Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'

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Lecture 25
Schrodinger, Heisenberg and Dirac "pictures" of QM

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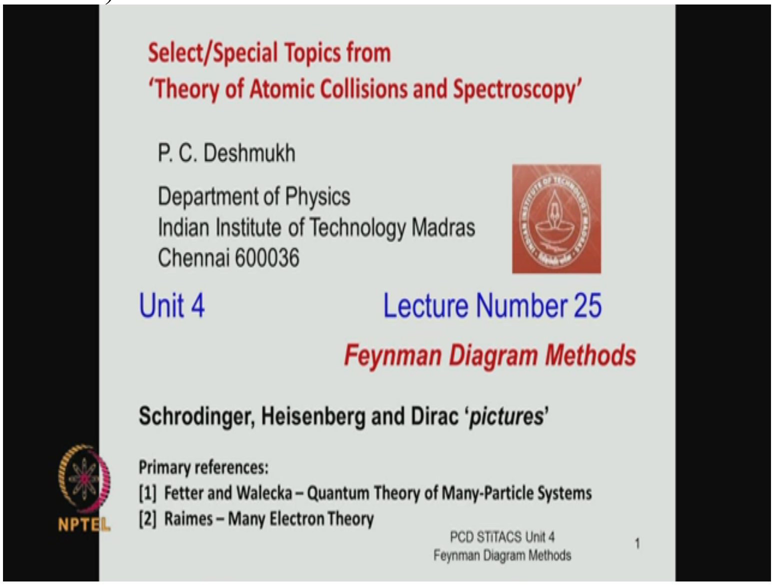

Select/Special Topics from
'Theory of Atomic Collisions and Spectroscopy'

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Unit 4

Lecture Number 25

Feynman Diagram Methods

Schrodinger, Heisenberg and Dirac '*pictures*'

Primary references:
[1] Fetter and Walecka – Quantum Theory of Many-Particle Systems
[2] Raimes – Many Electron Theory

Greetings, after doing the random phase approximation in unit 3 we will today start with the next unit. And in this unit we will introduce Feynman diagram methods, I would like to suggest these two references which you see on your screen Fetter and Walecka's book Quantum Theory of Many-Particle Systems and the book by Raimes Many Electron Theory. These will be the primary sources for this unit.

And before we get into the details of the Feynman diagram methods today's class will be like warming up for this topic. We will revisit a little bit of what you would have done in your quantum mechanics course on the Schrodinger picture, the Heisenberg picture and the Dirac picture. So, we will spend some time just warming up and that is what we will do today and then build the topic from there.

So, let me first remind you some results from the unit 3 from the previous unit and I will refer to the Hartree Fock model. And the Hartree Fock model which we discussed earlier in the course on atomic physics and later we dealt with it also in unit 3 of this course. And in particular I would like to refer to the lecture number 19 and 20 of unit 3 and slide number 96 and 97 from that lecture.

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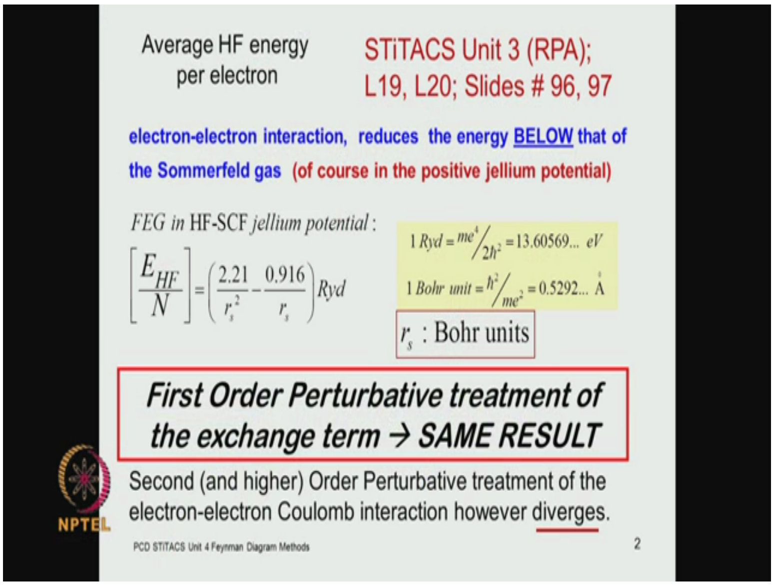

Average HF energy per electron

STiTACS Unit 3 (RPA); L19, L20; Slides # 96, 97

electron-electron interaction, reduces the energy BELOW that of the Sommerfeld gas (of course in the positive jellium potential)

FEG in HF-SCF *jellium potential*:

$$\left[\frac{E_{HF}}{N}\right]=\left(\frac{2.21}{r_s^2}-\frac{0.916}{r_s}\right)Ryd$$

$1\,Ryd = me^4/2\hbar^2 = 13.60569...\ eV$

$1\,Bohr\ unit = \hbar^2/me^2 = 0.5292...\ \mathring{A}$

r_s : Bohr units

First Order Perturbative treatment of the exchange term → SAME RESULT

Second (and higher) Order Perturbative treatment of the electron-electron Coulomb interaction however diverges.

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So, I will recollect one of the results from there and what we learnt over there that when you take into account the electron-electron interaction in the Hartree Fock, you get an energy which is actually lower than that of the Sommerfeld gas which is somewhat surprising because you have the electron-electron interaction and you expect that okay it will increase the energy because it is repulsive.

But then it has an attractive component which is the exchange energy and that is completely taken into account in the Hartree Fock model right. And what the exchange does is it, it is a result of the fact that the many electron wave function is an anti symmetrised wave function in consistency with the Fermi Dirac statistics the electrons being half integer spin particles. And what this does is to keep electrons with parallel spins away from each other okay.

And that is what reduces the energy as we have seen and what we found is that the average Hartree Fock energy per electron, so Hartree Fock average energy per electron if capital N is the number of electrons then this is given by a result which we have discussed in the previous unit and you will remember that result.

Now what we also discussed is the fact that if you obtain this result using first order perturbation Theory rather than the self-consistent field methodology of the Hartree Fock scheme you can essentially the same result. So, we discuss this in the previous unit in the lectures 19 and 20. However if you went to higher order perturbation theory, if you went to the second order okay or any order higher than the first.

Then you find that the methodology does not converge at all and you cannot use perturbative methods. So, you have to look for methods which are non perturbative and whereas the Hartree Fock self-consistent method is equivalent in a certain sense to the first order perturbation theory going beyond the perturbation method is important. Because Hartree Fock takes into account this exchange correlation.

The exchange interaction so it takes into account all the correlations which is coming from the Fermi Dirac statistics but then there are some correlations which are left out and the correlations which are left out are what we call as the Coulomb correlation. So, correlations in a many electron system are of two kinds one is the spin correlations they are equivalently the Fermi Dirac correlations or exchange correlations, statistical correlations.

They are all synonymous equivalent terms to describe this fact that the many electron system observes the Fermi Dirac statistics. But then there are other correlations and these are the Coulomb correlations and we are interested in taking account of these correlations that is what many-body theory is about.

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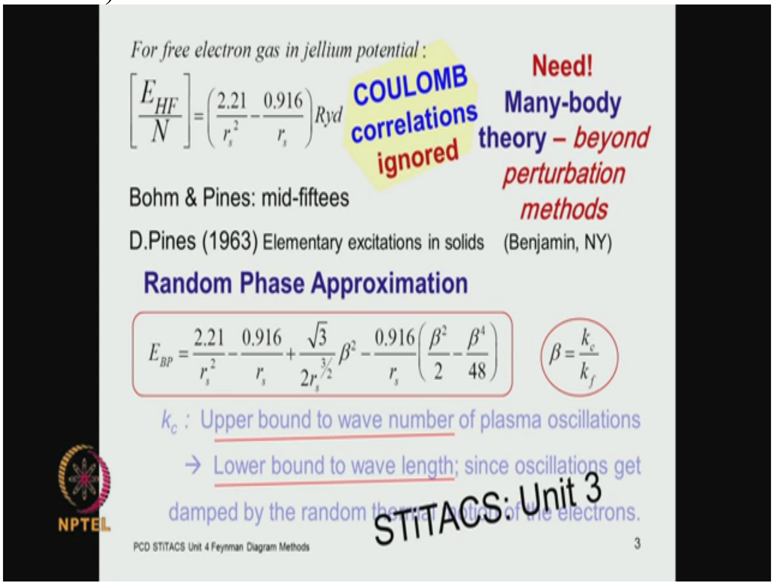

For free electron gas in jellium potential:

$$\left[\frac{E_{HF}}{N}\right]=\left(\frac{2.21}{r_s^2}-\frac{0.916}{r_s}\right)Ryd$$

COULOMB correlations ignored

Need! Many-body theory – *beyond perturbation methods*

Bohm & Pines: mid-fiftees

D.Pines (1963) Elementary excitations in solids (Benjamin, NY)

Random Phase Approximation

$$\boxed{E_{BP}=\frac{2.21}{r_s^2}-\frac{0.916}{r_s}+\frac{\sqrt{3}}{2r_s^{3/2}}\beta^2-\frac{0.916}{r_s}\left(\frac{\beta^2}{2}-\frac{\beta^4}{48}\right)}$$

$$\beta=\frac{k_c}{k_f}$$

k_c : Upper bound to wave number of plasma oscillations

→ Lower bound to wave length; since oscillations get damped by the random thermal motion of the electrons.

STITACS: Unit 3

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So, these Coulomb correlations are ignored in this result and these can be addressed using a variety of different techniques and we are in the process of discussing some of them. And for this you need a formal many-body theory this is where quantum field theory methods or many-body methods become necessary and they help us go beyond perturbation methods.

So, the technique that we discussed in the previous unit is the random phase approximation it is due to Bohm and Pines which was developed in the mid-50s of the previous century, very nicely described in the book by David Pines elementary excitations in solids and it gives you a result beyond the first order perturbation theory it gives you a correction and we haven't discussed some of these results in unit 3.

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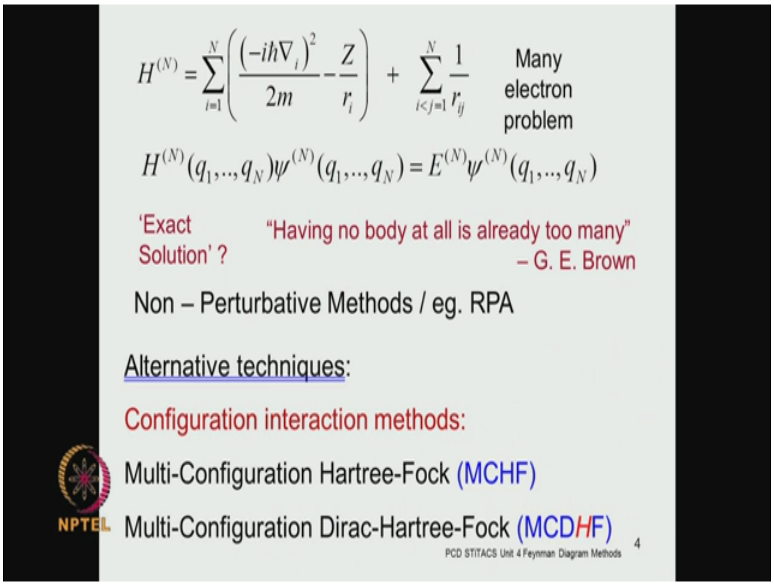

$$H^{(N)} = \sum_{i=1}^{N}\left(\frac{(-i\hbar\nabla_i)^2}{2m} - \frac{Z}{r_i}\right) + \sum_{i<j=1}^{N}\frac{1}{r_{ij}}$$

Many electron problem

$$H^{(N)}(q_1,..,q_N)\psi^{(N)}(q_1,..,q_N) = E^{(N)}\psi^{(N)}(q_1,..,q_N)$$

'Exact Solution' ?

