

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
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Lecture 29
Feynman Diagrams

Greetings, we will continue our discussion of the Feynman diagram methods and as you can see from the opening slide of today's lecture you are going to meet the Feynman diagrams for the first time in this unit although we will really be taking up the discussion and discuss the diagrams themselves more extensively in the next class but I think we are now approaching the diagrammatic diagrams themselves.

So, I am going to spend some time recapitulating on what we did in the previous class because everything has to be put in the right perspective.
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$\Delta E = \Delta E^{(1)} + \Delta E^{(2)} + \Delta E^{(3)} + ..$

$\Delta E = \lim_{\alpha \rightarrow 0} ih \frac{\partial}{\partial t} \left[\left((A_1 + A_2 + A_3 + \dots) - \frac{1}{2} \left(\begin{matrix} A_1^2 + A_2^2 + A_3^2 + \dots \\ + A_1 A_2 + A_2 A_1 + A_1 A_3 + \\ + A_3 A_1 + A_2 A_3 + A_3 A_2 + \dots \end{matrix} \right) \right) \right]_{t=0}$

Adiabatic 'switch' on the correlation / perturbation

Chronological operator

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$= \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_1(t_1) H_1(t_2) \dots H_1(t_n)] \right| \Phi_0 \right\rangle$$

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So, we were dealing with a problem in which we could solve a part of the problem which is the unperturbed part as we call it and then there is an additional part which was cumbersome which was difficult which was not amenable to usual methods in quantum theory. And this is the part which in our context we have to deal with the electron correlations particularly the Coulomb correlations.

The exchange correlations we could certainly handle but not the Coulomb correlations. And they would lead to a correction which we have written as delta E. And we can write this set of correction to various orders in perturbation expansion. So, you will have the first order perturbation correction the second order, the third order corrections and so on.

Now these are the corrections that we really wish to incorporate in our formalism and by developing this adiabatic switching technique which is a mathematical device to turn on the perturbation to turn on the correlations we arrived at an expression. So, alpha is the mathematical switch it is the adiabatic switch.

And by developing a formalism in terms of this alpha parameter but then finally our results must of course be independent of this mathematical device. So, we will take the limit alpha going to 0 and in this we got an expression which is quite complex it has got first order terms, second order terms higher order and goes all the way to infinity.

And there are fairly complex terms these A's are the nth A contains the nth order terms. So, there are you know the interaction term will appear n times once, twice, thrice and so on up to n times and what you have is a chronological order chronological operator which orders the latest operators to the left. So, the time ordering also has to be preserved because these operators do not automatically commute.

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$$\Delta E^{(1)} = \lim_{\alpha \rightarrow 0} ih \left[\frac{\partial}{\partial t} A_1 \right]_{t=0} \quad A_1 = \langle \Phi_0 | U_1 | \Phi_0 \rangle = \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right) \int_{-\infty}^t dt_1 H_I(t_1) \right| \Phi_0 \right\rangle$$

$$I = \int_{-\infty}^t dt_1 e^{(i\Delta_1 + \alpha)t_1} = \frac{e^{i\Delta_1 t} e^{\alpha t}}{(i\Delta_1 + \alpha)} \Bigg|_{-\infty}^t = \frac{e^{i\Delta_1 t} e^{\alpha t}}{(i\Delta_1 + \alpha)}$$

$$\frac{\partial A_1}{\partial t} = \frac{\partial}{\partial t} \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right) \int_{-\infty}^t dt_1 H_I(t_1) \right| \Phi_0 \right\rangle = \frac{-i}{\hbar} \langle \Phi_0 | H_I(t) | \Phi_0 \rangle$$

$$\Delta E^{(1)} = \lim_{\alpha \rightarrow 0} ih \left[\frac{\partial}{\partial t} \left\langle \Phi_0 \left| \sum_{i,j,k,l} c_i^\dagger c_j^\dagger \langle ij | v | lk \rangle c_k c_l \right| \Phi_0 \right\rangle \frac{e^{(i\Delta_1 + \alpha)t}}{(i\Delta_1 + \alpha)} \right]_{t=0}$$

$$\Delta E^{(1)} = \langle \Phi_0 | H' | \Phi_0 \rangle = \frac{1}{2} \sum_{i,j,k,l} \langle \Phi_0 | c_i^\dagger c_j^\dagger c_k c_l | \Phi_0 \rangle \langle ij | v | lk \rangle$$

$\alpha \rightarrow 0$ not relevant for first order correction; but not so for higher order terms....

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So what we did was to first consider the first order corrections. So, let me remind you of those results because we are going to use all of that in our discussion today. So, the first order term is given by this, so you have got only one term in the interaction here in the first order term. You have a time integral which is very easy to evaluate because it is just an exponential function. So, you can evaluate this time integral separately.

And typically you have in these integrals time integrals as well as space integrals and you can always carry them out separately as long as you do not mess up with the order of those operators wherever they are involved. So, as long as you do not do that you can carry out the

time integrals and the space integrals separately. So, in the limit alpha going to 0 as you can see when you take the first derivative with respect to time.

You have got e to the i delta 1 t and e to the alpha t over here in this integral and that will give you an i delta 1 + alpha when you take the time derivative and that will cancel the 1 in the denominator and then you are left with this exponential function which in the limit t going to alpha going to 0 will simply become unity okay, e to the alpha t in the limit alpha going to 0 will become unity.

And the first order alpha really does not show up in your final result at all. So, your correction is quite independent of alpha and the limit alpha going to 0 is not relevant for first order term. However for second order terms in higher order terms you will have to keep track of that.

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$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \left\{ \sum_{n=1}^{\infty} A_n - \frac{1}{2} \left(\sum_{n=1}^{\infty} A_n \right)^2 + \frac{1}{3} \left(\sum_{n=1}^{\infty} A_n \right)^3 - \frac{1}{4} \left(\sum_{n=1}^{\infty} A_n \right)^4 + \frac{1}{5} \left(\sum_{n=1}^{\infty} A_n \right)^5 - \dots \right\} \right]_{t=0}$$

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$= \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_I(t_1) H_I(t_2) \dots H_I(t_n)] \right| \Phi_0 \right\rangle$$

$$\Delta E^{(2)} = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \left\{ A_2 - \frac{1}{2} (A_1)^2 \right\} \right]_{t=0}$$

$$\Delta E^{(2)} = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} A_2 \right]_{t=0} - \lim_{\alpha \rightarrow 0} \frac{i\hbar}{2} \left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0}$$

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So, we subsequently dealt with the second-order terms and in the second-order terms you will have H the HI the interaction term appearing twice okay. So, that is the second order term and when we dealt with the second order terms we had contributions from the time derivative of A2 and from the time derivative of A1 squared which is actually half A1 square right.

So, these were the two contributors to the second order correction. What did it give us? It we, what we did was to separate these two terms and dealt with each separately. So, we dealt with the first one which I will quickly remind you how we did it and then we will proceed to work with the second term. So, the first term is the time derivative of A2 the second would be the time derivative of A1 square.


