Foundation of Quantum Theory: Relativistic Approach

Atom-Field Coupling

Prof . Kinjalk Lochan

Department of Physical Sciences

IISER Mohali

Transition rates

Lecture- 36

.

So, today we will move forward from the discussion of the last week where we obtained the expressions for transition probability across atomic states. When the case atom was in ground state and the field was in vacuum, we asked for the probability that the atom goes to its excited state while the field goes anywhere it wants. That means we do not care about the field's final state and sum over it.

We have established

For $|g\rangle \rightarrow |e\rangle$ transition in the atom for $T \gg \hbar/\Delta E$ when $|\psi_{in}\rangle_{field} = |0\rangle$

$$P_{|g\rangle \to |e\rangle} \rightarrow \frac{|\langle e|\hat{m}|g\rangle|^2}{(2\pi)^3 \hbar^2} \pi^2 \int \frac{d^3\vec{k}}{2\omega_{\vec{k}}} \left[\delta\left(\frac{\frac{\Delta E}{\hbar} + \omega_k}{2}\right)\right]^2$$

$$\rightarrow 0 \quad (\text{i.e. insignificantly small})$$

$$\ll 1$$

However if $|\psi_{in}\rangle_{field} = |1_{k_0}\rangle$

$$\frac{P_{|g\rangle \to |e\rangle}}{\langle 1_{k_0}|1_{k_0}\rangle} \rightarrow \frac{|\langle e|\hat{m}|g\rangle|^2}{\delta^{(3)}(0)(2\pi)^3 \hbar^2} \frac{\pi^2}{2\omega_{k_0}} \left[\delta\left(\frac{\frac{\Delta E}{\hbar} - \omega_{k_0}}{2}\right)\right]^2$$

$$= \frac{|\langle e|\hat{m}|g\rangle|^2}{4\pi\hbar^2} \frac{\left|\delta\left(\frac{\Delta E}{\hbar} - \omega_{k_0}\right)\right|^2}{\delta^{(3)}(0)}$$

/ 26:23

Survives only for $\omega_{k_0} = \frac{\Delta E}{\hbar}$

For finite time T

$$P_{g\to e} = \frac{1}{(2\pi)^3} \frac{|\langle e|\hat{m}|g\rangle|^2}{2\hbar^2 \, (2\omega_k)} \int dt\,dt' \left\{ e^{-i\left(\frac{\Delta E}{\hbar}+\omega_k\right)(t-t')} + e^{-i\left(\frac{\Delta E}{\hbar}-\omega_k\right)(t-t')} \right\}$$

$$\int_0^T dt\, e^{-i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)t} \int_0^T dt'\, e^{+i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)t'}$$

$$= \left[\frac{e^{-i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)T} - 1}{-i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)} \right] \left[\frac{e^{i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)T} - 1}{i\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)} \right]$$

$$= \left[\frac{\sin\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)\frac{T}{2}}{\frac{\left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)}{2}} \right]^2 \xrightarrow{T \gg \left(\frac{\Delta E}{\hbar}+\omega_{k_0}\right)^{-1}} \left(\delta\left(\frac{\Delta E}{\hbar}+\omega_k\right)\right)^2$$

We have established

For $|g\rangle \to |e\rangle$ transition in the atom for $T \gg \frac{\hbar}{\Delta E}$ when

$|\psi_{in.}\rangle_{field} = 0$

$$P_{|g\rangle\to|e\rangle} = \frac{-1}{(2\pi)^3 \hbar^2} |\langle e|m|g\rangle|^2 \pi^2 \int \frac{d^3\vec{k}}{2\omega_{\vec{k}}} \left[\delta \frac{\frac{\Delta E}{\hbar} - \omega_k}{2} \right]^2$$

$\to 0$ (ie, insignificant small)

$<< 1$

However if $|\psi_{in.}\rangle_{field} = |1_{k_0}\rangle$

$$\frac{P_{|e\rangle\to|g\rangle}}{\langle 1_{k_0}|1_{k_0}\rangle} \to \frac{|\langle e|m|g\rangle|^2}{\delta^1(0)(2\pi)^3\hbar^2} \frac{\pi^2}{2\omega_{k_0}} \left[\delta \frac{\frac{\Delta E}{\hbar} - \omega_{k_0}}{2} \right]^2$$

$$= \quad \frac{|\langle e|m|g\rangle|^2}{4\pi\hbar^2}\frac{\left[\delta\frac{\Delta E}{\hbar}-\omega_{k_0}\right]^2}{\delta^1(0)}$$

For finite time T

$$\frac{P_{|e\rangle\to|g\rangle}}{\langle 1_{k_0}|1_{k_0}\rangle}\to\frac{1}{(2\pi)^3}\frac{|\langle e|m|g\rangle|^2}{2\hbar^2(2\omega_k)}\iint dt\,dt'\{e^{\delta\frac{\Delta E}{\hbar}+\omega_{k_0}(t-t')}+e^{\delta\frac{\Delta E}{\hbar}-\omega_{k_0}(t-t')}\}$$