"Having no body at all is already too many"
– G. E. Brown

Non – Perturbative Methods / eg. RPA

Alternative techniques:

Configuration interaction methods:

Multi-Configuration Hartree-Fock (MCHF)

Multi-Configuration Dirac-Hartree-Fock (MCDHF)

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So, this is just a quick recapitulation of that and the basic problem that we are trying to solve is just the many-electron Schrodinger equation with this Hamiltonian. So, this is the one electron part and this is the Coulomb part but then all the statistical correlation is appearing in the Hartree Fock formalism because the N electron wave function has to be an anti symmetrised wave function.

And as I pointed out earlier you do not have an exact solution for this problem. I had quoted Brown, earlier also that if you are looking for exact analytical solutions then having nobody at all is already too many and you cannot have exact solutions even for the vacuum state let alone for the N electron problem.

So, what do you do; you have non perturbative methods one of which we discussed at length in the previous class, the random phase approximation. Then there are methods which are alternative to the RPA some of which turn out to be equivalent to RPA in some sense. Some of them are different and you can do them using techniques which are based on configuration interactions or CI methods.

And what they enable you to do is describe the N electron wave function not by a single Slater determinant as we do in the Hartree Fock but by a superposition of 2, 3, 4 or more or in principle it can be an infinite set of Slater determinants. And these are the configuration interaction methods. So, the methodology which comes out of this when it is based on the Hartree Fock is called as the multi configuration Hatree Fock.

But you can have its relativistic analog in which the starting elements which go into the Slater determinant are not the two component Hatree Fock spiners, spiner wave functions, the spin wave functions. But these are the four component Dirac wave functions the Dirac by spiner's as we call them right. So, if the Slater determinants are made up of these four components by spiners.

Then you have what we call as the multi configuration Dirac Fock and more correctly it should be called as multi configurational Dirac Hartree Fock and there is a whole scheme which has been developed pioneering works has been done by Frost Fisher for the multi configurational Hartree Fock by Ian Grant and some others on the multi configurational Dirac Hartree Fock.

So, we have the multi configurational Dirac Hartree Fock sometimes abbreviated as MCDF or MCDHF for the Dirac Hartree Fock as such. And then there are other methods which are the Feynman diagram methods and this unit will focus on the Feynman diagram method. So, all of these techniques are essentially they target the many-body problem.

And in particular they target the issue of how the Coulomb correlations must be dealt with in a many electron system.

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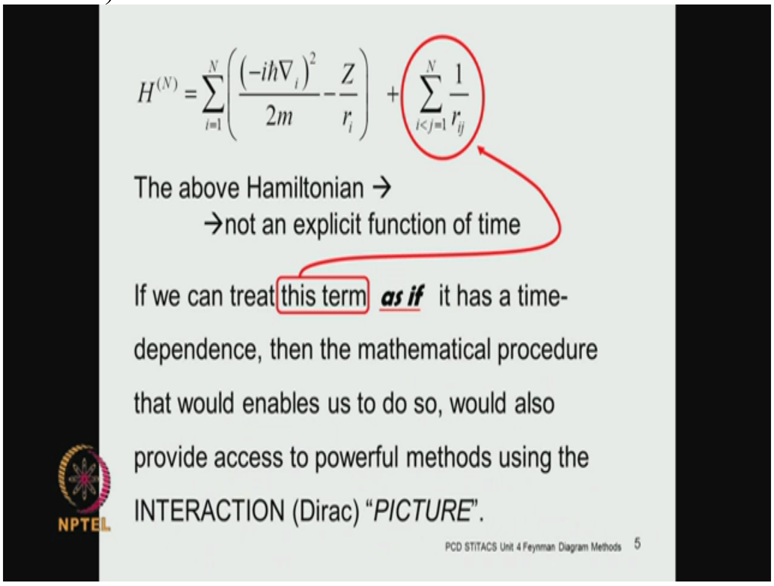

$$H^{(N)} = \sum_{i=1}^{N}\left(\frac{(-i\hbar\nabla_i)^2}{2m} - \frac{Z}{r_i}\right) + \boxed{\sum_{i<j=1}^{N}\frac{1}{r_{ij}}}$$

The above Hamiltonian →
→not an explicit function of time

If we can treat this term ***as if*** it has a time-dependence, then the mathematical procedure that would enables us to do so, would also provide access to powerful methods using the INTERACTION (Dirac) "*PICTURE*".

So, let us have a look at this Hamiltonian now notice that this Hamiltonian is not an explicit function of time there is no time dependence in this. Now what we can do is the correlations are of course coming from the electron-electron interaction. So, you have got the 1 over r12 or 1 over rij electron-electron interaction term and if we can deal with this term as if it were time-dependent okay.

Then we could use methodology in which the operators are time dependent okay. This is an operator 1 over r12 or 1 over rij is one of the terms in the N electron Hamiltonian and if we can treat it as if it were a time dependent term then we can use those methods in quantum theory in which time dependent operators are made use of.

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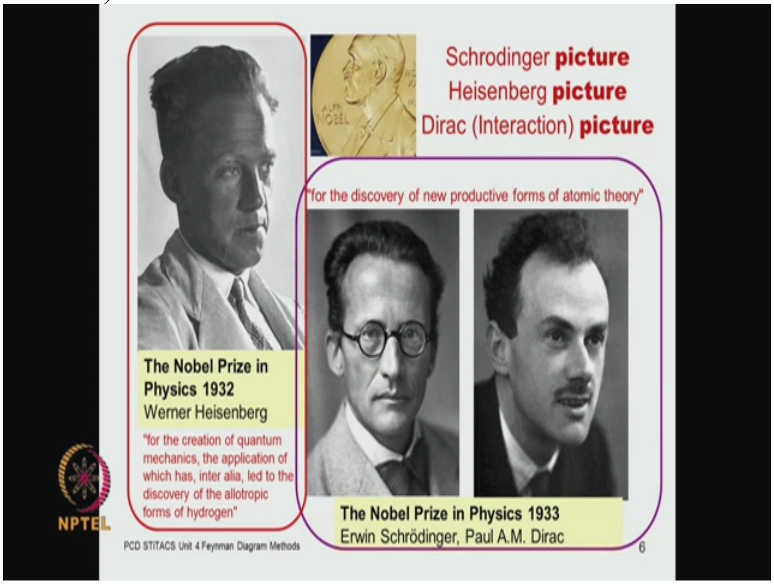

The Nobel Prize in Physics 1932
Werner Heisenberg

"for the creation of quantum mechanics, the application of which has, inter alia, led to the discovery of the allotropic forms of hydrogen"

Schrodinger **picture**
Heisenberg **picture**
Dirac (Interaction) **picture**

"for the discovery of new productive forms of atomic theory"

The Nobel Prize in Physics 1933
Erwin Schrödinger, Paul A.M. Dirac

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And in particular this is possible in what is called as the interaction picture or equivalently synonymously also called as a Dirac picture. So, I would like to introduce these three pictures the Schrodinger picture, the Heisenberg picture and the Dirac picture all of these essentially contributed to the development of quantum theory.

All of them got Nobel Prize, Heisenberg in 1932 and Schrodinger and Dirac share it in 1933 and the formalism of quantum theory which we most often make use of and which is what we have used in our in our earlier courses. We have made use of the Schrodinger picture but there are equivalent you know formulations in the so called Heisenberg picture and the Dirac picture. In today's class I will revisit these pictures.

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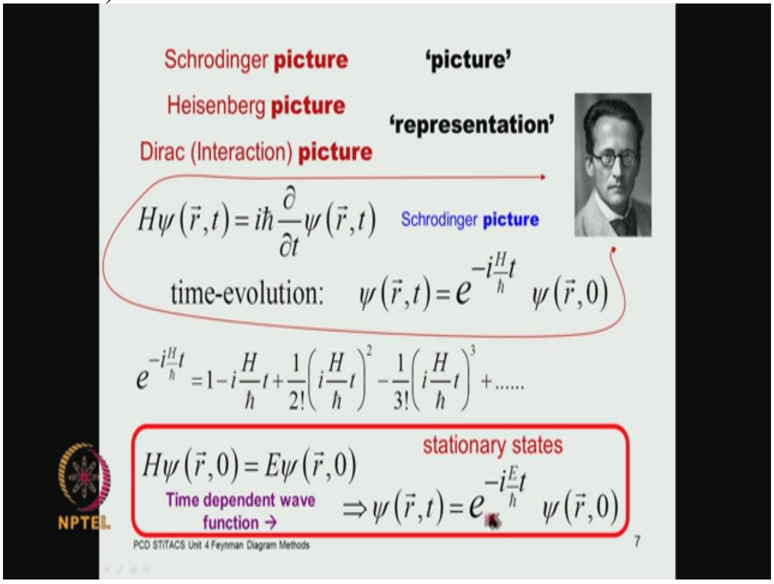

Schrodinger **picture**
Heisenberg **picture**
Dirac (Interaction) **picture**

'picture'

'representation'

$$H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$$

Schrodinger **picture**

time-evolution: $\psi(\vec{r},t) = e^{-i\frac{H}{\hbar}t}\,\psi(\vec{r},0)$

$$e^{-i\frac{H}{\hbar}t} = 1 - i\frac{H}{\hbar}t + \frac{1}{2!}\left(i\frac{H}{\hbar}t\right)^2 - \frac{1}{3!}\left(i\frac{H}{\hbar}t\right)^3 + \ldots\ldots$$

$$H\psi(\vec{r},0) = E\psi(\vec{r},0)$$

stationary states

Time dependent wave function →

$$\Rightarrow \psi(\vec{r},t) = e^{-i\frac{E}{\hbar}t}\,\psi(\vec{r},0)$$

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These are to be distinguished from what we often refer to as a representation. For example you will write the state of a system by a vector in the Hilbert space and then you can have a coordinate representation of the state vector which is the wave function. You can also have a momentum representation. So, these are different representations and you can go from one representation to another by carrying out appropriate transformations.

A picture is somewhat different. So, it is also you know different kind of representation in a certain sense. But these are achieved through what are called as generalized rotations in the Hilbert space rather than usual rotations in the Hilbert space. So, let me explain this. So let us begin with a Schrodinger equation H Psi = ih cross time derivative of the wave function. It what the Schrodinger equation does is to give you the time evolution of the system.

And the time evolution operator tells you how the wave function evolves from an initial time 0 to a later time t and the evolution is through this time evolution operator which includes the Hamiltonian right. So, this is what gives you the Schrodinger equation and this is the typical Schrodinger picture of quantum mechanics that we are used to.

So, this is the description of state of a vector at time t. And we are essentially looking at stationary state solutions. So, this exponential of an operator is understood as a power series expansion. So, that the Hamiltonian can operate as many times depending on whether it is the first term or the next term and so on. And the stationary state solution then is given by the solution e to the -i omega t omega is e over h cross.

And most often we write this solution that the time dependent part of the time dependent solution is given by e to the minus i omega t or - i e over h cross t and the time independent Schrodinger equation has got the solution which is E is the Eigen value and Eigen function is Psi of r at time equal to 0. So, this is the time independent Schrodinger equation for a stationary state.