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$$\Delta E^{(2)} = \lim_{\alpha \rightarrow 0} ih \left[\frac{\partial}{\partial t} A_2 \right]_{t=0} - \lim_{\alpha \rightarrow 0} \frac{ih}{2} \left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0}$$

$$A_2 = \langle \Phi_0 | U_2 | \Phi_0 \rangle; \text{ hence } \frac{\partial}{\partial t} A_2 = \frac{\partial}{\partial t} \langle \Phi_0 | U_2 | \Phi_0 \rangle$$

$$\frac{\partial}{\partial t} A_2 = \frac{-1}{\hbar^2} \left(\frac{\partial}{\partial t} \left\langle \Phi_0 \left| \int_{-\infty}^t dt_1 H_1(t_1) \int_{-\infty}^{t_1} dt_2 H_1(t_2) \right| \Phi_0 \right\rangle \right)$$

at t=0

$$\frac{\partial}{\partial t} A_2 = \frac{-1}{\hbar^2} \left\langle \Phi_0 \left| H_1(t) \int_{-\infty}^t dt_2 H_1(t_2) \right| \Phi_0 \right\rangle$$


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So, the first one is this which is del by del t of A2 you have to take this partial derivative at t = 0 and let us deal with this first term alone. So, what is A2, A2 is this matrix element of U2 in the unperturbed ground state. And now this time derivative will involve but U2 will involve these time integrals. Now this time integral what you see there is a time integral over here of which you have to take the time derivative.

So, the other integration variable is the dummy label which goes from which is a t1 which is a dummy label which goes from minus infinity to the upper limit which is t and it is this t with respect to which the time derivative is taken okay. So, this integral we have handled already when we did the first order term it is exactly the same kind of term.

And what it gives us is a result for this. So, you get the HI t here and then of course you will have to take this time derivative at t = 0. So, when you take the time derivative at t = 0 this t will become t = 0 and this upper limit will also become 0 right. This is the next dummy label whose range is also from minus infinity to t.
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$$\left[\frac{\partial}{\partial t} A_2 \right]_{t=0} = \frac{-1}{\hbar^2} \sum_{n=0}^{\infty} \left| \langle \Phi_n | H_1 | \Phi_0 \rangle \right|^2 \int_{-\infty}^0 dt e^{-i \left(\frac{E_0 - E_n + i\hbar\alpha}{\hbar} \right) t}$$

$$\int_{-\infty}^0 dt e^{-i \left(\frac{E_0 - E_n + i\hbar\alpha}{\hbar} \right) t} = \frac{e^{-i \left(\frac{E_0 - E_n}{\hbar} \right) t} e^{at}}{-i \left(\frac{E_0 - E_n + i\hbar\alpha}{\hbar} \right)} \Bigg|_{-\infty}^0 = \frac{\hbar}{-i(E_0 - E_n + i\hbar\alpha)}$$

$$\left[\frac{\partial}{\partial t} A_2 \right]_{t=0} = \frac{1}{\hbar} \sum_{n=0}^{\infty} \frac{\left| \langle \Phi_n | H_1 | \Phi_0 \rangle \right|^2}{i(E_0 - E_n + i\hbar\alpha)}$$

?

$$\Delta E^{(2)} = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} A_2 \right]_{t=0} - \lim_{\alpha \rightarrow 0} \frac{i\hbar}{2} \left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0}$$

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So, that is what we now have over here, so this is $t = 0$, here okay and here the upper limit is now 0, so that has been taken care of. Now here have a look at this integral and this integral is I have written it explicitly as an integral thing this is the Dirac notation and this is a usual De Broglie Schrodinger notation and this is the integral that you have to work with.

And H_1 operating on Φ_0 can always be expressed as a linear superposition of the entire basis set. And the basis set is the Eigen basis of the unperturbed Hamiltonian. So, the premise of perturbation theory is that the Eigen function of the unperturbed Hamiltonian is sufficient to expand an arbitrary state.

So, we use this expansion of the H_1 operating on Φ_0 but then you also have H_1 operating on Φ_0 to the left over here okay. So, the; which is nothing but the adjoint of this expression. And we use the adjoint of this expression that gives us a modular square over here and then by doing some simple you know transformations we arrived at this result. So, this was the result of last time and then we had this time integral.

So, this time integral is again a simple function the exponential function and you can evaluate this time integral. So, you get this function divided by this exponent this part of the exponent which is which multiplies time and then you take the difference at the upper limit which is 0 and the lower limit which is minus infinity, so that term will go to 0 and this is what you get right.

So, this is your result now this result is good and we still have to determine the second term. So, we came as far as getting the first term in our previous class. And this is the term that we now have to discuss today okay. Now in this case you not only have to get the time derivative

at $t = 0$ which is what we get over here but subsequently you have to take the limit α going to 0 okay.

So, you might wonder that here the summation is from 0 through infinity. And if you look at the term for $n = 0$ you will get $E_0 - E_n$ with $n = 0$. So, $E_0 - E_0$ will vanish then you have got the $i\hbar$ cross α that is what you are left with. And then you are going to have to take the limit α going to 0. So, you will end up taking the limit α going to 0 of a term whose denominator vanishes in the limit α going to 0.

So, you will sort of worry about the divergence that it is going to blow up and you might meet some infinities over there. So, you probably are worried about it and you ought to be worried about it but just leave this worry on the shelf for a moment. Because we are we have another term and that is the term that we have to work with. So, let us see what we get from the other term.

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So, this is the second term that we have to evaluate. So, let us go ahead and do that what we need to do over here is to take the time derivative of A_1 square. Now both are A_1 , so this is even into A_1 , so this will work okay. So, this is twice A_1 and the time derivative of A_1 , now A_1 we already know we have worked with A_1 earlier in our previous class. So, given this even we know that its time derivative is given by this term.

So, this result we have already got. So, now all you have to do is to multiply this A_1 with this to get $A_1 \frac{\partial A_1}{\partial t}$ by $\frac{\partial}{\partial t}$ and of course you have a factor of 2. So, you take twice A_1 into A_1 square, so here you will get the time derivative of A_1 square which is just the product of these two pre multiplied by the factor of 2.

So, you have got a -i here, you have got a -i here, so that is what gives you a minus sign here. And then you have 2h cross square because there is an h cross in the denominator of both. So, you have got the h cross square in the denominator and then you have got these two terms in the particular order in which we want them okay.

So, now we take the limiting value because this time derivative we are interested in the value of the time derivative at $t = 0$, so we put $t = 0$ over here okay. And over here as well this is of course a dummy label which goes from minus infinity to $t = 0$. So, this is where you pick up the interaction term at $t = 0$. So this is your net result.

