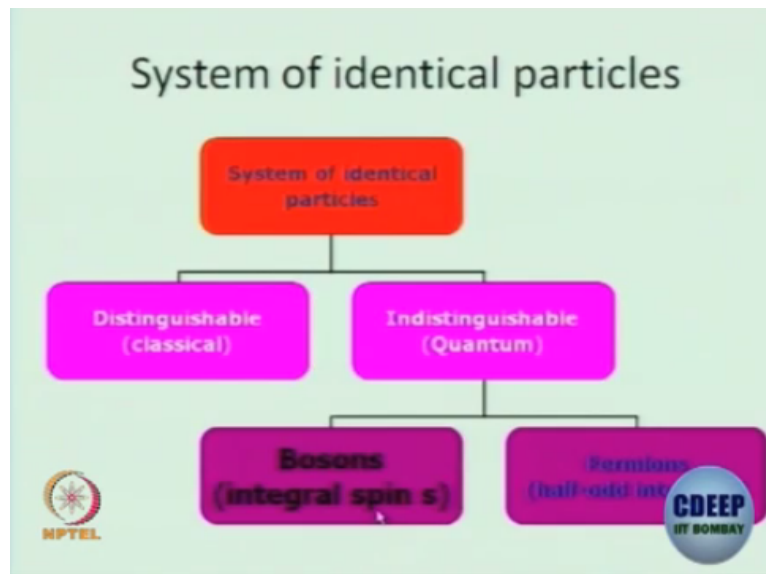


So, no 2 electrons can share the same set of quantum numbers, so what does that tell us whether the electrons are interacting or non-interacting, Pauli's exclusion principle has to be obeyed, how do you incorporate Pauli's exclusion principle for 2 electrons which are non-interacting, take the 2 electrons to be very far away position, the interaction is really feeble that you treat it to be almost non interacting.

It is like a dilute system, what is the dilute system; different atoms are so far away that you can pretend as if there is no interaction only when they start becoming concentrated, then you start seeing the  $1/r$  interactions between the repulsive interaction between the electrons also, right, so but how do you write if you have given 2 electrons far away in position, how do you write the wave function, how will you write the Hamiltonian?

There will be a Hamiltonian for the first electron, there will be a Hamiltonian for the second electron, if there is no interaction between these 2, you can write  $h_1 + h_2$  and you can write  $\psi_1$  wave function for the first electron,  $\psi_2$  wave function for the second electron, those 2 are not talking to each other which means, the total wave function of the system given by  $h_1 + h_2$  is  $\psi_1 * \psi_2$ .

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But you have to also obey the Pauli's exclusion principle, how do you do that? This is where you need to know the formal classification which I am sure you would have studied in your first year course, why is it distinguishable in classical physics, suppose I take 2 electrons, I can actually distinguish them in classical physics, what is the reason, they do not have a wave associated with it, it is the point particle in classical physics.

Only, when 2 of the electrons have a wave, they may start overlapping, then you cannot say whether this overlap region, this part is this electron and the other part is other electron, so the indistinguishable concept will start coming only in quantum physics classically, you can keep an eye on that electron okay, so it is distinguishable, even though they are identical, classical physics they will be distinguishable.

But quantum because you will give the wave form to those particles, the waves can overlap in the overlapping region, it becomes fuzzy you do not know what is your electron which you are keeping track okay, so it becomes indistinguishable and there are also 2 categories for particle which are seen in the experiments, so in the context of Stern-Gerlach, there were 2 splitting's which 1 due to right  $s = 1/2$  but there are other particles which higher spins also okay.

So, there of 2 categories; one is Bosons, where the spin, this is an internal space, this is not your orbital angular momentum, this is the new quantum number, everyone had heard about this great news about god particle right, the god particle belongs to the  $s = 0$ , at least, there are signatures that it has been; we have got god particle and then  $s = 0$  is also more or less 0, okay, so they are Bosons.