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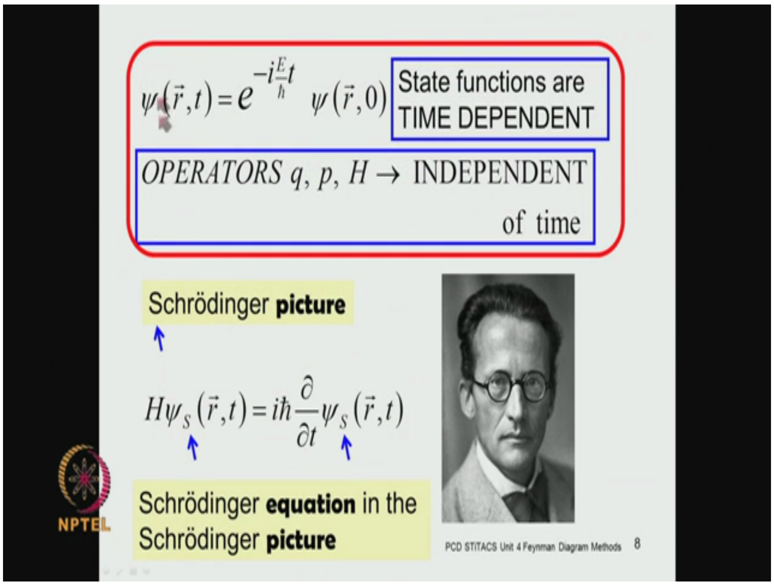

$$\psi(\vec{r},t) = e^{-i\frac{E}{\hbar}t}\,\psi(\vec{r},0)$$

State functions are TIME DEPENDENT

OPERATORS q, p, H → INDEPENDENT of time

Schrödinger **picture**

$$H\psi_S(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_S(\vec{r},t)$$

Schrödinger **equation** in the Schrödinger **picture**

Now notice that the state functions are a time dependent and the entire time evolution is contained in this e to the minus i omega t term or e to the -i e over h cross t term okay. This is the entire time dependence, the state function is a time dependent function. And the operators the operators are made up of the position operator the momentum operator right.

The Hamiltonian operator is made up of the potential energy operator and the kinetic energy operator and all of these operators you write in terms of the q and p and these are completely independent of time. So, in this picture it is the state function which is time dependent and the operators are completely independent of time and this is the signature of the Schrodinger picture.

So, this is the usual quantum mechanics that we do and that is the reason I have added a subscript s to emphasize that what we are looking at over here is the Schrodinge equation in the Schrodinger picture okay. But you can have alternative formulations in which the time dependence is not necessarily in the wave function.

You can actually transfer the time dependence to the operators rather than the wave function. And still do equivalent quantum mechanics.

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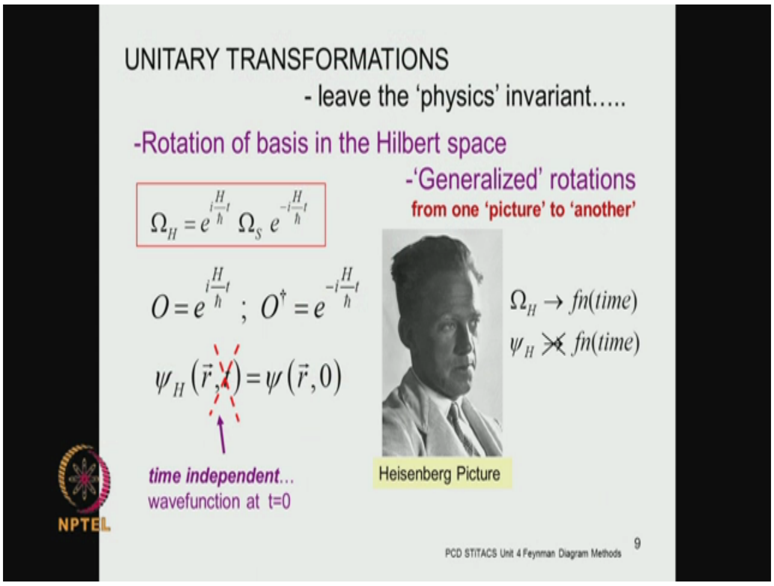

UNITARY TRANSFORMATIONS

- leave the 'physics' invariant.....

-Rotation of basis in the Hilbert space

-'Generalized' rotations

from one 'picture' to 'another'

$$\boxed{\Omega_H = e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}}$$

$$O = e^{i\frac{H}{\hbar}t}\ ;\ O^{\dagger} = e^{-i\frac{H}{\hbar}t}$$

$$\psi_H(\vec{r},\cancel{t}) = \psi(\vec{r},0)$$

time independent...

wavefunction at t=0

$\Omega_H \rightarrow fn(time)$

$\psi_H \not\rightarrow fn(time)$

Heisenberg Picture

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And let us see how this is done, this is done through certain transformations unitary transformations we know that they leave the physics invariant okay. The physics of such remains invariant you can have unitary transformations even in time independent Schrodinger picture formalism.

And essentially by and large what it amounts to is that you can expand the wave function in any linearly independent basis. You can have; you can orthogonalize that basis and then you have got an orthonormal basis and you can have an orthonormal basis made up of you know like in three dimensional space you have this you can twist it turn it move it right and any basis which is equivalent will work.

And you can carry out transformation of the wave function from one basis to another through unitary transformations the coefficients are then the cosine functions which connect the two orthogonal basis okay. So, that is something that you know very well and they leave the physics invariant. We will introduce what are called as generalized rotations.

So, a rotation from one basis to another, this is the usual rotation that we talk about when we talk about unitary transformations. Now what I am introducing are generalized rotations we not transformations of this kind but there are transformations which are very similar but with a difference. And this difference tells you how you carry out the transformation from the Schrodinger picture to the Heisenberg picture or to the Dirac picture.

So, this is how you carry out the transformation of an operator from the Schrodinger picture. So, if omega with subscript s is an operator in the Schrodinger picture then the corresponding operator in the Heisenberg picture is given by this transformation. This is the transformation rule which tells you how you carry out a transformation from the Schrodinger picture to the Heisenberg picture.

And this transformation is effected through these time-dependent operators in which the Hamiltonian plays a big role okay. So, the Hamiltonian has to appear in this transformation there is a time dependence which is explicit as you can see and this gives you a new operator. So, this operator it is what you call as the Heisenberg picture operator and this is the Schrodinger picture operator.

This is the relation between Heisenberg picture and Schrodinger picture. So, the operator which is affecting this transformation is this e to the i Ht over h cross this is operator. So, you have got O omega s omega dagger which gives you the Heisenberg picture operator okay. Correspondingly when you carry out the transformation the states will also be transformed.

And you get new se which are then called as the Heisenberg picture states and these pictures in the Heisenberg picture, these states the Heisenberg states will become independent of time. So, the Schrodinger picture the wave functions are time dependent the operators are not, in the Heisenberg picture it is the other way around.

The operators become time dependent but the wave functions become independent of time and we will see how they become independent of time. So, this is the main difference between the Schrodinger picture and the Heisenberg picture. So, you still need a time-dependent formulation but the time dependence is transferred from the wave function to the operators.

To do quantum mechanics there are two things that you do one is represent the state of the system by the state vector and then deal with operators instead of the classical dynamical variables. And these operators we are looking at the properties of these operators and now we will introduce time-dependent operators which we did not use in the Schrodinger picture.
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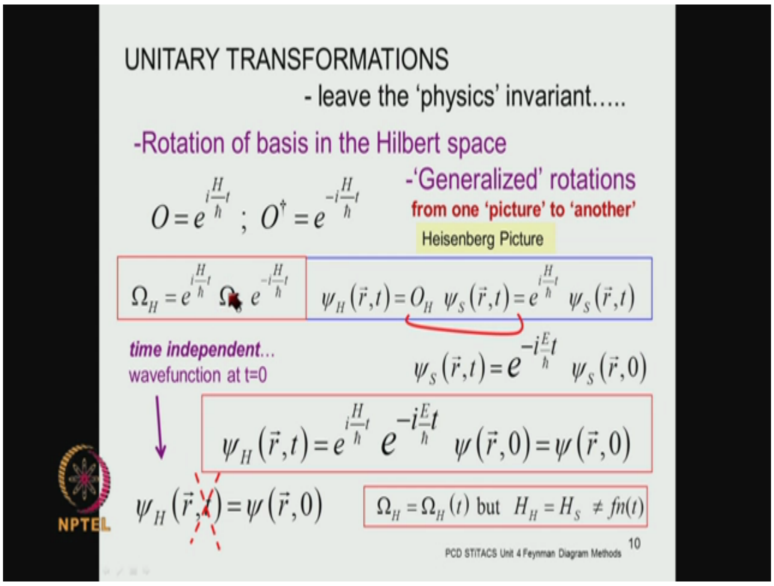

UNITARY TRANSFORMATIONS

- leave the 'physics' invariant.....

-Rotation of basis in the Hilbert space

$O = e^{i\frac{H}{\hbar}t}$; $O^{\dagger} = e^{-i\frac{H}{\hbar}t}$

-'Generalized' rotations

from one 'picture' to 'another'

Heisenberg Picture

$\boxed{\Omega_H = e^{i\frac{H}{\hbar}t}\,\Omega\,e^{-i\frac{H}{\hbar}t}}$ $\boxed{\psi_H(\vec{r},t) = \underbrace{O_H\ \psi_S(\vec{r},t) = e^{i\frac{H}{\hbar}t}}\ \psi_S(\vec{r},t)}$

time independent...

wavefunction at t=0

$\psi_S(\vec{r},t) = e^{-i\frac{E}{\hbar}t}\ \psi_S(\vec{r},0)$

$\boxed{\psi_H(\vec{r},t) = e^{i\frac{H}{\hbar}t}\ e^{-i\frac{E}{\hbar}t}\ \psi(\vec{r},0) = \psi(\vec{r},0)}$

$\psi_H(\vec{r},\cancel{t}) = \psi(\vec{r},0)$

$\boxed{\Omega_H = \Omega_H(t) \text{ but } H_H = H_S \neq fn(t)}$

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So, you have a generalized rotation effected through the transformation operator O which is e to the iH over h cross t. And the corresponding wave function when you carry out transformation of the operators omega s to omega H there is a transformation of the wave functions Psi s to Psi H essentially through the same transformation which is operator O.

And because we are dealing with the operator O which affects the transformation to the Heisenberg picture I have now added a subscript H over here okay. So, this operator transforms the Schrodinger picture wave function to a Heisenberg picture wave function okay. And this Heisenberg picture wave function is now e to the i H over h cross t operating on Psi s.

So, this is an operator which is made up of the Hamiltonian and when this operates on the Schrodinger picture wave function you get a new wave function which is the wave function in the Heisenberg picture. And notice that you can write the Schrodinger picture wave function is an Eigen function of the Hamiltonian belonging to an Eigen value e.

So, this e the i H over h cross t is equivalently replaced by the corresponding Eigen value which is e to the -i E over H cross t. So, this is the stationary state solution the time-dependent Schrodinger equation. And if you now put this back in the Heisenberg picture wave function, so this is the Heisenberg picture wave function.

How do we get it by operating by this transformation for generalized rotation operating on the Schrodinger picture time-dependent wave function which is now e to the -i omega t times the time independent wave function at t =0, right. But then e to the -i omega t can be pulled out. And then you have got this operator operating on the Schrodinger picture wave function at t = 0 and that will give you e to the +ie omega t.

And these two terms will then cancel each other and you get Psi at r 0. So, you have what a time dependence a formal time dependence over here but it turns out that it really does not depend on time because this is the wave function at t =0 okay. So, essentially what we see is that the time dependence is lost.

So, all the time dependence is in the operator here, this is where you have got the time dependence. So, far as the wave functions are concerned in the Heisenberg picture there is no time dependence. But the physics remains the same and that is the reason this is called as a generalized rotation from one picture to another. However remember that if the operator which is being transformed.