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The slide contains the following mathematical expressions:

$$\left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0} = \frac{-2}{\hbar^2} \langle \Phi_0 | \int_{-\infty}^0 dt_1 H_I(t_1) | \Phi_0 \rangle \langle \Phi_0 | H_I(t=0) | \Phi_0 \rangle$$

$$H_I(t) = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iH_0 t}{\hbar}} \quad | H_I(t \rightarrow -\infty) = 0 \quad | H_I(t=0) = H_1$$

$$\left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0} = \frac{-2}{\hbar^2} \langle \Phi_0 | \int_{-\infty}^0 dt H_I(t) | \Phi_0 \rangle \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$\langle \Phi_0 | \int_{-\infty}^0 dt \{ H_I(t) \} | \Phi_0 \rangle = \langle \Phi_0 | \int_{-\infty}^0 dt \left\{ e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iH_0 t}{\hbar}} \right\} | \Phi_0 \rangle$$

$$\langle \Phi_0 | \int_{-\infty}^0 dt H_I(t) | \Phi_0 \rangle = \int_{-\infty}^0 dt \langle \Phi_0 | e^{\frac{iE_0 t}{\hbar}} (e^{\alpha t} H_1) e^{-\frac{iE_0 t}{\hbar}} | \Phi_0 \rangle$$

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And what we do know is that the interaction term Hamiltonian at $t = 0$ is nothing but H_1 itself okay. So, let us write that, so this one is H_1 you have rest of the terms and let us now evaluate this matrix element. So, this matrix element has got this H_1 which I have written in this beautiful bracket.

And here this is nothing but the transformation to the Dirac picture of the Schrodinger picture interaction okay. And this transformation to the Dirac picture is through the operator e to the iH_0 over \hbar cross t right. So, it is this transformation operator and you are sandwiching the Schrodinger picture operator in the middle.

Except that you have plugged in this adiabatic factor e to the αt which we know that eventually we will end up taking the limit α going to 0, so that will be all fine okay. So, you have plugged in this e to the αt as well in addition to the H_1 . Now look at this term over here you have got the H_0 operator here, so this is an infinite power series in H_0 but Φ_0 is an Eigen state of H_0 .

So, you will get an Eigen value equation from this infinite series and when you sum up that infinite series you will recover the exponential function but with the Eigen value of H0 rather than the operator H0 okay. So, you will have the e to the -iE0 over h cross t over here from this operation. And you have the same on the left because this H0 would operate on this Phi 0 and this is a hermitian operator.

So, you will have a similar power series and again you will be able to exploit an Eigen value equation. So, these terms can be handled rather easily and instead of this e to the iH0 h cross t you get E0 instead of this H0 here, in the last step and so also over here. And now you have got these are just scalar numbers okay.

And it does not matter where you put them in the expression. So, these two terms will cancel each other, so e to the iE0 over h cross t cancels e to the -i E0 over h cross t and you get rid of that so let me bring this result to the top of the next slide okay.

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$$\left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0} = \frac{-2}{\hbar^2} \langle \Phi_0 | \int_{-\infty}^0 dt H_I(t) | \Phi_0 \rangle \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$\langle \Phi_0 | \int_{-\infty}^0 dt H_I(t) | \Phi_0 \rangle = \int_{-\infty}^0 dt \langle \Phi_0 | e^{i\frac{E_0}{\hbar}t} (e^{\alpha H_1}) e^{-i\frac{E_0}{\hbar}t} | \Phi_0 \rangle$$

$$= \int_{-\infty}^0 dt e^{\alpha t} \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$= \left(\frac{e^{\alpha t}}{\alpha} \right)_{-\infty}^0 \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

$$= \frac{\langle \Phi_0 | H_1 | \Phi_0 \rangle}{\alpha}$$

$$\left[\frac{\partial}{\partial t} (A_1)^2 \right]_{t=0} = \frac{-2}{\hbar^2} \frac{\langle \Phi_0 | H_1 | \Phi_0 \rangle}{\alpha} \langle \Phi_0 | H_1 | \Phi_0 \rangle$$

So, these terms have cancelled and you are now left with a rather simpler expression and now you separate the time integral okay. And the only term which is time dependent the integrand will only be this e to the alpha t everything else has been taken care of okay. So, now here you are and this is a very simple integral to determine.

And this is just e to the alpha t over alpha between the limits you will have to take the difference for t = 0 and t equal to minus infinity. So, that will give you 1 over alpha and this matrix element of H1 and these states in the unperturbed ground state of H0 okay. So, this is your result now, so this is your del over del t of A1 square at t = 0.

So, you have now evaluated it and you get a product of these two terms and notice that you have an alpha in the denominator. So, which is good news and bad news, bad news because you meet a divergence good news because it is going to cancel the other divergence that we were worried about earlier.

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So, these are the two terms that you now have to combine okay. So, this $\Delta E^{(2)}$ by Δt we determined earlier. Now we have determined $\Delta E^{(2)}$ by Δt of A_1 square, so now you put both the terms together and this is what you have got okay. Now here you have got an infinite sum n going from 0 through infinity okay that is the infinite sum that you have got, here these two are complex conjugate.

So, I just take the modulus squares, so that I can write it in a simpler fashion okay, so this is $|\langle \Phi_0 | H_1 | \Phi_0 \rangle|^2$. And here you have a sum over n you have got an infinite series and I separate the term for $n = 0$ and then the remaining sum is $n = 1$ through infinity okay. So, the sum going from 0 to infinity is now separated into two pieces one term corresponds to $n = 0$ which is the first term here.

And the other term which will again be an infinite series because even if you remove one term from infinity you are still left with infinite terms that is the beauty of infinity. So, you still have infinite challenge but beginning with $n = 1$ and for $n = 1$ $E_0 - E_n$ is not going to vanish. So, there is no divergence coming from here.

The only divergence to worry with, worry about was over here and this $E_0 - E_0$ will cancel you will have 1 over α . But then you have got 1 over $i\hbar$ cross α whereas over here you have i over \hbar cross α . So, the 1 over i and the i over 1 will cancel each other. So, the first term and the third term cancel.


And now you are left with only what is in the middle okay. So, now there is no divergence that is left the first term and the third term cancel you are left only with this middle term but then with a restricted sum from which to the $n = 0$ term has been removed. So, this is now your result but the second order correction is an infinite power series you do have to take the limit alpha going to 0 okay.
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$$\Delta E^{(2)} = \lim_{\alpha \rightarrow 0} \sum_{n=1}^{\infty} \frac{|\langle \Phi_n | H_1 | \Phi_0 \rangle|^2}{(E_0 - E_n + i\hbar\alpha)}$$

$$= \sum_{n=1}^{\infty} \frac{|\langle \Phi_n | H_1 | \Phi_0 \rangle|^2}{(E_0 - E_n)} \quad \leftarrow \text{Same as 2}^{\text{nd}} \text{ order Rayleigh-Schrodinger perturbation theory.}$$

$\alpha \rightarrow 0$ was needed to see correspondence with Rayleigh-Schrodinger perturbation theory.

Same result holds good for higher order terms.


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So, let us look at this result alright. So, now let us take the limit alpha going to 0 okay, what do you have now this is just the result you get from the Rayleigh Schrodinger perturbation theory okay which is fine which is just what one would want to have okay. So, it is a very desirable result and that is exactly what you get.

So, no worries but this is one might wonder that okay if you are getting the same thing as Rayleigh Schrodinger perturbation theory. But how did we get it, we went about getting this result in a slightly round about manner by taking the limit alpha going to 0. So, we first inserted an ϵ to the α term and then we get rid of it.