Bosons have integer spin, what about photon, photon; how many possible polarizations are there? Y2, what about the longitudinal one; photons are mass less, so you have only the transverse polarization, there are 2 of them but if you make it massive, then you can also have the longitudinal polarisation, so there will be 3 for a massive object and that 3; how will you account;  $s =$ ; if there are 3 states,  $s$  has to be 1 and so on.

So, every object which we see in experiments in particle scenario, either will have an integer spin or a half integer spin, so how did they see the spin is that they go to the refrain where the orbital angular momentum is 0, they are still see there are 3 states, if they see 3 states, then they will say this particle should belong to the  $s = r$  in the restraint because the orbital angular momentum  $l$  is 0.

In spite of that they see 3 states, then they will say that that object is a Boson with  $s = 1$ , what are the other Bosons which we see in the experiments in particle physics is that we have weak interaction, weak nuclear force interactions, where we P see the vector Bosons, the  $W + W - z$ , I am sure you would have just read as data, they have 3 states, so they are like the spin 1 Boson that is why it is called vector boson.

Vector means that there are 3 components is what we are familiar right, Fermions also one of the fermions which you have seen in the hydrogen atom and Stern-Gerlach, anomalous is  $s = 1/2$  but you can also have other kind of higher  $1/2$  odd integral like spin  $3/2$  so, if you have spin  $1/2$  odd integral you call them to be fermions okay, so these are 2 classes, there is no way a Boson can become a fermion.

Bosons have a different property, what is the property; it does not need to obey Pauli's exclusion principle that is why you had this famous Bose Einstein condensed state, you can put any number of Bosons in the ground state whereas, if I give you any number of electrons, you cannot put everything in the ground state, Pauli's exclusion principle prevents it and you have to stack it and you will get a Fermi energy, right.

So, this is a formal classification if you have a system of identical particles in quantum physics, there can be integral spin particles which is Bosons or  $1/2$  odd integrals spin particles which is

fermions, electron is a fermion and Bosons are all the vector particles including the photon you can call it as an integral as well, okay.

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Let's take two identical particles - for example, two electron system.

In **classical physics**, these identical particles are **distinguishable**.  
By distinguishable, we mean that we can keep track of the trajectory of the two particles by marking electron 1 and electron 2.

In **quantum physics**, these identical particles are described by wavefunctions which will have a spread and hence the individual labelling of the two electrons is not possible when the two wavefunctions overlap- That's why, the system of identical particles are considered **indistinguishable in quantum physics**.

These indistinguishable system of identical particles can have integer spin  $s$  or half-odd integer spin  $1/2, 3/2, 5/2, \dots$

The integral spin  $s$  particles are called **Bosons**  
The half-odd integer spin particles are called **fermions**

How do we write this wave function? so I have already said that identical particles are distinguishable because we can keep track of the trajectory of the 2 particles by putting some colour on it or marking on it but in quantum physics, they will have wave functions and they start overlapping so, there is they become indistinguishable and you can try to classify them as integral spin or half odd integral spins.

And the integral spins are called Bosons, half odd integral spins are fermions yeah, so there is this; one is when we have composite objects, we have a particle which has in a; it is called delta plus particle okay, there are particles which are made of 3 quarks, proton is also made of 3 quarks but that belongs to the spin half but there are particles where you can combine 3 quarks which can give you spin  $3/2$  which are like the delta + particle omega particle and so on.

If suppose, you have 5 electrons and you make a bound state of 5 electrons, it can have the total spin of that bound state, maximum value could be a  $5/2$ , some subset of it can behave like a spin  $5/2$ , there would be some subset will behave like a spin  $3/2$ , some subset will behave like a spin  $1/2$ , so these things will get into it at some point, okay, yeah, but the upper bound is that if you have a composite of 3 quarks, which each one is spin half.

I am trying to say that you can have a spin  $3/2$  object which is a composite, you can have a spin half object which is a composite and so on, proton belongs to spin half composite whereas your

delta + and omega particle belong to the spin 3/2 object but you do not find in the lab as spin 5/2, in the composite particle physics, they are all called hadrons, the zoo of hadrons, do not have a spin 5/2.