This is any Schrodinger picture operator if this is the Hamiltonian itself okay then this Hamiltonian operator of course commutes with e to the - ie Ht over h cross it will commute with every term in that infinite series right. And you can then write swap the positions of this operator H with this and then essentially you find that if the operator which is being transformed happens to be the Hamiltonian itself then it remains the same.

So, the Hamiltonian in the Heisenberg picture is the same as the Hamiltonian in the Schrodinger picture and this is not a function of time okay. Otherwise there is a time dependence for all of the other operators okay.

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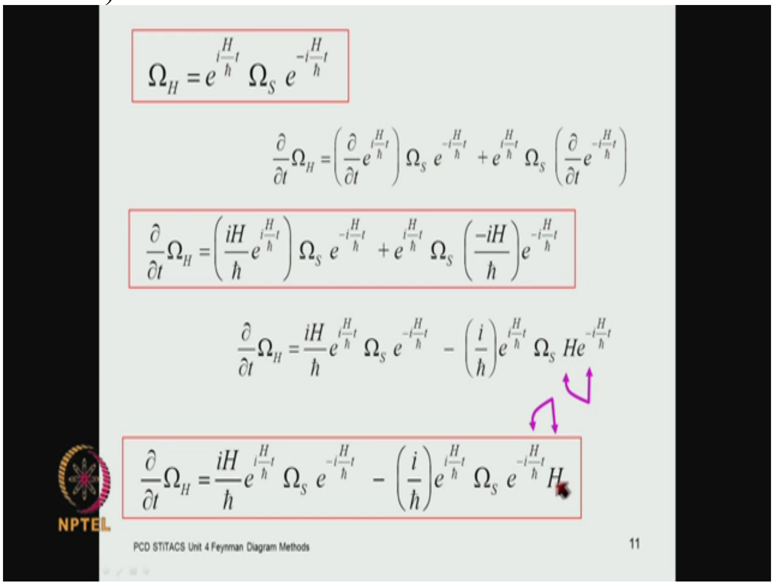

$$\boxed{\Omega_H = e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}}$$

$$\frac{\partial}{\partial t}\Omega_H = \left(\frac{\partial}{\partial t}e^{i\frac{H}{\hbar}t}\right)\Omega_S\,e^{-i\frac{H}{\hbar}t} + e^{i\frac{H}{\hbar}t}\,\Omega_S\left(\frac{\partial}{\partial t}e^{-i\frac{H}{\hbar}t}\right)$$

$$\boxed{\frac{\partial}{\partial t}\Omega_H = \left(\frac{iH}{\hbar}e^{i\frac{H}{\hbar}t}\right)\Omega_S\,e^{-i\frac{H}{\hbar}t} + e^{i\frac{H}{\hbar}t}\,\Omega_S\left(\frac{-iH}{\hbar}\right)e^{-i\frac{H}{\hbar}t}}$$

$$\frac{\partial}{\partial t}\Omega_H = \frac{iH}{\hbar}e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t} - \left(\frac{i}{\hbar}\right)e^{i\frac{H}{\hbar}t}\,\Omega_S\,He^{-i\frac{H}{\hbar}t}$$

$$\boxed{\frac{\partial}{\partial t}\Omega_H = \frac{iH}{\hbar}e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t} - \left(\frac{i}{\hbar}\right)e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}H}$$

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So, this is let me summarize the essence of this. So, you have got the Heisenberg picture operator which is time dependent and therefore its time evolution can be studied because it is time dependent. And its time evolution is given by the rate at which it changes with time. So, now you have got the rate at which omega H changes with time and the time dependence will come from this term and also from this term.

And you can treat it just as if it is a function of three products of three functions two of which the first and the third are time dependent, the middle one is time independent right. So, you get the time derivative of this and then you have got omega s e to the -i H over h cross t + you have got the this term omega s is not dependent on time. So, it stays as it is and then you have got to the partial derivative of the third operator which is e to the -i H over h cross t okay.

So, now let us take these derivatives, so you will get i H over h cross here and you will get -iH over h cross here. So, now you have got these two terms the third term is missing because omega s is independent of time. Now you have got these two terms and let us write them in a slightly different way because the operator products are associative.

So, you can look at these terms in a slightly different way by recognizing that this Hamiltonian here and this function of the Hamiltonian which is e to the -i H over h cross t these two operators can be swapped, their positions can be swapped because they obviously commute, one is made up of the other.

So, naturally the two operators swap, so if you interchange the positions of these two you bring e to the -i H over h cross t to the left of this omega s and to the left of this operator H. So, this H now is written at the end rather than the penultimate position that it had in the previous set.

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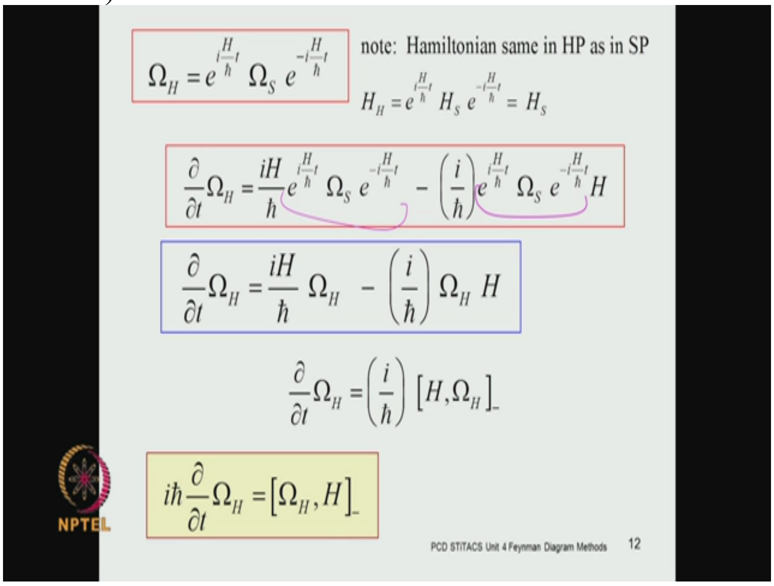

$$\boxed{\Omega_H = e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}}$$

note: Hamiltonian same in HP as in SP

$$H_H = e^{i\frac{H}{\hbar}t}\,H_S\,e^{-i\frac{H}{\hbar}t} = H_S$$

$$\boxed{\frac{\partial}{\partial t}\Omega_H = \frac{iH}{\hbar}\underbrace{e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}} - \left(\frac{i}{\hbar}\right)\underbrace{e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}}H}$$

$$\boxed{\frac{\partial}{\partial t}\Omega_H = \frac{iH}{\hbar}\,\Omega_H - \left(\frac{i}{\hbar}\right)\Omega_H\,H}$$

$$\frac{\partial}{\partial t}\Omega_H = \left(\frac{i}{\hbar}\right)[H,\Omega_H]_-$$

$$\boxed{i\hbar\frac{\partial}{\partial t}\Omega_H = [\Omega_H, H]_-}$$

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So, the Hamiltonian as I pointed out is the same as the Heisenberg picture as in the Schrodinger picture. The time dependence of an arbitrary operator in the Heisenberg picture is given by these two terms. And what is this? This is nothing but the transformed operator omega in the Heisenberg picture right.

So, you have got a commutator over here. So, if you factor out ih cross is common you find that the time derivative of the Heisenberg picture operator is given by i over h cross times the commutator of H the Hamiltonian with this operator H right. So, obviously this gives you the time evolution and this is sometimes called as the Heisenberg equation of motion for the operator omega okay.

So, this is how the time derivative of the operator is expressed in the Heisenberg picture. It is the operators which are time-dependent. The wave functions are independent of time.

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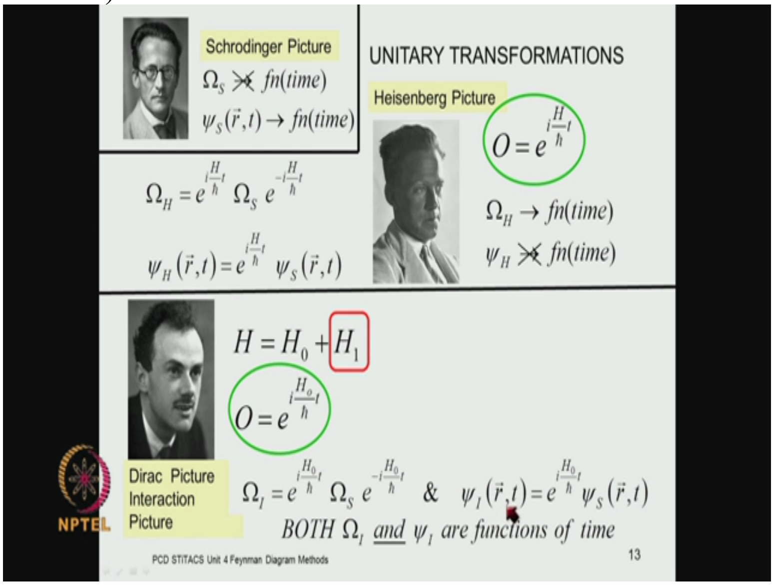

Schrodinger Picture

$\Omega_S \not\to fn(time)$

$\psi_S(\vec{r},t) \to fn(time)$

UNITARY TRANSFORMATIONS

Heisenberg Picture

$$\boxed{O = e^{i\frac{H}{\hbar}t}}$$

$$\Omega_H = e^{i\frac{H}{\hbar}t}\,\Omega_S\,e^{-i\frac{H}{\hbar}t}$$

$$\psi_H(\vec{r},t) = e^{i\frac{H}{\hbar}t}\,\psi_S(\vec{r},t)$$

$\Omega_H \to fn(time)$

$\psi_H \not\to fn(time)$

$$H = H_0 + \boxed{H_1}$$

$$\boxed{O = e^{i\frac{H_0}{\hbar}t}}$$

Dirac Picture
Interaction
Picture

$$\Omega_I = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\,e^{-i\frac{H_0}{\hbar}t} \quad \& \quad \psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t)$$

BOTH Ω_I $\underline{\text{and}}$ ψ_I are functions of time

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Now this is contrasted with the Schrodinger picture in which the operator is not a function of time whereas the wave function was and the relationship was affected through the generalized transformations which are unitary transformations but generalized rotations in the Hilbert's space through operator.

This is the transformation operator e to the iH over h cross t. So, this gives you the transformation from the Schrodinger picture to the Heisenberg picture. Now there is another picture that is the Dirac picture it is also called as the interaction picture and in this picture quantum mechanics of those problems which cannot be solved perturbatively using perturbation methods.

This is particularly useful for such problems like the Coulomb correlations in our problem. In the many electron problem we recognized that the statistical correlations the spin correlations could be handled using the anti-symmetrised wave function which is the Hartree Fock theory which we learnt is equivalent to the first order perturbation theory result.

But there is a residual correlation in the main electron system that is the Coulomb correlation and that is something we cannot handle using perturbative methods. Because; whereas the first order perturbation theory gives you a result which is the same as the Hartree Fock theory, the second order and higher order perturbative methods do not give any converged result.

So, now we are looking of ways to deal with this term the electron-electron interaction which is responsible for the Coulomb correlations and for these problems for which you cannot solve using perturbative methods. The interaction picture provides you with very powerful tools to solve the problem. So, how do you do that you again carry out generalized rotations in the Hilbert's space.

But this time the transformation operator is e to the iH over h cross t but mind you this is the H0 which is a soluble part of the Hamiltonian. So, this Hamiltonian consists of two parts one is H0 for which you can get exact solutions. Then there is a residual part which is the culprit in a certain sense which gives you these complications that you cannot handle using perturbative methods.