So, it is like you know you insert something which you do not seem to need which you do not seem to want and then get rid of it and say that everything is fine. So, why do we do that okay? So, one might wonder as to what is the advantage of this inserting this mathematical device which is through this adiabatic switch which is affected through the parameter alpha.
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$$\Delta E^{(2)} = \sum_{n=1}^{\infty} \frac{|\langle \Phi_n | H_1 | \Phi_0 \rangle|^2}{(E_0 - E_n)}$$

If it is the same result as Rayleigh-Schrodinger Perturbation Theory, what is the advantage?

Combined with time-dependent methods and FEYNMAN DIAGRAMS, the present method offers tremendous convenience, specially in addressing higher order corrections.



So, there is a definite advantage of this and the reason you see this advantage is because what the ϵ has enabled us to do is to carry out transformations to the interaction picture then we develop a certain formalism, we develop this mathematical device of you know adiabatic switching we know how the limits are taken. And we have done all that exercise, so we will quickly recapitulate all of that.

Because all of this when you use this in conjunction with the Feynman diagrammatic methods because now we have done it using the time dependent operators. And the operators are time dependent in the Dirac picture in the interaction picture. So, what the ϵ has allowed us to do is to use the Dirac picture and the interaction picture and that turns out to be a great convenience when we use the Feynman diagram.

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The technique of adiabatic switching, and addressing the perturbations using the methods we discussed can be applied to many other situations; not just a many-electron system.



So, as you will see apart from the fact that these methods are also applicable in any other situations. So, the techniques are very powerful are the nice things you learn okay. So, this


adiabatic switching means it is not to be dismissed as something that is redundant just because you got the same result as what you get from perturbation theory.

In fact you get the same results even for higher order. But then you are now equipped with very powerful tools that these tools which will make use of the interaction picture operators and you will see how the Feynman diagrammatic methods exploits this. (Refer Slide Time: 22:44)

We have seen the second order term:

$$A_2 = \frac{-1}{\hbar^2} \left\langle \Phi_0 \left| \int_{-\infty}^t dt_1 H_I(t_1) \int_{-\infty}^{t_1} dt_2 H_I(t_2) \right| \Phi_0 \right\rangle$$

Let us get an *advance* glance at the nth order term:



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So, we worked with the first order term then we worked with the second order term and the interaction appears twice in this. And let me give you a slight advance glance and the nth order term okay. And we are going to get that term by generalizing these forms but before we do it systematically let me just give you what you might call as a preview okay of what is to come.



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$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle = \left(\frac{-i}{2\hbar} \right)^n \left\langle \Phi_0 \left| \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n H_I(t_1) H_I(t_2) \dots H_I(t_n) \right| \Phi_0 \right\rangle$$

Feynman Diagrams

~~complex?~~

What if today, we were just grateful for everything?

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So, just have a look at that so this is the nth order term and do you like it do you like it means there are these multiple summations okay. Each single summation is a summation over four

indices okay i, j, k, l you saw that already in the first order term right. And then you have these multiple summations then you have these two center integrals and you have plenty of them okay, 1, 2 and many okay.

Then you have these terms which are coming from the time integrals and there are several of them okay. And then you have got the expectation value of the second quantized creation and destruction operators. So, it is a mess and it is awful right and instead of you know looking at this kind of mess just imagine that you could work with some fun diagrams instead of these complex mathematical expressions.

If you were to work with pictures of this kind okay, it would be so much nicer and that is what the Feynman diagrams are about okay. So, you are going to meet them very soon now. So, all this complexity will be removed or it will be reduced to handling certain diagrams and that will make your analysis that much easier and a lot of fun, so here these diagrams will represent all these processes you know what is happening over here.

There is a destruction operator for c_k there is a creation operator for c_j^\dagger look at the $c_p^\dagger c_q^\dagger$ dagger term then there is a $c_r c_s$. So, there are these creation and destruction in different one particle states okay and a lot of it is happening if you look at this complete expression. That many particles are being destroyed some other are being created you are conserving the total number of particles okay.

We are working in you know in atomic physics we are not really working with actual creation of particles from energy okay. But we are changing their states from one occupied state to an unoccupied state and vice versa. So, that is what the second quantization is doing for us in atomic physics. So, this will be represented using rather lovely Feynman diagrams and that is what we are going to introduce now.

(Refer Slide Time: 25:58)

"I learned very early the difference between knowing the *name of* something, and *knowing something.*" — Richard P. Feynman (1918-1988)

http://www.goodreads.com/author/quotes/1429989_Richard_P_Feynman
Downloaded on December 09, 2013

particle creation
particle destruction
Vertex is where an interaction between interacting particles is indicated
Mediator (Boson) PHOTON
hole creation
hole destruction

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So, the Feynman diagrams they look like this okay this is just an example of some of the simplest ones you have these Wiggles and you have got these arrows and these arrows seem to get into the vertex they seem to get it out of the vertex and what we will do is introduce all of this systematically and define these terms carefully okay. So the first thing to note are the vertices okay.

These are the vertices and the vertex is where the interaction between the interacting articles is indicated. So, these are pictorial representations of physical process and what the vertex represents is the location okay this is it is just an indication of where the interaction is taking place and what you find in between the vertices are these wiggles which represent the mediator which effects the interaction.

Because after all the interaction between two electrons is affected by the electronic field, so what is a virtual photon which is involved? So, that is what this wiggles represents and then you have got these arrows which go into the vertex and arrows which go out of the vertex. So, the convention here is that the arrow which goes into the vertex represents the destruction of a particle.

And the arrow which goes out of the vertex represents the creation of a particle because you saw in the previous slide that you have to work with various second quantized operators okay and these are the creation and destruction operators. So, any operator in quantum theory you can always write in terms of the creation and destruction operators. So, you will always have to work with them.

And the creation of a particle will be indicated by an arrow going out of the vertex and pointed upward okay. So, I will define all these rules in fact you will notice if you have

noticed already and if you have not let me bring it to your notice. That this p is written in italics here okay and there is a reason for it and I am following the discussion as given in the book by Raimes, Stanley Raimes the main electron theory.

And this is a nice notation that he has introduced over here, so that is the one that I am using. So, he uses particle in two different fonts one with an upright P as usual and one with a slant which is written in italics and these have got different meanings which I will define very soon. So, you have these particle states which are created or destroyed and if you have an arrow pointing upward these are particle states.

Likewise if you have arrows pointing downward these are hole states okay and here again the h is written in italics with a slant. So, I will define them okay and you have not either hole creation or hole destruction okay. So, you have these different processes which are taking place over the Fermi sea. So, if not an electron gas in the Fermi sea and then you can bounce off these particles into unoccupied states.


And then you can create holes below the Fermi level, you can create particles above the Fermi level, you can destroy the particles above the Fermi level right. So, all of these processes will be this you know described by these pictures. So, you have got hole creation all the hole operators both creation and destruction are indicated by arrows pointing downward, arrows pointing upward our particle operators.