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**System of two identical particles**

Let's look at Schrodinger equation for a system of two non-interacting particles placed inside **an one-dimensional infinite potential well**:

$$\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} \Psi(x_1, x_2) + \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} \Psi(x_1, x_2) = E \Psi(x_1, x_2)$$

where  $x_1, x_2$  denotes the coordinates of particle 1 and particle 2 respectively and  $\Psi(x_1, x_2)$  is the two-particle wavefunction.

The differential operator for particle 1 and particle 2 are separate and

$$\Psi(x_1, x_2) = \phi(x_1)\phi(x_2)$$

So that is why we try to say that at most, these composites should be made of only 3 spin half particles so for, I have try to take you on the bosons and the fermions and let us just take a simplest situation, 2 particle system in one dimensional potential well and write the wave function should be a function of position of the first electron, position of the second electron, this x1 and x2 is still in one dimension.

But this subscript 1 for the first electrons, subscript 2 for the second electron, this is the kinetic energy for the first electron, this is the kinetic energy for the second electron and it has to be satisfying your time independent Schrodinger equation. So, what is this solution? So, you can write the solution to this equation as a product of solutions to each electron if they are non-interacting, why is it non interacting? I have not put a v, which is coupling x1 and x2 that is why it is not interacting.

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$\Psi(x_1, x_2) = \phi(x_1)\phi(x_2)$

where  $\phi(x_1)$  and  $\phi(x_2)$  are exactly the particle in a box wavefunctions.

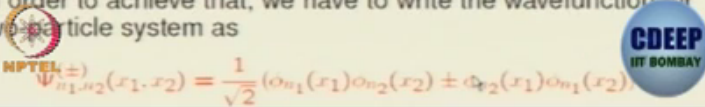
If the two identical particles are in quantum state  $n_1$  and  $n_2$ , then the solution to the Schrodinger equation will be

$$\Psi_{n_1, n_2}(x_1, x_2) = \phi_{n_1}(x_1)\phi_{n_2}(x_2) = \phi_{n_2}(x_1)\phi_{n_1}(x_2)$$

Prob. Densit  
Not same

Suppose the particles are electrons, Pauli's exclusion principle requires that the wavefunction  $\Psi_{n_1=n, n_2=n}$  has to be zero.

In order to achieve that, we have to write the wavefunction for two particle system as

$$\Psi_{n_1, n_2}^{(\pm)}(x_1, x_2) = \frac{1}{\sqrt{2}} (\phi_{n_1}(x_1)\phi_{n_2}(x_2) \pm \phi_{n_2}(x_1)\phi_{n_1}(x_2))$$


So, for such a non-interacting electrons, so particle in a box will have only 1 quantum number which is the  $n_1$  and for the particle 1 and  $n_2$  for the particle 2 and they are identical, what will you do; you can write the composite wave function to be product of particle 1 in quantum state  $n_1$  and particle 2 in quantum state  $n_2$  or you could also write particle 1 in quantum state  $n_2$  because they are identical, you cannot distinguish, what else can be possible?

Both are equally possible, a linear superposition is also possible right, you can take a linear superposition of them that is also possible but you should take a linear superposition in such a way that when I put both the electrons in the same quantum suppose, i put both the electrons in the same ground state or same first excited state, what is the meaning of that;  $n_1$  has to be =  $n_2$  but Pauli's exclusion principle does not allow, so what linear combination you can take?

You have to take a linear combination, so that composites when both  $n_1 = n_2$ , it has to be 0 but do we see that here, if you put  $n_1 = n_2$ , the solution exists, if you put  $n_1 = n_2$ , this solution also exists, so these are not valid by Pauli's exclusion principle, what is valid is; you have to take a linear combination, when I put  $n_1 = n_2$ , the wave function has to vanish that is it, there is no such solution possible, only trivial.

So, probability density if you try to work for this case, it is not the same and you want the Pauli's exclusion principle to be satisfied that is the wave function has to be 0 when you put  $n_1 = n$  and  $n_2 = n$ , so how will you achieve both of them, you can write + or -, which one is right; it is the minus sign which is right, for the electrons suppose, I replace the electron by a boson, we will put a plus sign.