You can get approximate solutions Hartree Fock is a solution to this problem H0 + H1 but it is only an approximate solution. It is approximation to the extent that it has taken into account the statistical correlations but not the Coulomb correlations. And it is the Coulomb correlations that we are now interested in handling. So this is left out in the transformation Hamiltonian.

So, notice the difference between this transformation operator which is the full Hamiltonian here in the Heisenberg picture. But over here it is only the unperturbed soluble part of the Hamiltonian which is used to affect the generalized rotation. So, that is the big difference and this is what gives you the Dirac picture operators omega i.

And the corresponding interaction picture wave functions are obtained from the Schrodinger picture wave functions. By operating these Schrodinger picture wave functions by the same transformation operator which is e to the i H0 over h cross t right. So this is the Dirac picture and in this picture there is time dependence in the wave functions.

The interaction picture wave function is time dependent okay. There is an explicit time dependence over here as well as here and then there is explicit time dependents over here. So both the operators and the wave functions depend on time. In the Schrodinger picture only the wave functions depend on time the operators do not.

In the Heisenberg picture it is our operators which depend on time but the wave functions do not. And in the interaction picture both depend on time but the physics remains invariant. So, the important difference in the Heisenberg picture in the Schrodinger picture is that the transformation operator consists only of the soluble part of the Hamiltonian.

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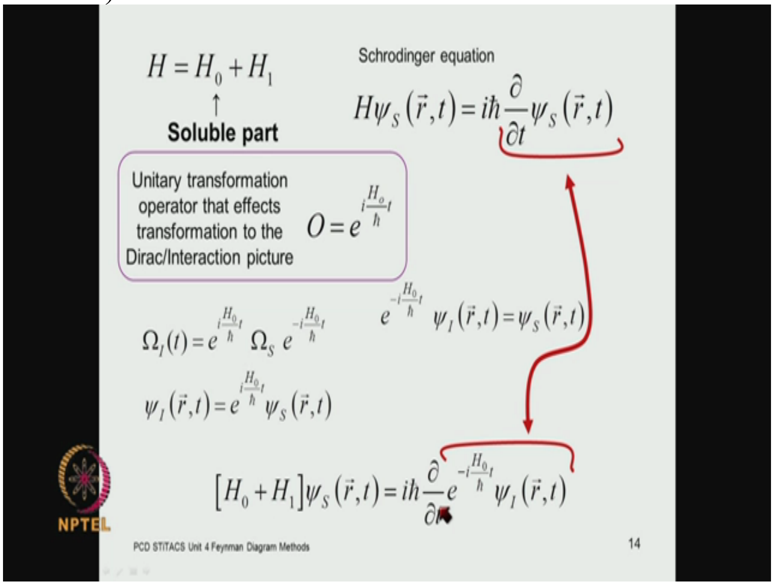

$H = H_0 + H_1$

$\uparrow$

Soluble part

Schrodinger equation

$H\psi_S(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_S(\vec{r},t)$

Unitary transformation operator that effects transformation to the Dirac/Interaction picture $O = e^{i\frac{H_0}{\hbar}t}$

$e^{-i\frac{H_0}{\hbar}t}\psi_I(\vec{r},t) = \psi_S(\vec{r},t)$

$\Omega_I(t) = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\,e^{-i\frac{H_0}{\hbar}t}$

$\psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\psi_S(\vec{r},t)$

$[H_0 + H_1]\psi_S(\vec{r},t) = i\hbar\frac{\partial}{\partial t}e^{-i\frac{H_0}{\hbar}t}\psi_I(\vec{r},t)$

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So, here we are this is what we get for the interaction picture operator and the wave function. And if you now operate on the interaction picture wave function by the adjoint of this operator which will be e to the -i iH0 over h cross t then you get the Schrodinger picture wave function right.

And the Schrodinger picture wave function you know what we can do is rewrite this wave function this Schrodinger equation. Because this H is nothing but H0 + H1, so that is what we have over here. Then you have got the Schrodinger picture wave function which is Psi of s, then you have got ih cross del over del t of the Schrodinger picture time-dependent wave function.

But the Schrodinger picture time-dependent wave function is related to the interaction picture wave function by operating upon this by e to the -i H0 over h cross t okay. So, if this is an equation which looks very similar to the Schrodinger equation as such but then there are these subtle differences that you have to keep track of and get used to.

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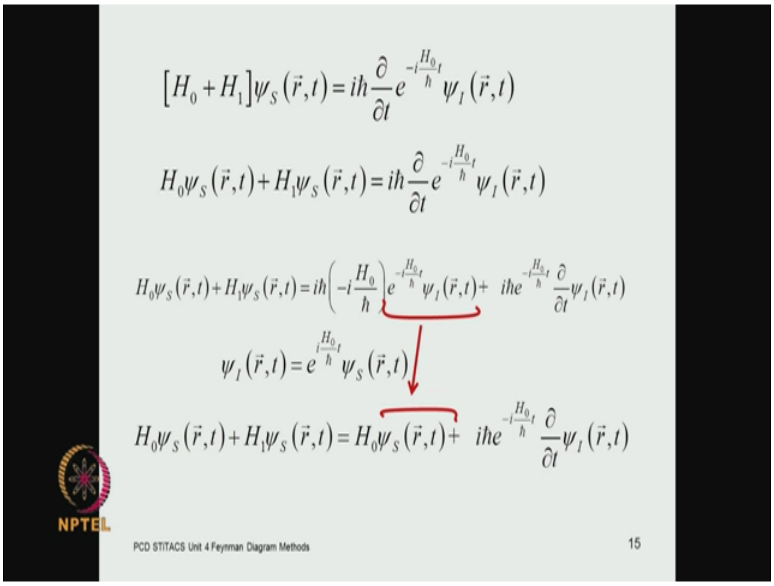

$$\left[H_0+H_1\right]\psi_S(\vec{r},t)=i\hbar\frac{\partial}{\partial t}e^{-i\frac{H_0}{\hbar}t}\psi_I(\vec{r},t)$$

$$H_0\psi_S(\vec{r},t)+H_1\psi_S(\vec{r},t)=i\hbar\frac{\partial}{\partial t}e^{-i\frac{H_0}{\hbar}t}\psi_I(\vec{r},t)$$

$$H_0\psi_S(\vec{r},t)+H_1\psi_S(\vec{r},t)=i\hbar\left(-i\frac{H_0}{\hbar}\right)\underbrace{e^{-i\frac{H_0}{\hbar}t}\psi_I(\vec{r},t)}+\ i\hbar e^{-i\frac{H_0}{\hbar}t}\frac{\partial}{\partial t}\psi_I(\vec{r},t)$$

$$\psi_I(\vec{r},t)=e^{i\frac{H_0}{\hbar}t}\psi_S(\vec{r},t)$$

$$H_0\psi_S(\vec{r},t)+H_1\psi_S(\vec{r},t)=H_0\overbrace{\psi_S(\vec{r},t)}+\ i\hbar e^{-i\frac{H_0}{\hbar}t}\frac{\partial}{\partial t}\psi_I(\vec{r},t)$$

So, this is; the physics is the same as we had in the Schrodinger equation in the Schrodinger picture. What are the consequences? Let us take the time derivative of the right hand side, so there is time dependence over here and the time dependence over here right. So, you have two terms on the left hand side one coming from the operation on Psi s by H0.

And the other which comes from the operation on Psi s by H1 which contains the complicated terms leading to electron-electron correlations, so you have two terms of the left hand side on the right hand again you expect two terms because there is a time derivative which has to be taken of this term as well as this term, so the time derivative of the operator here gives you -iH 0 over h cross and then this function right.

And then you take the time derivative of the interaction picture wave function which we also know is time dependent. So, you get a time dependent term over here so there are two terms. However this term Psi irt is related to the Schrodinger picture wave function through this generalized transformation operator e to the i H0 over h cross right.

So, you have you plug it in and using this you find that e to the -iH0 t over h cross operating on Psi i gives you the Schrodinger picture wave function. Now notice that both sides have got this term. The left-hand side has got this coming from one of the two terms which comes from the time derivative.

And the left-hand side has got this term because the left-hand side Hamiltonian was written in two pieces one the soluble part H0 and the other is the correlation part. So, these two terms cancel each other right. So, these two terms are essentially the same they cancel each other and you are left with the remaining relationship.

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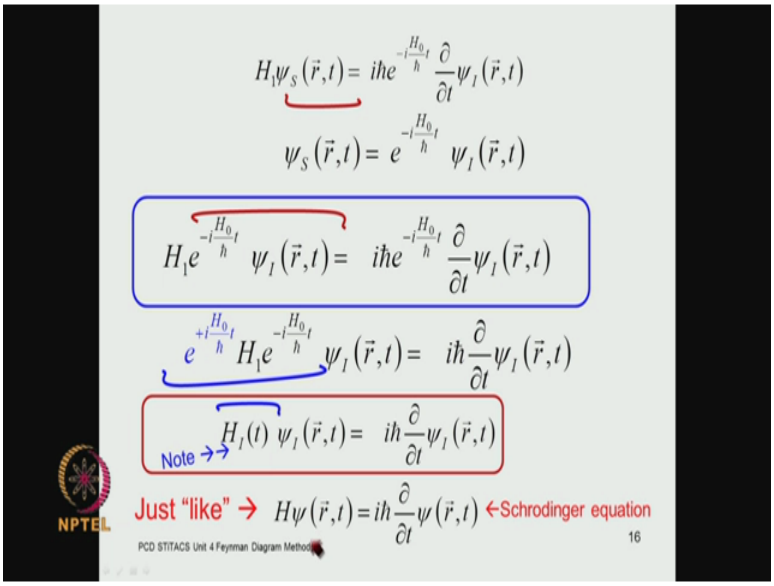

$$H_1\underbrace{\psi_S(\vec{r},t)}= i\hbar e^{-i\frac{H_0}{\hbar}t}\frac{\partial}{\partial t}\psi_I(\vec{r},t)$$

$$\psi_S(\vec{r},t)= e^{-i\frac{H_0}{\hbar}t}\,\psi_I(\vec{r},t)$$

$$\boxed{H_1\overbrace{e^{-i\frac{H_0}{\hbar}t}\,\psi_I(\vec{r},t)}= i\hbar e^{-i\frac{H_0}{\hbar}t}\frac{\partial}{\partial t}\psi_I(\vec{r},t)}$$

$$\underbrace{e^{+i\frac{H_0}{\hbar}t}H_1e^{-i\frac{H_0}{\hbar}t}}\psi_I(\vec{r},t)= i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)$$

$$\boxed{\text{Note}\rightarrow\rightarrow\ \overbrace{H_I(t)}\,\psi_I(\vec{r},t)= i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)}$$

Just "like" → $H\psi(\vec{r},t)=i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$ ←Schrodinger equation

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Which again looks like the Schrodinger equation but there are subtle differences and important differences. So, this Schrodinger picture wave function is now given by this. This is the transformation, what it does is if you now write this only in terms of the interaction picture terms okay.

You write this wave function in terms of interaction picture wave function but to do that you must operate upon this by –i H0 over h cross t. The right hand side is the same at this stage. And now on this result you operate on both sides by e to the + i H0 over h cross t this is the transformation operator O which affects the generalized rotation to the Dirac picture.

So, you take this relation in this blue box okay and operate on both sides by this e to the i H0 over h cross. So, this term together with this term on the right hand side will give you the unit operator and you are left only with iH cross times del over del t of Psi i on the right side. And on the left side you have got this transformation of H1.