What goes into the vertex is the particle destruction and what goes out of the vertex is particle creation likewise for hole the convention is that an arrow getting into the vertex is the hole creation and an arrow getting out of the vertex but pointed downward is the hole destruction. So, this is a convention that we will follow.

And if these quantum labels are the same you can actually close this and you get what is called as a nice double bubble okay. So, they not only look nice they also have nice names. So, you will actually have fun in this,
(Refer Slide Time: 30:55)

Our interest in the present course:
Select/Special Topics
 in the
Theory of Atomic Collisions and Spectroscopy
 Study of electron-correlation effects in atomic
 collision / photoabsorption processes -

- Random Phase Approximation
- Many Body Perturbation Theory
- Configuration Interactions etc.
- RRPA: Relativistic Random Phase Approximation
- MCTD: MultiConfiguration Tamm Dancoff method
- MQDT: Multichannel Quantum Defect Theory etc...

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Now what is our interest in this course? So, we have a rather restricted interest in this our focus is on studying atomic collisions and spectroscopy and in particular we will be interested in studying the electron correlation effects in atomic physics. An atomic physics is done using some experiments in which you have got a target.

You have a certain probe the probe is either an electron or some other particle or a collection of particle like the alpha particle it can also be an ion or some other atom or else you shine electromagnetic radiation on it and then look at ion photo absorption or photon scattering. So, that is the kind of processes that we are interested in. So, I will present this discussion specifically in the context of our interest and atomic physics.

At most specifically we are interested in dealing with the electron correlations. We know that the statistical correlations have been accounted for in our discussion using the Hartree Fock formalism which we have studied in a previous course. So, we are quite familiar with the Hartree Fock technique it takes into account of all the statistical correlation. And what went beyond the Hartree Fock are the Coulomb correlations.

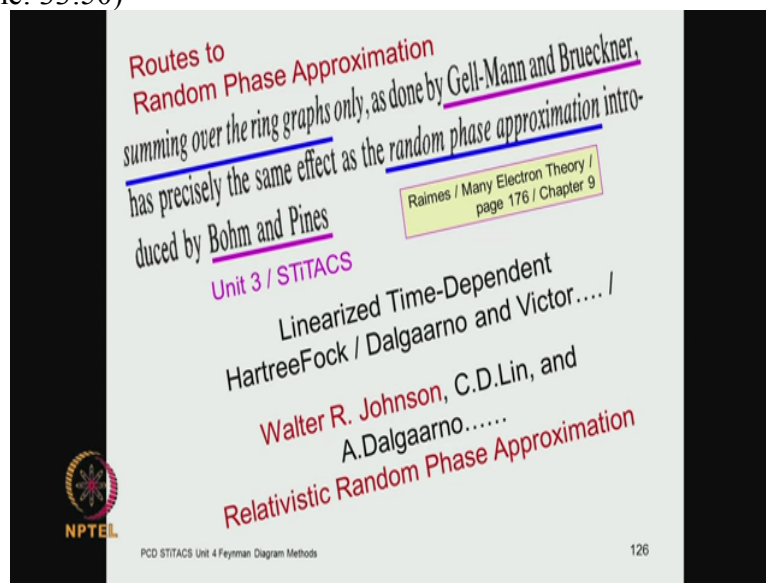
For which we are going to be using the Feynman diagrammatic methods and in the previous unit we actually did different many body theory namely the random phase approximation which we did using the Bohm Pines approach. So, we will be able to see the correspondence between the Bohm Pines approach and the diagrammatic perturbation theory as well.

So, essentially it boils down to doing configuration interactions okay. You have a single Slater determinant is not adequate to represent the N electron wave function. So, you have a configuration interaction between a numbers of Slater determinants. So, this is the situation

that we have to work with and then there are, there is the non relativistic random phase approximation.

You have you can begin with the Dirac equation rather than the Schrodinger equation. And then you have the relativistic random phase approximation one can go to go on to address the residual correlations using some other techniques. And some of you are already using the multi configuration Tamm Dancoff method or the quantum defect theory.

And these are the techniques in which we as atomic physicists are interested in okay. So, what I hope to do is to provide some sort of a background which is which will take us into these techniques and we will see how these methods are used in atomic physics.
(Refer Slide Time: 33:50)



So, there are actually different routes to random face approximation when we did the previous unit 3 we did the Bohm Pines method quite extensively. And I did it specifically to explain the term random face approximation okay. So, this term random face approximation actually has only a historical importance. But the historical importance came from the method of Bohm and Pines.

And you actually saw the terms you identify the terms that to get the RPA you eliminated certain terms in unit 3 and that elimination was possible on the basis of those terms which came with random phases which cancelled each other. So, that was the manifestation of the random phase approximation.

But that was not the foundation of the RPA the foundation came from the linearization of certain terms okay. And that linearization is fundamental that is more fundamental than the nomenclature random phase because now we are going to use the same linearization

techniques and arrive at equivalent but alternate routes to random phase approximation. So, one can do the Gell-Mann Brurckner formalism.

For example in what you have seen these diagrams and you will see that there are some of these diagrams have these pictures the Feynman diagrams they look like ring diagrams. There will be the loops, there will be these rings that you will see in these diagrams when we develop this formalism the next one or two classes okay. So, you have these ring graphs but you also have some other graphs which are not expressible like ring diagrams.

And the process of linearization would involve the exclusion of these non during diagrams and the retention of the ring diagrams. So, the linearization process will be common to this as it was the Bohm Pines method. So, the method continues to be called as the random phase approximation okay. So, I am following the discussion from Raimis, so this is the reference that you might want to look up.

We did this quite extensively in unit 3 of this course and the essential element of this is the linearization process. So, this linearization process you can do it in many different ways you can do it as we did in the Bohm Pines method. You can do it as we will now do in this unit using the Gell-Mann and Brurckner method which will amount to the retention of the ring diagrams.

You can also do it using an extension of the Hartree Fock method. But we know that the Hartree Fock is not sufficient to address the Coulomb correlations, so you have to make use of what is called as the time-dependent Hartree Fock and then you will get nonlinear terms. But in those nonlinear terms you can then make an approximation keep only the linear terms. So, the linearization process will be common to all of them.

And they are all equivalent mathematically equivalent formalisms of the RPA of the random phase of transformation okay. So, the linearization of the time dependent Hartree Fock was done earlier by Dalgaarno and Victor. And then it is relativistic formalism was developed by Walter Johnson which is what we refer to as a relativistic random phase approximation.