Because it should be nonzero you cannot have a minus sign clear and this will also take care that the probability density, the plus sign; + 1 and – 1 is very important, so you can see that for a 2 particle system, even for non-interacting, the wave function should be either the plus sign can be also interpreted as symmetric and exchange of particle 1 and particle 2, minus sign can be interchange as if you exchange particle 1.

And particle 2, you get a negative sign, these are like your odd functions and even functions which you are studying, where you took  $x_2 - x_1$ , here I am saying make the first particle and the second particle exchange under exchange, the wave function is anti-symmetric for electrons and symmetric for bosons, so this will extrapolate if you had 3 particles, you have to make it totally anti symmetric and for bosons you can make it to be totally symmetric, okay.

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$$\Psi_{n_1, n_2}^{(\pm)}(x_1, x_2) = \frac{1}{\sqrt{2}} (\phi_{n_1}(x_1)\phi_{n_2}(x_2) \pm \phi_{n_2}(x_1)\phi_{n_1}(x_2))$$

where  $\Psi_{n_1, n_2}^{(-)}$  is an odd-function under exchange and obeys Pauli's exclusion principle. This will represent two-electron system.

Similarly the even function  $\Psi_{n_1, n_2}^{(+)}$  allows both the particles to be in the same quantum state. This is the property of bosons allowing any number of integral spin particles to occupy a quantum state.

This procedure done for two-particle system inside a infinite well can be done for electrons subjected to  $1/r$  potential energy. Instead of writing all the four quantum numbers for those particles, we can say

one electron is in state  $\alpha = (n_\alpha, l_\alpha, m_{l_\alpha}, m_{s_\alpha})$

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So, I have just giving you a flavour that you can try to write the wave function for a 2 electron system as an odd function with the - sign, this is should become the - sign similarly, the even functions is allowed for bosons. What do you do for the hydrogen atom problem, I did this for a particle in a box you formally, say that the fs electron is in a state alpha, alpha is a compact notation which tells you it has this alpha is n alpha is the principal quantum number, L alpha is azimuthal quantum number, ml alpha, ms alpha, the s can be suppressed.

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The set of four quantum numbers which is associated with the state  $\alpha$  **must not be same** as the state  $\beta$  for the two electron system

$$\Psi_{\alpha,\beta}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} (\psi_{\alpha}(\vec{r}_1)\psi_{\beta}(\vec{r}_2) - \psi_{\beta}(\vec{r}_1)\psi_{\alpha}(\vec{r}_2))$$

where  $\psi_{\alpha}(\vec{r}_1) = \psi_{n_{\alpha}, l_{\alpha}, m_{l_{\alpha}}}(\vec{r}_1)\phi_{m_{s_{\alpha}}}$

$\phi_{m_{s_{\alpha}}}$  is independent of  $\vec{r}_1$  and is introduced by hand to match with experimental data in **non-relativistic theories**

For almost zero velocity particles, the spin part of the wavefunction looks like binary bits 0, 1 in classical computers. Further, quantum physics allows superposition and these two spin states are called **qubits**

Because for electrons you know  $s$  is  $1/2$  you do not need to explicitly put the  $1/2$ , okay, similarly put  $\beta$  for the other state, write down the total anti symmetric where  $\alpha$ , the long hand notation for  $\alpha$  is the 4 quantum numbers similarly,  $\beta$  it is again the 4 quantum numbers and those 2 should be different at least one of them should be different, clear and this is what I was trying to say.