And what is this transformation this is the transformation of the H1 operator from the Schrodinger to the Dirac picture okay, because that transformation is effected through the operator O which is O omega O dagger. And you have essentially the interaction picture Hamiltonian.

But now even if this equation looks just like the Schrodinger equation there are important differences the physics is the same when we looked at a similar relation in the Schrodinger picture. We had the wave functions which had the entire time dependence. We had the operators which had no time dependence.

But now you have this interaction picture Hamiltonian but what is this Hamiltonian? It has got information coming in from both the soluble part as well as the part which is not soluble. The soluble part is coming over here H0 is the part of the Hamiltonian which is the soluble part. H1 is the one which we are not able to deal with.

So, you have got a relation which looks very similar to the Schrodinger equation. It has got the same physics but here the focus; the central term is H1. It does not mean that it has nothing to do with the soluble part. It is of course implicit because after all it is this product of these three operators in that particular order which gives you the Hi t. So, this is the subscript i for the interaction picture correlation part of the term okay.

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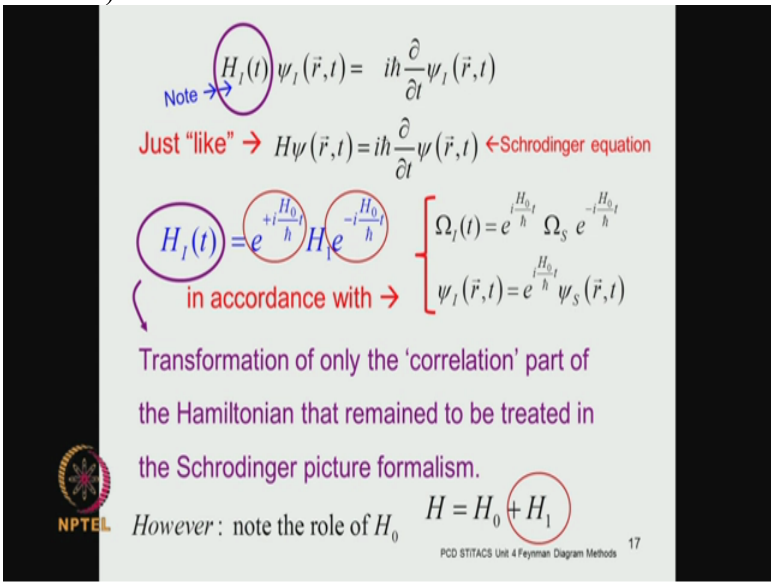

$$\boxed{H_I(t)}\,\psi_I(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)$$

Note →

Just "like" → $H\psi(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t)$ ←Schrodinger equation

$$\boxed{H_I(t)} = \boxed{e^{+i\frac{H_0}{\hbar}t}}\,H_1\,\boxed{e^{-i\frac{H_0}{\hbar}t}}$$

in accordance with →

$$\begin{cases} \Omega_I(t) = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\,e^{-i\frac{H_0}{\hbar}t} \\ \psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t) \end{cases}$$

Transformation of only the 'correlation' part of the Hamiltonian that remained to be treated in the Schrodinger picture formalism.

However: note the role of H_0

$$H = H_0 \boxed{+H_1}$$

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So, this is a very similar relation but it has important differences and it is a result of these transformations effected through the generalized transformation, generalized rotation in the Hilbert space affected through the soluble part H0 of the Hamiltonian. Now this is a transformation only of the difficult part or the trouble monger if you might call it right, but then note that H0 the soluble part also plays a role. Because O and O dagger involve the transformation terms okay.

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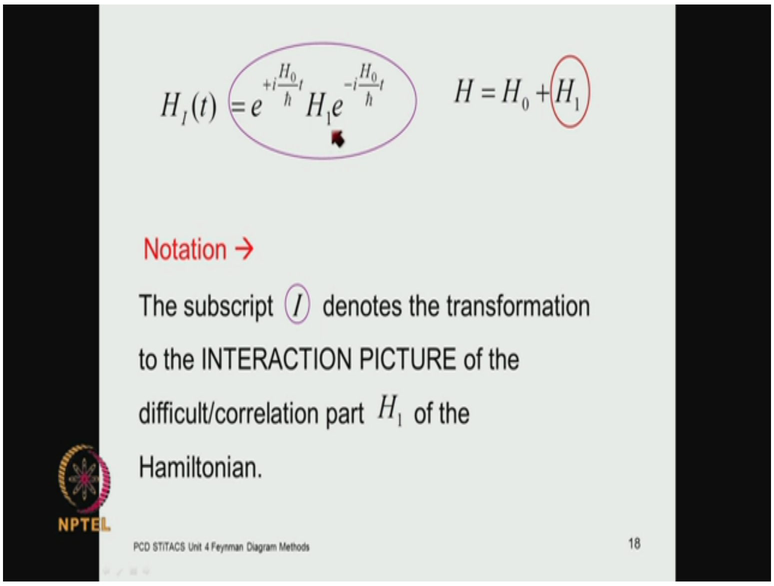

$$H_I(t) = e^{+i\frac{H_0}{\hbar}t} H_1 e^{-i\frac{H_0}{\hbar}t} \qquad H = H_0 + H_1$$

Notation →

The subscript I denotes the transformation to the INTERACTION PICTURE of the difficult/correlation part H_1 of the Hamiltonian.

So, this is the interaction picture term interaction picture Hamiltonian. This is the transformation of the difficult the trouble part but it is effected through the simple nice (Question time: 42:02) yeah the interaction picture term yeah I mean as the only we are using the interaction picture only because of the other term the wave function.

The act of the x not on Psi only easier phase that is only reason why we are using the interaction picture right, yeah the interaction picture is going to render the operators time dependent. The Schrodinger picture operators are not dependent on time okay. The Hamiltonian in the Schrodinger picture is completely independent of time.

We are developing methods so that we can use a formulation in which the operators become time dependent. And the operators become time dependent in the Heisenberg picture they also become time dependent in the interaction picture and to develop the powerful techniques of Feynman diagrams the most convenient framework is that of the interaction picture. So, I am laying down the groundwork for that.

You are doing essentially the same physics, so as of this stage we have not introduced any methodology to deal with the residual correlation. But that is something that we are going to develop in the next few classes in this unit. So, the first task in today's class is to show how you affect these transformations and these are necessary because our essential problem is that we are not able to deal with the electron-electron correlations in the Schrodinger picture.

We tried using perturbation theory we succeeded with first order perturbation theory but then when we use the second order or higher order perturbation theory we fail, so; but perturbative methods are not useful to deal with that one way of dealing with it was the RPA which we discussed in the previous unit.

But now we are using we are developing other methods which make use of Feynman diagram methods and these will make use of the interaction picture. But to be able to use the interaction picture we need the operators to be time dependent. So, what we have done through this transformation? The transformation is effected through this transformation operator e to the i H0 over h cross t.

So, this is the transformation operator O it provides a generalized rotation of the state vectors. So, this is the wave function and this is transformed to a new function which is on the left hand side and the new wave function is obtained from the previous old wave function of the Schrodinger picture by a transformation operator which is made up of this exponential function operator.

But it has only the unperturbed part of the Hamiltonian only the H0. And this makes both the wave function Psi i time-dependent and the operators omega also time dependent. Now when you carry out this transformation on the electron-electron term and that is where the correlations are coming from. That is where the Coulomb correlations are coming from, the statistical correlations we know how to handle.

But the coulomb correlations have to be handled and through this transformation this operator H1 which is otherwise independent of time. This operator H1 which is independent of time now becomes time dependent, the time dependence is coming here. So, we have succeeded in expressing the electron-electron interaction term this is the difficult term which was otherwise independent of time.

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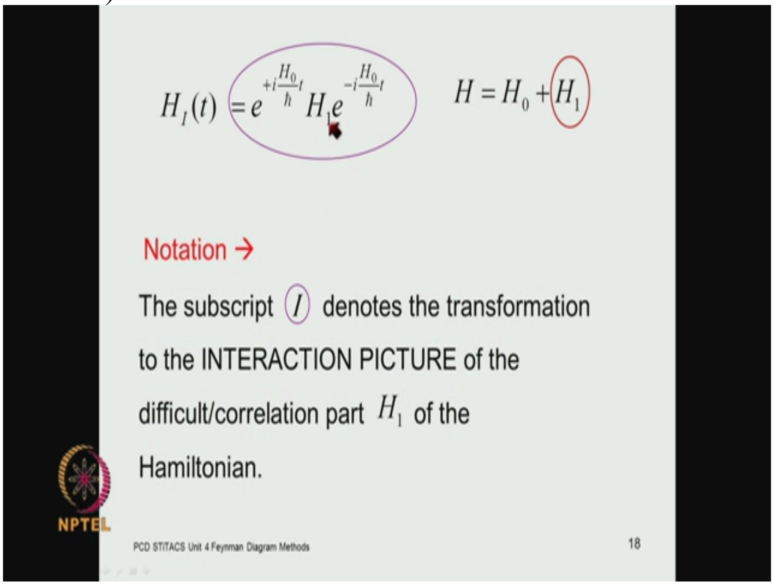

$$H_I(t) = e^{+i\frac{H_0}{\hbar}t} H_1 e^{-i\frac{H_0}{\hbar}t} \qquad H = H_0 + H_1$$

Notation →

The subscript I denotes the transformation to the INTERACTION PICTURE of the difficult/correlation part H_1 of the Hamiltonian.

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But we have not succeeded in expressing it as a time dependent operator but correspondingly the wave functions are also transformed and then we will do physics in the interaction picture rather than the Schrodinger picture. So, the subscript i over here look similar to the number one over here. So, the two fonts are very similar but keep track of the fact that H1 is the electron-electron interaction term.

Hi is the corresponding interaction picture term which is a transformation of H1 through the generalized rotation affected by the operator which carry out the transformation from the Schrodinger picture to the interaction picture.

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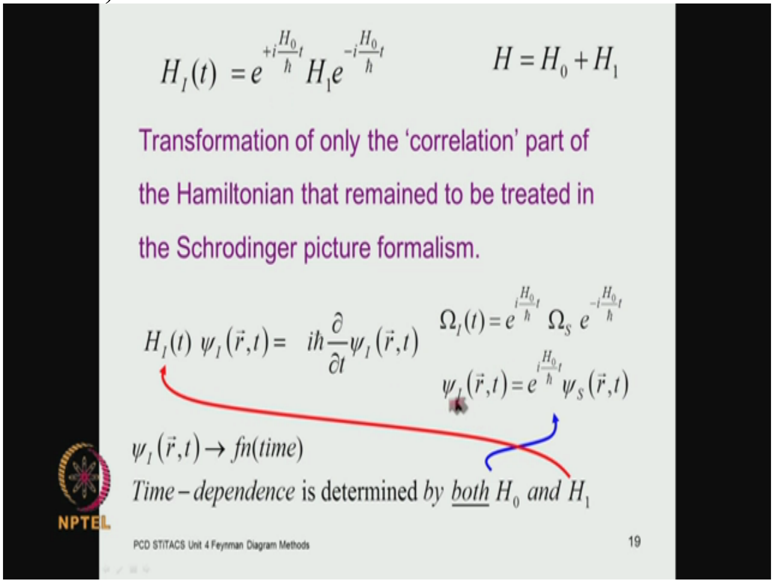

$H_I(t) = e^{+i\frac{H_0}{\hbar}t} H_1 e^{-i\frac{H_0}{\hbar}t}$ $\qquad H = H_0 + H_1$

Transformation of only the 'correlation' part of the Hamiltonian that remained to be treated in the Schrodinger picture formalism.