So, this was done by Johnson, Lin and Dalgaarno, Dalgaarno did it earlier for the non-relativistic formalism with Victor for the non relativistic time dependent Hartree Fock. What Walter did for the time dependent Dirac Fock okay.
(Refer Slide Time: 37:53)

$$H_1 = \frac{1}{2} \sum_i \sum_j \sum_k \sum_l c_i^\dagger c_j^\dagger \langle ij|v|lk \rangle c_k c_l$$

We shall use the INTERACTION PICTURE formalism.


$$\Omega_I = e^{\frac{iH_0 t}{\hbar}} \Omega_S e^{-\frac{iH_0 t}{\hbar}}$$

$$\psi_I(\vec{r}, t) = e^{\frac{iH_0 t}{\hbar}} \psi_S(\vec{r}, t)$$

$$H_I(t) = e^{\frac{iH_0 t}{\hbar}} H_1 e^{-\frac{iH_0 t}{\hbar}}$$

$H = H_0 + e^{\alpha t} H_1$ ← **Adiabatic switching on of the interaction.**

$$H_I(t) = e^{\frac{iH_0 t}{\hbar}} \left(e^{\alpha t} H_1 \right) e^{-\frac{iH_0 t}{\hbar}}$$



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So, how do we go about doing it, so we have the, this is the tricky part, this is the interaction part, this is the two electron interaction we already have this expression. We will use the interaction picture and do not get cheated because you are going to see some of the terms that you have seen earlier.

I am putting all of that together in the present context, so that we can develop the Feynman diagrams from here. So, we will be using the interaction picture formalism and this is how you go through an interaction picture operator from a Schrodinger picture operator. You get the interaction pictures state wave functions from the Schrodinger picture wave functions the transformation is through the unperturbed Hamiltonian H_0 .

So, this is your interaction picture Hamiltonian corresponding to the two electron interaction. But we will be inserting the adiabatic switch which is the $e^{\alpha t}$ okay. So, this is our; you know model, so we will use this.
(Refer Slide Time: 39:03)

$$H_I(t) = e^{\frac{iH_0 t}{\hbar}} (e^{\alpha t} H_I) e^{-\frac{iH_0 t}{\hbar}}$$

$$H_I(t \rightarrow -\infty) = 0$$

α : adiabatic switch control parameter

$$H_I(t) = \frac{1}{2} \sum_i \sum_j \sum_k \sum_l c_i^\dagger(t) c_j^\dagger(t) \langle ij|v|lk \rangle c_k(t) c_l(t) e^{\alpha t}$$

From U4L26/Slide 66: $H = (H_0 + e^{\alpha t} H_I)$

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle \right]_{t=0}$$

Correction to the energy due to the interaction between the many-particle electron system.

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Then we know that this will reduce to the unperturbed Hamiltonian in the limit t going to minus infinity because this term vanishes, so those solutions are known. And this is the term that we will use, this is the control parameter the alpha adiabatic switch which is the mathematical device.

And we know that when we use this adiabatic hypothesis we do get a correction which is represented by the time derivative of this logarithmic expectation value of the time evolution operator in the unperturbed ground state of the unperturbed Hamiltonian. The time derivatives evaluated at t = 0 and they and finally you must take the limit alpha are going to 0. So, that is our overall prescription that we are going to use okay. (Refer Slide Time: 40:02)

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle \right]_{t=0}$$

From U4L26 STITACS

$$\log \langle \Phi_0 | U_\alpha(t, -\infty) | \Phi_0 \rangle = \sum_{n=1}^{\infty} A_n - \frac{1}{2} \left(\sum_{n=1}^{\infty} A_n \right)^2 + \frac{1}{3} \left(\sum_{n=1}^{\infty} A_n \right)^3 - \frac{1}{4} \left(\sum_{n=1}^{\infty} A_n \right)^4 + \frac{1}{5} \left(\sum_{n=1}^{\infty} A_n \right)^5 - \dots$$

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$= \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_I(t_1) H_I(t_2) \dots H_I(t_n)] \right| \Phi_0 \right\rangle$$

All these time integrals have to be obtained

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \left[\sum_{n=1}^{\infty} A_n - \frac{1}{2} \left(\sum_{n=1}^{\infty} A_n \right)^2 + \frac{1}{3} \left(\sum_{n=1}^{\infty} A_n \right)^3 - \frac{1}{4} \left(\sum_{n=1}^{\infty} A_n \right)^4 + \frac{1}{5} \left(\sum_{n=1}^{\infty} A_n \right)^5 - \dots \right] \right]_{t=0}$$

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So, we have discussed this we know that it has got a very complex form we have seen this okay. So, it leads to energy corrections two different orders first order corrections, second

order, third order and so on. So, you get a large number of terms infinite terms and then you have got a large number of these time integrals which also have to be evaluated right. (Refer Slide Time: 40:33)

Slide 80 / UAL27 : Raimis / Many Electron Theory / Eq. 7.18, page 114

$$A_i = \langle \Phi_0 | U_i | \Phi_0 \rangle = \frac{-i}{2\hbar} \sum_{i,j,k,l} \langle ij|v|lk \rangle \langle \Phi_0 | c_i^\dagger c_j^\dagger c_k c_l | \Phi_0 \rangle \frac{e^{i(\omega_i + \alpha)t}}{(i\Delta_i + \alpha)}$$

$$\Delta_i = (\omega_i + \omega_j - \omega_l - \omega_k)$$

Two equivalent forms of the Time Evolution Operator:

(A)

$$U(t, -\infty) = 1 + \left(\frac{-i}{\hbar}\right) \int_{-\infty}^t dt^* H_I(t^*) + \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt^* \int_{-\infty}^{t^*} dt'' H_I(t^*) H_I(t'') + \dots$$

(B)

$$U(t, -\infty) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T[H_I(t_1) H_I(t_2) \dots H_I(t_n)]$$

We must use $U_{\alpha}(t, -\infty)$ since $H_I(t) = e^{\frac{iH_0 t}{\hbar}} (e^{at} H_1) e^{-\frac{iH_0 t}{\hbar}}$

We shall now consider the 2nd order term; use (A)

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Now there are these two equivalent forms of the time evolution operator that we have introduced. This is one form which is an infinite series you have got infinite terms here. We also use another form which is completely equivalent to one at the top which does not have these dots over here but it has got an infinite sum over here.

And these two expressions are mathematically completely equivalent to each other. And this we have established in some of our earlier classes okay. So, these are the forms that we have used you have of course a time operator over here. The chronological operator and finally you are going to take the limit alpha going to 0 okay.

What we will do is these two forms are equivalent form A and form B. So, I will use the form A and consider the second order term. So, we have dealt with it but we will recapitulate some of the main results. So, that we have the right context for introducing the Feynman diagrams. (Refer Slide Time: 41:50)

$$U(t, -\infty) = 1 + \left(\frac{-i}{\hbar}\right) \int_{-\infty}^t dt' H_I(t') + \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt' \int_{-\infty}^{t'} dt'' H_I(t') H_I(t'') + \dots$$

$$U_{2,\alpha}(t, -\infty) = \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 H_I(t_1) H_I(t_2)$$

$$A_2 = \langle \Phi_0 | U_2 | \Phi_0 \rangle = \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 H_I(t_1) H_I(t_2) \right| \Phi_0 \right\rangle$$

$$H_I(t) = \frac{1}{2} \sum_i \sum_j \sum_k \sum_l c_i^\dagger(t) c_j^\dagger(t) \langle ij | v | lk \rangle c_k(t) c_l(t) e^{i\alpha t}$$

$$\langle ij | v | lk \rangle = \int dq_1 \int dq_2 \phi_j^*(q_1) \phi_i^*(q_2) v(q_1, q_2) \phi_l(q_1) \phi_k(q_2)$$

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So, here this is the form A and this is the second order term. So, the interaction term appears twice once here and once here okay. So, you have the two time integrals over to dummy time labels t2 will go for my ready to t1 and subsequently t1 will get integrated from minus infinity to t, the final time derivative will be with respect to this okay.