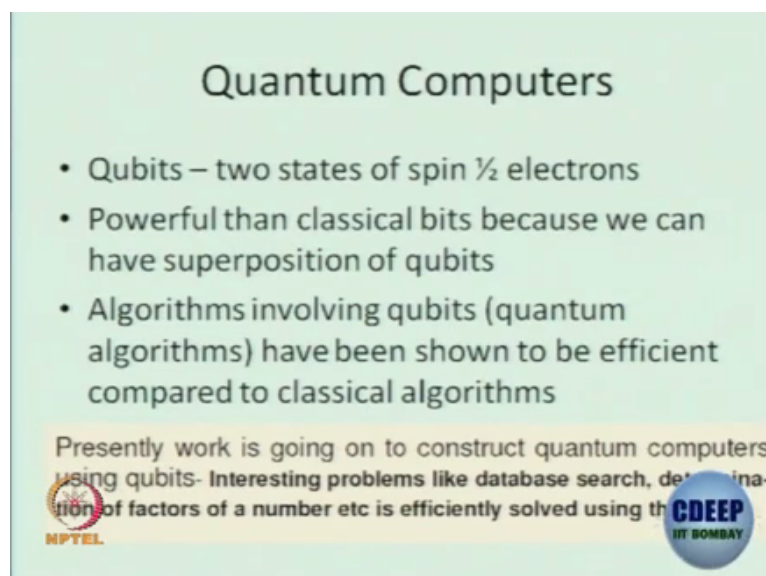
You can write the position space wave function which depends on only the orbital quantum number and magnetic quantum number but you can put a product which is the new space which does not talk to them put that wave function with an  $m$ , the magnetic quantum number okay, so this is a formal way in which you can write your wave function as a product of the position space wave function times the spin state.

A spin state does not have any projection on the position basis, it is an internal spaces, so this one is independent of  $r_1$  and it is introduced by hand to match with the experiments in non-relativist theories, so if you take zero velocity, you can ignore that this wave function is almost like the S wave and you can concentrate on the spin part of the; take  $n = 1$  or even for any  $n$ ,  $l$  to be 0 situation, then you can concentrate on this part of the wave function.

This is the beautiful concept that these 2 states are like the 2 bits in your computer's; binary operation which we do all the computations which are done involves only playing around with 0 and 1, right, 0 and 1 binary then bytes is how many bits; 8 of them, each one is called as a bit which is 0 and 1 and you can have a byte which is 8 of such bits. What is quantum mechanics tells us?

These are also 2 states, so just to keep track it is quantum mechanics, we call them as qubits okay and there also 2 states but there is much more; in the 0 and 1, you can keep adding 0 and 1 but in the context of qubits, you can take superposition, you can start taking superposition of various possible qubits, so this is you know, this is suppose, to increase your speed, suppose, to enhance what all you want to do in a much more efficient way, is what is the; is what we all feel, okay.

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The slide is titled "Quantum Computers" and features a light green background. It contains three bullet points: "Qubits – two states of spin 1/2 electrons", "Powerful than classical bits because we can have superposition of qubits", and "Algorithms involving qubits (quantum algorithms) have been shown to be efficient compared to classical algorithms". Below the text, there is a line of smaller text: "Presently work is going on to construct quantum computers using qubits- Interesting problems like database search, determination of factors of a number etc is efficiently solved using the". At the bottom left, there is a logo for NPTEL, and at the bottom right, there is a logo for CDEEP IIT BOMBAY.

So, just to give you that qubits are two states of the spin 1/2 electrons, powerful than classical bits because there you just play around with only 0 and 1 but here you have superposition of qubits, algorithms have already been written in the literature, so some of you would have known at least, so they have called quantum algorithms, they are definitely efficient especially, the factorisation problem can be solved in polynomial time shows algorithm okay.

So, these have been achievable using qubits and lot of work, there are lot of problems you know gravitational wave, wave detection, why could not we detected, it took so long why, there is so much of these background noise and it is such a feeble thing so similarly, this quantum computer construction even though theory can be a lot of in coherence, so how many things have to be taken care of and that is itself a challenge, people are working on it.

They have try to make a couple of qubits together, couple of qubits together, still it has not reached a level that we have a quantum computer but people are at it because theory wise we do see that there will be lot of efficiency in the computation, you can do things faster, still it is at

the research level okay, so I thought I should give you some motivation before we get into doing this hard core calculation since Stern-Gerlach experiments that why it is spin  $1/2$  and why lot of excitement are going on, okay. I will stop here.