$H_I(t)\,\psi_I(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)$

$\Omega_I(t) = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\, e^{-i\frac{H_0}{\hbar}t}$

$\psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t)$

$\psi_I(\vec{r},t) \rightarrow fn(time)$

Time-dependence is determined *by both* H_0 *and* H_1

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So, this is the interaction picture term and this is a transformation of what only the H1 part not the H0 part. This is the transformation only of the H1 part but the transformation is by the operator omega by the operator e to the iH0 over h cross t and this is where the soluble part of the Hamiltonian shows up.

So, you have got time dependence which is contained in the wave function Psi i the interaction picture wave functions are time dependent. And the interaction picture operators are also time dependent both are time dependent and the time dependence is governed both by H0 as well as by H1 as it ought to be because the physics is the same.

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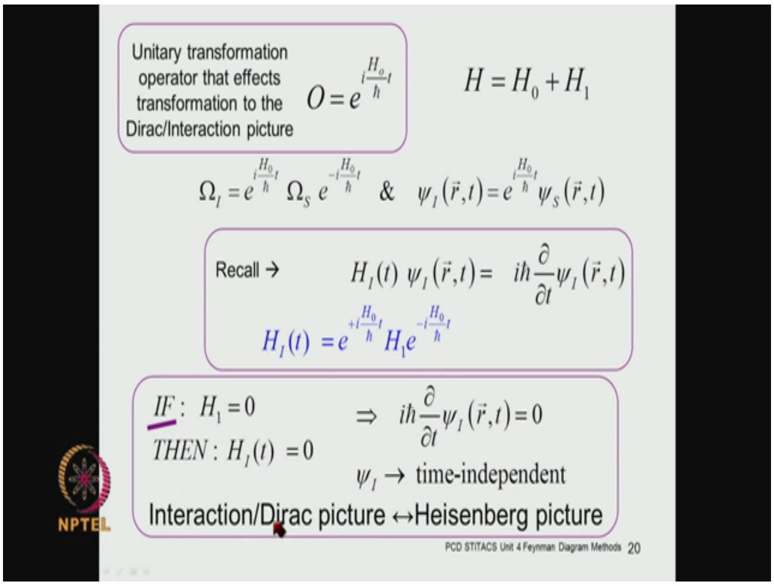

Unitary transformation operator that effects transformation to the Dirac/Interaction picture $O = e^{i\frac{H_0}{\hbar}t}$

$H = H_0 + H_1$

$\Omega_I = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\, e^{-i\frac{H_0}{\hbar}t}$ & $\psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\psi_S(\vec{r},t)$

Recall → $H_I(t)\,\psi_I(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)$

$H_I(t) = e^{+i\frac{H_0}{\hbar}t} H_1 e^{-i\frac{H_0}{\hbar}t}$

$IF:\ H_1 = 0$ $\Rightarrow\ i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t) = 0$

$THEN:\ H_I(t) = 0$

$\psi_I \rightarrow$ time-independent

Interaction/Dirac picture ↔ Heisenberg picture

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So, this is again a unitary transformation and notice that if there were no interaction the electron-electron interaction were 0, then this H1 would be 0 Hi would be 0 and what if Hi is 0 then the time derivative of the interaction picture would also be 0 and then the interaction picture becomes independent of time okay. So, it is particularly tailored to deal with the electron-electron term which is the one which we really want to focus on.

The soluble part we already know how to do it in quantum mechanics you know it in your first course in quantum theory. So, it is the difficult part and that is what is the focus in the Dirac picture. So, if there were no electron-electron interaction then the interaction picture wave function becomes time independent.

And you get a result similar to the Heisenberg picture but that is a special case. When there is no electron-electron interaction all right. Let us study task time development operator now.
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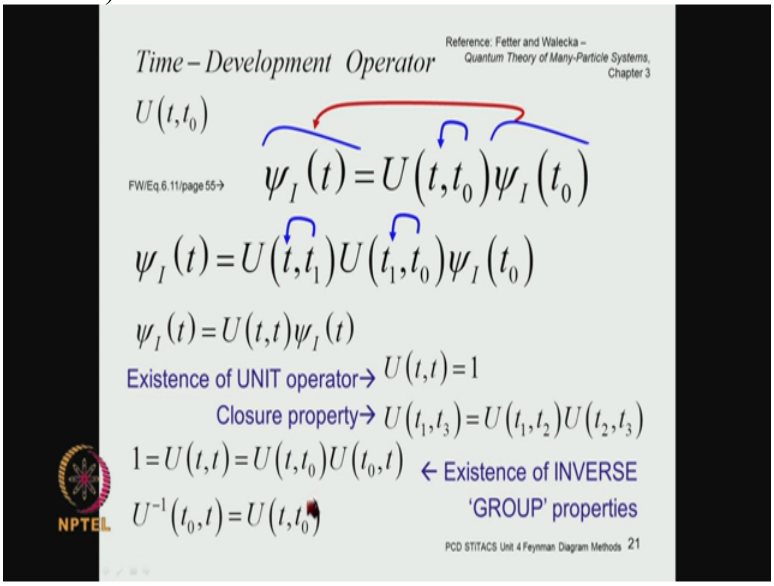

Time – Development Operator

Reference: Fetter and Walecka – *Quantum Theory of Many-Particle Systems*, Chapter 3

$U(t,t_0)$

FW/Eq.6.11/page 55→ $\psi_I(t) = U(t,t_0)\psi_I(t_0)$

$\psi_I(t) = U(t,t_1)U(t_1,t_0)\psi_I(t_0)$

$\psi_I(t) = U(t,t)\psi_I(t)$

Existence of UNIT operator→ $U(t,t) = 1$

Closure property→ $U(t_1,t_3) = U(t_1,t_2)U(t_2,t_3)$

$1 = U(t,t) = U(t,t_0)U(t_0,t)$ ← Existence of INVERSE

$U^{-1}(t_0,t) = U(t,t_0)$

'GROUP' properties

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Now what the time development operator does is it gives you the wave function at a later time t from an earlier time t0. So, this is the time evolution from the time t 0 to the time t and this is the result of the time evolution operator and its properties are quite familiar to you because you can carry out a transformation from t0 to t through an intermediate instant of time t1.

So, first carry out look at the evolution from t0 to t1 and then the evolution from t1 to t. So, you can have a cascading effect like this. So, this is an essential property of the time evolution operator. You can also see that if you look at the evolution from instant of time t to the same instant of time t then of course you have the unit operator right.

So, if you break this into any intermediate step you have U t ,t = 1 from t1 evolution from t3 to t1 can be done in two stages t3 to t2 and then t2 to t1 you can do it you can break that time interval into 2 pieces, 3 pieces or even infinite pieces okay. It is the continuous time interval you can break it into infinite pieces.

So, these are the properties of the time evolution operator we have already seen that if you break it from; If you look at the time evolution from t to t0 and then from t0 to t then you find that the inverse of t0 to t evolution is the same as t, t0, essentially if you look at these properties.

You find that the inverse exists there is a closure property, the unit operator exists and these are the properties of operators which constitute a group okay. Because you have the closure, you have got the existence of the unit operator and you also have the inverse. So, they these time evolution operators they constitute a group.

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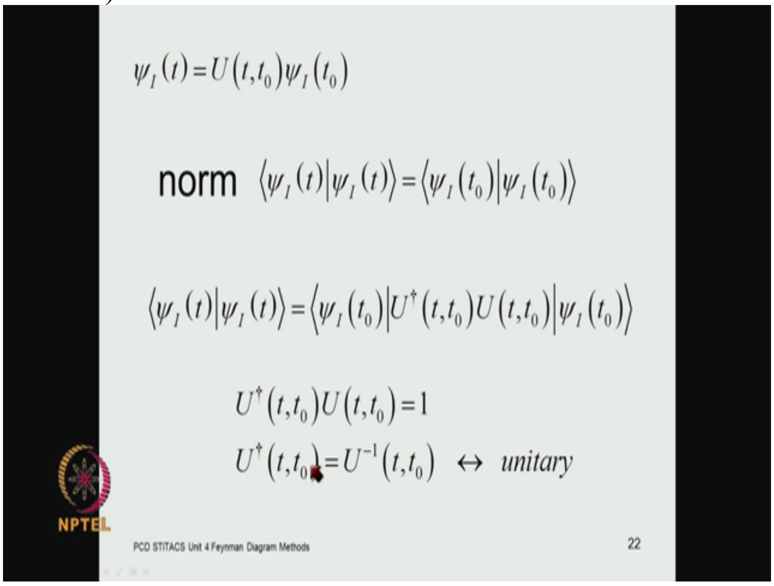

$$\psi_I(t) = U(t,t_0)\psi_I(t_0)$$

norm $\langle \psi_I(t) | \psi_I(t) \rangle = \langle \psi_I(t_0) | \psi_I(t_0) \rangle$

$$\langle \psi_I(t) | \psi_I(t) \rangle = \langle \psi_I(t_0) | U^\dagger(t,t_0) U(t,t_0) | \psi_I(t_0) \rangle$$

$$U^\dagger(t,t_0) U(t,t_0) = 1$$

$$U^\dagger(t,t_0) = U^{-1}(t,t_0) \leftrightarrow \textit{unitary}$$

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So, this is the unitary transformation the reason it is unitary is because it preserves the norm. You look at the wave function you construct its norm. So, this is the norm of the wave function in the interaction picture and you obtain it by looking at the evolution from t0 to t on the; this adjoint vector is given over here.

And this operator being unitary you have U dagger U = 1. And what you find is that the time evolution operator is essentially a unitary operator because it preserves the norm.
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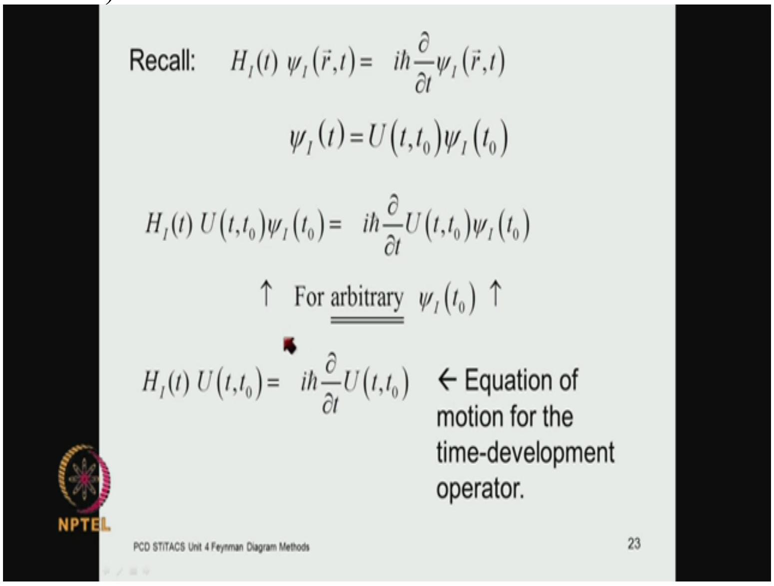

Recall: $H_I(t)\,\psi_I(\vec{r},t) = i\hbar\frac{\partial}{\partial t}\psi_I(\vec{r},t)$

$$\psi_I(t) = U(t,t_0)\psi_I(t_0)$$

$$H_I(t)\,U(t,t_0)\psi_I(t_0) = i\hbar\frac{\partial}{\partial t}U(t,t_0)\psi_I(t_0)$$

↑ For arbitrary $\psi_I(t_0)$ ↑

$$H_I(t)\,U(t,t_0) = i\hbar\frac{\partial}{\partial t}U(t,t_0)$$

← Equation of motion for the time-development operator.