So, this is your interaction term and these are the two center integrals which you are quite familiar with you had them also in Hartree Fock. But here in the time integrals you have got a parameter t2 and a parameter t1 over here. So, the adiabatic alpha will come twice once with t2 and once with t1 okay.

And this will then be e to the alpha t1 and e to the alpha t2, so you have to keep track of these indices. And so these dummy labels are dummy, but where you use 1 you cannot use the other okay. So, you will have to use them carefully.
(Refer Slide Time: 43:01)

$$A_2 = \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar}\right)^2 \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 H_I(t_1) H_I(t_2) \right| \Phi_0 \right\rangle$$

$$H_I(t) = \frac{1}{2} \sum_i \sum_j \sum_k \sum_l c_i^\dagger(t) c_j^\dagger(t) \langle ij | v | lk \rangle c_k(t) c_l(t) e^{i\alpha t}$$

$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\langle ij | v | lk \rangle \times \langle pq | v | sr \rangle \right) \left\langle \Phi_0 \left| \begin{array}{c} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \\ c_i^\dagger(t_1) c_j^\dagger(t_1) c_k(t_1) c_l(t_1) \\ e^{i\alpha t_1} \\ c_r^\dagger(t_2) c_q^\dagger(t_2) c_s(t_2) c_t(t_2) \\ e^{i\alpha t_2} \end{array} \right| \Phi_0 \right\rangle$$

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So, here you are, so this is your expression for the second order term, you have got these two time integrals, you have got the creation and annihilation operators with appropriate time parameters t_1, t_1 over here are the first four operators. And t_2 in the next four okay, you have got the two center integrals and you have got a multiple sum over here i, j, k, l .

You can of course go on to show spin labels as well and have some more summation indices if you like okay. So, that is something which is implicit in this, so here mind the fact that you have got an αt_1 and an αt_2 okay. And then you have these two center integrals. (Refer Slide Time: 43:54)

The slide displays the following mathematical content:

$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\langle ij|v|lk \rangle \times \langle pq|v|sr \rangle \right) \left\langle \Phi_0 \left| \begin{array}{c} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \\ c_i^\dagger(t_1) c_j^\dagger(t_1) c_k(t_1) c_l(t_1) \\ e^{i\alpha t_1} \\ c_p^\dagger(t_2) c_q^\dagger(t_2) c_r(t_2) c_s(t_2) \\ e^{i\alpha t_2} \end{array} \right| \Phi_0 \right\rangle$$

Operator definitions:

$$c_{l,k}(t) = c_k e^{-i\omega_k t}$$

$$c_{l,k}^\dagger(t) = c_k^\dagger e^{+i\omega_k t}$$

$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\langle ij|v|lk \rangle \times \langle pq|v|sr \rangle \right) \left[\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{i\alpha t_1} \int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{i\alpha t_2} \times \left\langle \Phi_0 \left| c_i^\dagger c_j^\dagger c_k c_l c_p^\dagger c_q^\dagger c_r c_s \right| \Phi_0 \right\rangle \right]$$

Energy differences:

$$\Delta_1 = (\omega_i + \omega_j - \omega_l - \omega_k) \quad \Delta_2 = (\omega_p + \omega_q - \omega_r - \omega_s)$$


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So, this is your expression for A_2 which is already not so pleasing to the eye okay, you have the creation and destruction operators in the interaction picture which are related to the corresponding Schrodinger picture operators. We obtain these results quite extensively in some of our earlier classes and using them.

I have rewritten, so when you use the complete form of this interaction picture creation operator it will have this e to the $-i$ $\omega_k t$ okay from here and so this is the creation operator. So, it will have an e to the $+i$ $\omega_k t$ the destruction operators will have e to the $-i$ $\omega_k t$. But then of course the ω will be subscript inappropriately by i, j, k, l and then you have to keep track of the sign.

So, that is done using these short notation, so I will use Δ_1 because I have creation operators for i and j . So, I have got ω comes with a plus sign for i and j . And then I have got the destruction operators for k and l . So, these ω s come with a minus sign for ω_l and ω_k right. So, this is the short symbol Δ_1 for $\omega_i + \omega_j - \omega_l - \omega_k$.

And likewise I have for delta2 omega p plus omega q which is coming from these two creation operators minus omega r - omega s which is coming from these two destruction operators and they are just coming from the transformation from the Schrodinger picture to the interaction picture creation and destruction operator's right.
 (Refer Slide Time: 45:46)



$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\langle ij|v|lk \rangle \times \langle pq|v|sr \rangle \right) \left[\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} \times \left\langle \Phi_0 \left| c_i^\dagger c_j^\dagger c_k c_l c_p^\dagger c_q^\dagger c_r c_s \right| \Phi_0 \right\rangle \right]$$

$$\Delta_1 = (\omega_i + \omega_j - \omega_l - \omega_k) \quad \Delta_2 = (\omega_p + \omega_q - \omega_r - \omega_s)$$

$$\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = ?$$


$$\int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = ?$$

$$\int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = \int_{-\infty}^{t_1} dt_2 e^{(i\Delta_2 + \alpha) t_2} = \frac{e^{(i\Delta_2 + \alpha) t_2}}{(i\Delta_2 + \alpha)} \Big|_{-\infty}^{t_1} = \frac{e^{(i\Delta_2 + \alpha) t_1}}{(i\Delta_2 + \alpha)}$$

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So, this is now your expression e2 along with the delta 1 and delta 2 and now you have to evaluate these time integrals which are quite easy to be determined. So, let us evaluate these two time integrals one by one. So, this is the first one to be evaluated and that when you put the limit -m infinity to t1 take the difference at the top limit subtract from it the value at the bottom limit.