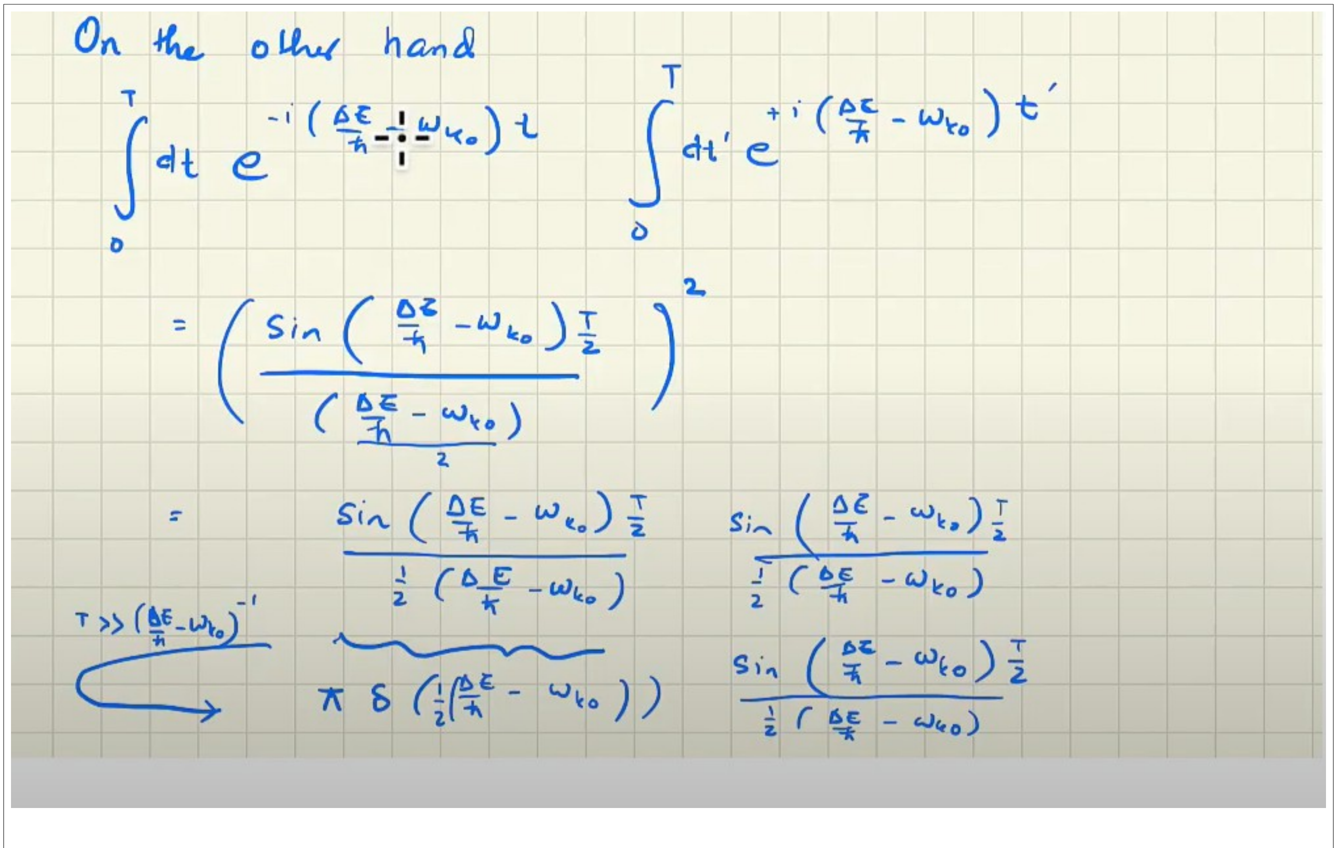
$$=$$

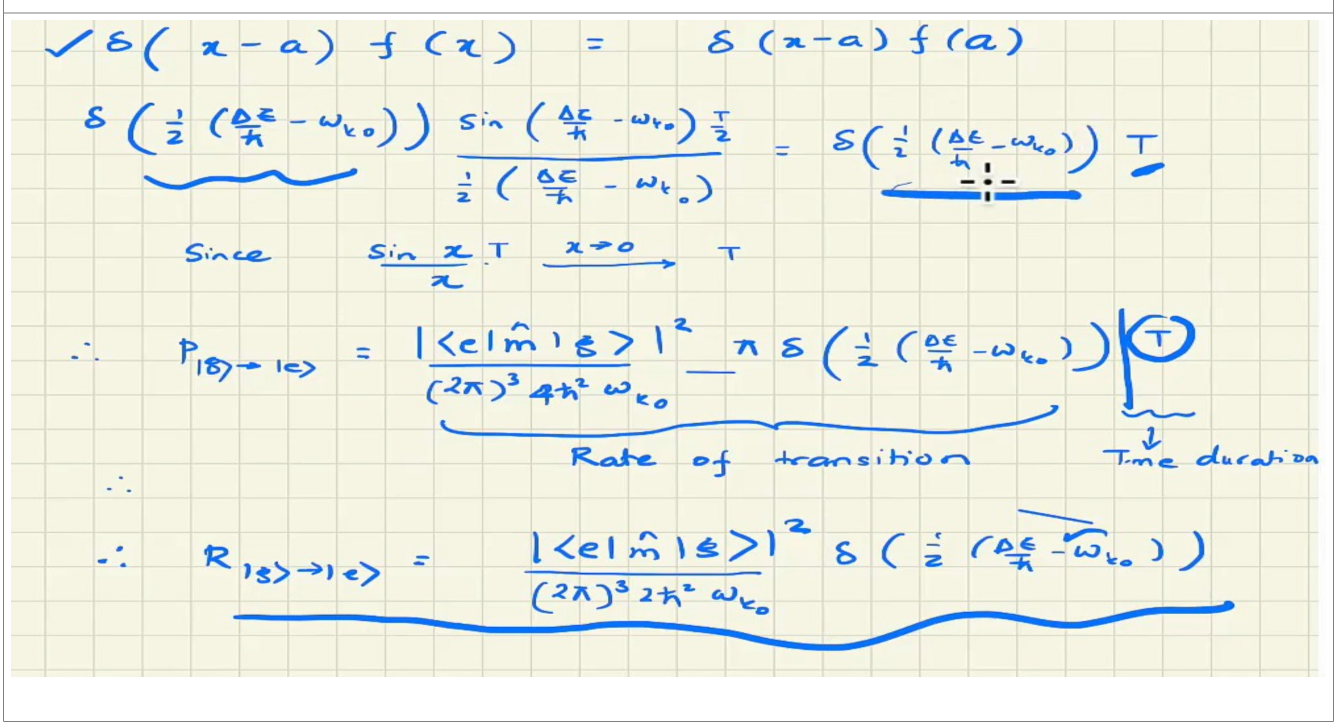
$$\left[\frac{e^{-i(\frac{\Delta E}{\hbar}+\omega_{k_0})T}-1}{-i\frac{\Delta E}{\hbar}+\omega_{k_0}}\right]\left[\frac{e^{(\frac{\Delta E}{\hbar}+\omega_{k_0})T}-1}{i\frac{\Delta E}{\hbar}+\omega_{k_0}}\right]$$

$$= \left[\frac{\sin(\frac{\Delta E}{\hbar}+\omega_{k_0})T/2}{\frac{(\frac{\Delta E}{\hbar}+\omega_{k_0})}{2}}\right]^2\to T\gg\frac{\Delta E}{\hbar}+\omega_{k_0}\to(\delta(\frac{\Delta E}{\hbar}+\omega_{k_0}))$$

Then we obtain the probability of transition to have these kind of expressions for long time durations. By long time durations, I typically mean this. The time scales much, much greater than h over ΔE. I will get the probability of transitions like that. Now, when we discussed in the last week, we realized that the time should not literally be infinity. We have done this analysis assuming T is much, much greater than h over ΔE. However, if I approximate it to infinity, I am not going to make much of an error in this computation. Only thing would be the higher order computations would be required if I literally want to take T tending to infinity. So, ideally one have to think that this expression is valid up to the limitation of the first order perturbation theory, which is much larger than the internal time scale of the system. And in that time window, we see that the probability of automatic excitation of the ground state, from the ground state of atom to excited state of the atom is very small. We have obtained it to be 0 in infinity T tending to infinity limit, but practically in the spot where the perturbation theory is valid, it is a very small number, ignorably small number. So, there is a very less likelihood, almost negligible likelihood of the atoms spontaneously getting excited. On the other hand, we realize that if I put the field initially in the excited state like 1_{k_0}, where one photon is present at the moment at k_0. In that case, the probability of transition, which we can obtain again from the previous version, happens to