So, these properties will be utilized in our analysis. So you have got the interaction picture Schrodinger equation now. This is the time evolution from time t0 to t of the interaction picture wave function. This is for an arbitrary time t0 okay and essentially you get from this because this result holds good for any arbitrary interaction picture wave function.

So, there is a corresponding operator equivalence of the operator which is operating on this. So, that operator equivalence is HiU on the left hand side is equal to ih cross del over del t of the time evolution operator. So, this is the equation of motion of the time development operator.
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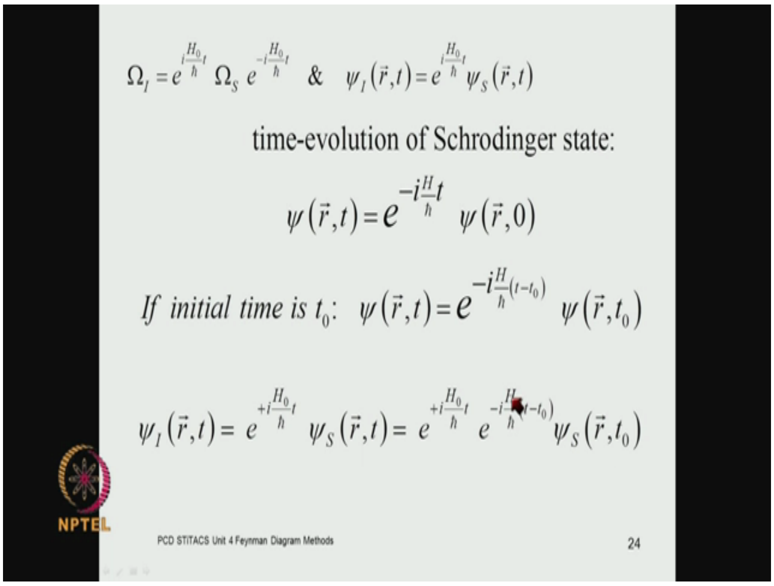

$$\Omega_I = e^{i\frac{H_0}{\hbar}t}\,\Omega_S\, e^{-i\frac{H_0}{\hbar}t} \quad \& \quad \psi_I(\vec{r},t) = e^{i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t)$$

time-evolution of Schrodinger state:

$$\psi(\vec{r},t) = e^{-i\frac{H}{\hbar}t}\,\psi(\vec{r},0)$$

$$\text{If initial time is } t_0: \quad \psi(\vec{r},t) = e^{-i\frac{H}{\hbar}(t-t_0)}\,\psi(\vec{r},t_0)$$

$$\psi_I(\vec{r},t) = e^{+i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t) = e^{+i\frac{H_0}{\hbar}t}\,e^{-i\frac{H}{\hbar}(t-t_0)}\,\psi_S(\vec{r},t_0)$$

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So, we have got in this the initial state was recognized at t =0 but if the initial time is some arbitrary time t0 then here instead of this -i over H cross ht instead of this t you will have t - t0. So, it is just an offset of the 0 of your time scale, so if your 0 of the time scale is at t0 you have this more general form and for this form you have the t - t0 coming over here.

Keep track of the fact that there are two exponential operators one containing the unperturbed part of the Hamiltonian which is H0 that is the soluble part. Here also you have got a similar term but this is the full Hamiltonian okay. So, you have to keep track of these details okay.
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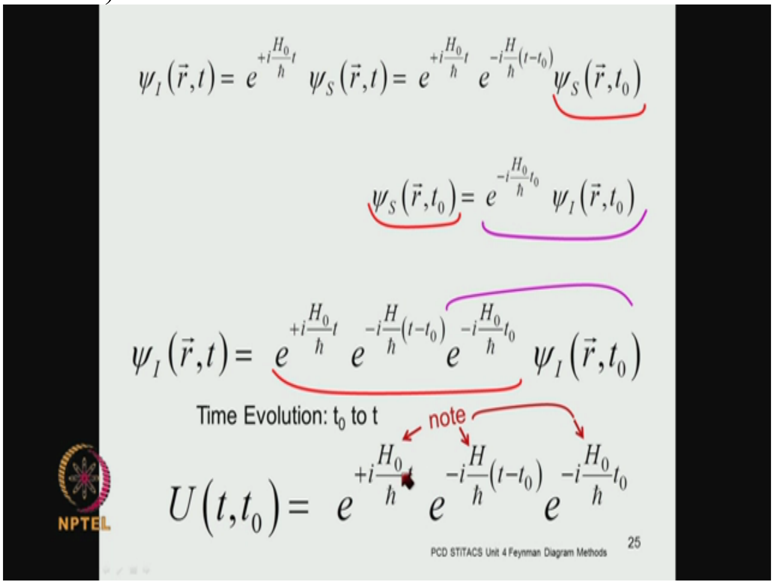

$$\psi_I(\vec{r},t) = e^{+i\frac{H_0}{\hbar}t}\,\psi_S(\vec{r},t) = e^{+i\frac{H_0}{\hbar}t}\,e^{-i\frac{H}{\hbar}(t-t_0)}\,\underline{\psi_S(\vec{r},t_0)}$$

$$\underline{\psi_S(\vec{r},t_0)} = \underline{e^{-i\frac{H_0}{\hbar}t_0}\,\psi_I(\vec{r},t_0)}$$

$$\psi_I(\vec{r},t) = \underbrace{e^{+i\frac{H_0}{\hbar}t}\,e^{-i\frac{H}{\hbar}(t-t_0)}\,e^{-i\frac{H_0}{\hbar}t_0}}\,\psi_I(\vec{r},t_0)$$

Time Evolution: t_0 to t

note

$$U(t,t_0) = e^{+i\frac{H_0}{\hbar}t}\,e^{-i\frac{H}{\hbar}(t-t_0)}\,e^{-i\frac{H_0}{\hbar}t_0}$$

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So that is where what we have got this is the Schrodinger picture wave function which is related to the interaction picture wave function. So, you can write this result for the interaction picture in terms of the interaction picture wave functions. So, now this term which is equivalently written by this term and now you have this left hand side Psi irt coming over here and at the right hand side you have got this term which comes here.

You have got the middle term which has got the full Hamiltonian which comes over here with the t - t0 and then the last term is given over here. So, this becomes your time evolution operator for the interaction picture okay. This is one describes the time evolution from t0 to time t for the interaction picture time evolution operator.

So, this is the time evolution operator in the interaction picture and you can explore its properties also okay. So, you must remember that you have got the exponential operators in which you have got the Hamiltonian but you have got the unperturbed Hamiltonian here, you have got the unperturbed Hamiltonian H0 over here, you have got the full Hamiltonian over here right.

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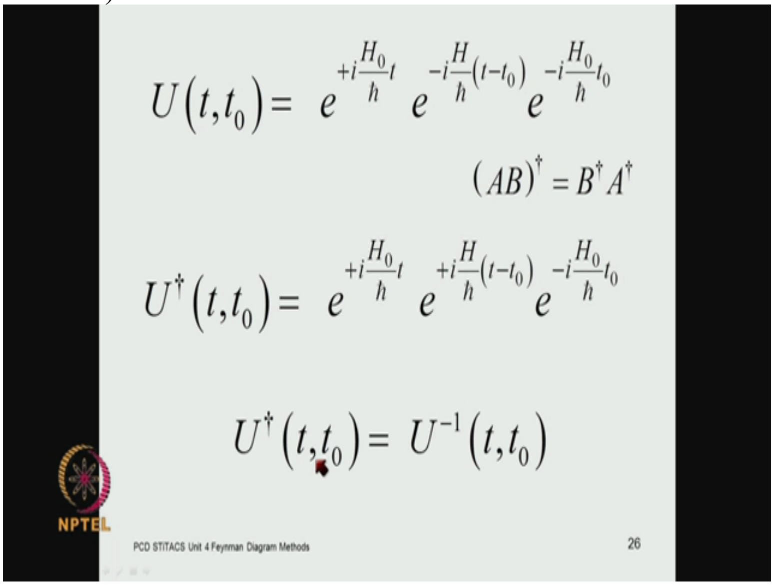

$$U(t,t_0) = e^{+i\frac{H_0}{h}t}\, e^{-i\frac{H}{h}(t-t_0)}\, e^{-i\frac{H_0}{h}t_0}$$

$$(AB)^\dagger = B^\dagger A^\dagger$$

$$U^\dagger(t,t_0) = e^{+i\frac{H_0}{h}t}\, e^{+i\frac{H}{h}(t-t_0)}\, e^{-i\frac{H_0}{h}t_0}$$

$$U^\dagger(t,t_0) = U^{-1}(t,t_0)$$

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So, we know the usual property when you take the joint of an operator of a adjoint of the product of an operators you get this relation. So, if you take the adjoint of this operator you get the adjoint of this then the joint of this and the adjoint of this comes over here. And essentially you find that this is also a unitary operator okay. So, in the interaction picture also you have got the time evolution described by a unitary operator.

So, these are you know more or less obvious properties but then you have to demonstrate their properties using explicit transformations. And the transformations have to be done carefully because you have got the Hamiltonian in the exponential terms but the unperturbed Hamiltonian here and here with the full Hamiltonian over here.

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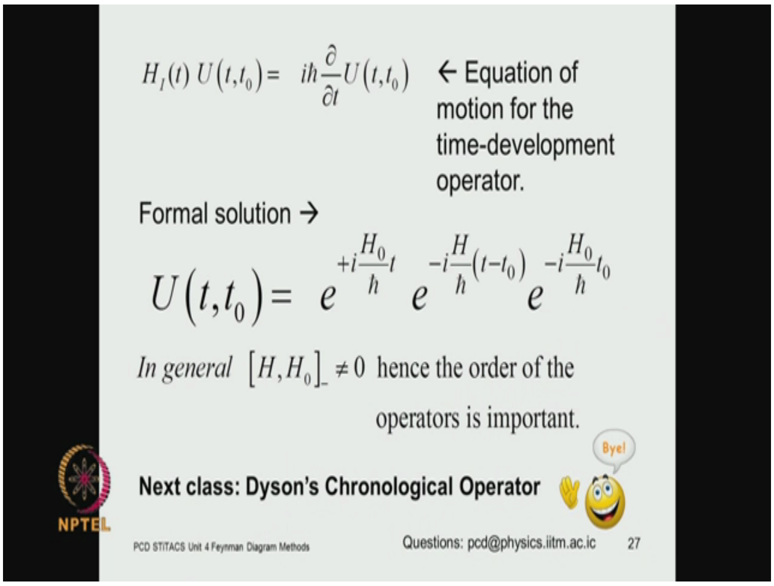

$H_I(t)\,U(t,t_0) = ih\frac{\partial}{\partial t}U(t,t_0)$ ← Equation of motion for the time-development operator.

Formal solution →

$$U(t,t_0) = e^{+i\frac{H_0}{h}t}\, e^{-i\frac{H}{h}(t-t_0)}\, e^{-i\frac{H_0}{h}t_0}$$

In general $[H,H_0]_- \neq 0$ hence the order of the operators is important.

Next class: Dyson's Chronological Operator

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Questions: pcd@physics.iitm.ac.ic 27

So, this is the equation of motion for the time development operator now and it has got a formal solution which we have just seen which is given by this product. And this is where I will take a break and stop for the day and we will continue from here in the next class. Remember that in general the full Hamiltonian does not commute with the unperturbed part. So, the order in which you carry out this product is critical okay.

That is absolutely important and that is where I will stop and with this platform I will introduce the chronological operator which is known as the Dyson's chronological operator in the next class. If there is any question I will be happy to take otherwise we break here and resume in the next class.