Now these are reasoning teachers we have evaluated number of number of times so this is what you get from one of these integrals integration over t2. And then this result together with this integrand you have to integrate from minus infinity to t okay.
 (Refer Slide Time: 46:33)



$$\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = ?$$

$$\int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = \frac{e^{(i\Delta_2 + a)t_1}}{(i\Delta_2 + \alpha)}$$

$$\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \frac{e^{(i\Delta_2 + \alpha)t_1}}{(i\Delta_2 + \alpha)} = \frac{1}{(i\Delta_2 + \alpha)} \int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} e^{(i\Delta_2 + \alpha)t_1}$$


$$= \frac{1}{(i\Delta_2 + \alpha)} \int_{-\infty}^t dt_1 e^{(i(\Delta_1 + \Delta_2) + 2\alpha)t_1}$$

$$\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \frac{e^{(i\Delta_2 + \alpha)t_1}}{(i\Delta_2 + \alpha)} = \frac{1}{(i\Delta_2 + \alpha)} \frac{e^{(i(\Delta_1 + \Delta_2) + 2\alpha)t}}{(i(\Delta_1 + \Delta_2) + 2\alpha)} \Big|_{-\infty}^t$$

$$\int_{-\infty}^t dt_1 e^{i\Delta_1 t_1} e^{a t_1} \int_{-\infty}^{t_1} dt_2 e^{i\Delta_2 t_2} e^{a t_2} = \frac{1}{(i\Delta_2 + \alpha)} \frac{e^{(i(\Delta_1 + \Delta_2) + 2\alpha)t}}{(i(\Delta_1 + \Delta_2) + 2\alpha)}$$

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So, this is the one that you have to evaluate this integral has already been evaluated on the previous slide. So, you put that result over here and now evaluate the second integral which is over t1 and what do you get again a very similar expression. So, again you have to put the limits get the value of the result of the upper limit subtract from it the value that you get at the lower limit and this is the result that you get okay.
(Refer Slide Time: 47:10)



$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\frac{\langle ij|v|lk\rangle}{\langle pq|v|sr\rangle} \right) \left(\frac{1}{(i\Delta_2 + \alpha)} \times \frac{e^{(i(\Delta_1 + \Delta_2) + 2\alpha)t}}{(i(\Delta_1 + \Delta_2) + 2\alpha)} \right) \left\langle \Phi_0 \left| c'_i c'_j c'_k c'_l c'_p c'_q c'_r c'_s \right| \Phi_0 \right\rangle$$

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \frac{\partial}{\partial t} \left[\sum_{n=1}^{\infty} A_n - \frac{1}{2} \left(\sum_{n=1}^{\infty} A_n \right)^2 + \frac{1}{3} \left(\sum_{n=1}^{\infty} A_n \right)^3 - \frac{1}{4} \left(\sum_{n=1}^{\infty} A_n \right)^4 + \frac{1}{5} \left(\sum_{n=1}^{\infty} A_n \right)^5 - \dots \right]_{t=0}$$

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle$$

$$= \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t \int_{-\infty}^{t_1} \int_{-\infty}^{t_2} \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_i(t_n) H_i(t_{n-1}) \dots H_i(t_1)] \right| \Phi_0 \right\rangle$$

nth order term....
One may generalize the pattern we have seen above....

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So, having got it, now you have got the complete expression for A2 with the delta1 and delta2 defined as here. These are the time integrals and when you put everything together you already have a result which one would rather not work with because it is quite complicated already just for the second order term. And what would it be if you just extend it.

So, there are similar terms and all you have to do is to recognize the pattern okay. Look at the pattern you have what a summation over four indices i, j, k, l. Then you have got the summation over p, q, r, s okay. Then you have got the product of these two center integrals

but this is coming twice. Then you have got these one over delta 2 + alpha multiplied by this and here you need to recognize the pattern.

And then you can extend it to higher order terms okay. So, observe this pattern very carefully and then see that you now have the Schrodinger picture operators. And you have their expectation value in the vacuum state of the unperturbed Hamiltonian okay. (Refer Slide Time: 48:40)

$$A_2 = \frac{-1}{2\hbar^2} \sum_{i,j,k,l} \sum_{p,q,r,s} \left(\langle ij|v|lk \rangle \times \langle pq|v|sr \rangle \right) \left(\frac{1}{(i\Delta_2 + \alpha)^2} \times \frac{e^{i(\Delta_1 + \Delta_2 + 2\alpha)t}}{(i(\Delta_1 + \Delta_2) + 2\alpha)} \right) \left\langle \Phi_0 \left| c_i^\dagger c_j^\dagger c_k c_l c_p^\dagger c_q^\dagger c_r c_s \right| \Phi_0 \right\rangle$$

$$\Delta E = \lim_{\alpha \rightarrow 0} i\hbar \left[\frac{\partial}{\partial t} \left[\sum_{n=1}^{\infty} A_n - \frac{1}{2} \left(\sum_{n=1}^{\infty} A_n \right)^2 + \frac{1}{3} \left(\sum_{n=1}^{\infty} A_n \right)^3 - \frac{1}{4} \left(\sum_{n=1}^{\infty} A_n \right)^4 + \frac{1}{5} \left(\sum_{n=1}^{\infty} A_n \right)^5 - \dots \right] \right]_{t=0}$$

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle = \left\langle \Phi_0 \left| \left(\frac{-i}{\hbar} \right)^n \frac{1}{n!} \int_{-\infty}^t dt_1 \int_{-\infty}^{t_1} dt_2 \dots \int_{-\infty}^{t_{n-1}} dt_n T [H_I(t_1) H_I(t_2) \dots H_I(t_n)] \right| \Phi_0 \right\rangle$$

nth order term....
One may generalize the pattern we have seen above....

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So, if you carry out this extension then with those extensions for An you will then be able to develop this infinite series and then plug it in to get your delta e. So, that is what you are going to do. So, that is the reason it is good to recognize this pattern and the nth order term you can get by extending this pattern. (Refer Slide Time: 49:04)

$$A_n = \langle \Phi_0 | U_n | \Phi_0 \rangle = \left(\frac{-i}{2\hbar} \right)^n \sum_{i,j,k,l} \sum_{p,q,r,s} \dots \sum_{u,v,x,y} \left(\langle ij|v|lk \rangle \times \langle pq|v|sr \rangle \right) \left[\frac{1}{(i(\Delta_2 + \Delta_2 + \dots + \Delta_n) + (n-1)\alpha)} \times \frac{1}{i\Delta_n + \alpha} \times \frac{e^{i(\Delta_1 + \Delta_2 + \dots + \Delta_n)t}}{(i(\Delta_1 + \Delta_2 + \dots + \Delta_n) + n\alpha)} \right] \left\langle \Phi_0 \left| c_i^\dagger c_j^\dagger c_k c_l c_p^\dagger c_q^\dagger c_r c_s \dots c_u^\dagger c_v^\dagger c_x c_y \right| \Phi_0 \right\rangle$$

Feynman Diagrams

~~complex?~~

What if today, we were just grateful for everything?

Bye!

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It is exactly the same pattern, so you have got these my summation indices over these four labels but they come several times okay. Then you have got these two center integrals and

they will come several times. Then you had this 1 over Δ^2 and so on okay and then you have got this expression over here.

So, this is where it is quite complicated but the pictures will make it easy because you are going to handle this particular term using these pictures. These time integrals are not all that difficult because they are just time integrals of exponential functions you know how to get them and how to put the limits.

But here you have fairly complicated process of creation and destruction of a large number of single particle states in principle there are infinite single particle states and you are talking as if you have got a boiling water and then some molecules of the water are boiled off they go above they start flying and then they bounce back they go back into the main water they condense okay.

So, you have got this creation and destruction of particles below the Fermi level and above the Fermi level okay. And you have got an infinite number of particle creation and destruction processes to work with. So, that is the most complicated part and that is what we are going to represent using these beautiful diagrams or we go and that is where I will pick up the discussion in the next class.