be proportional to a delta function with a possible argument which can survive, $\Delta E/\hbar - \Delta E/\hbar_0$. If the frequency of the wave number k_0 is commensurate with the energy gap of the system, then this expression can survive. we had divides the expressions to with, we had divided this expression with the initial normalization of the initial state out of field. That is one of the customary normalization one can do which brings about this $\delta^3(0)$. So, one thing one should make, one should correct in the previous week's note.

So, one thing one should make, one should correct in the previous week's note. These delta functions were all supposed to be three-dimensional delta functions. The commutators between $\hat{a}_{k1},\hat{a}_{k2}$ and other things. They are supposed to be the three-dimensional delta function and not the one-dimensional delta function which it might appear. So, at one stage this might have led to a confusion that when I did this time integral over here dt integral for this quantity, these are the square of one-dimensional delta function which is this. However, the normalization downstairs is a three-dimensional delta function. So, it should be $\delta^3(0)$ over here. In the denominator, I should have a $\delta^3(0)$. In the numerator, I should have a delta one-dimensional 0 because the numerator delta function is coming from the one-dimensional integral. So, that I have corrected in this week's note. You should also do it in your notes if you have made. Otherwise, the notes which are uploaded has already corrected it. Anyway, so let us go back to this week's discussion and you see now this normalization is $\delta^3(0)$ which is over here. So, all point taken in consideration, the central thing is that there is a proportionality to a delta function square which might survive. And it will survive whenever the photon frequency is the same as the, the photon frequency is same as the energy gap of the atom. So, this is what we had learned previously. So, now let us go forward and try to see what do we get as a transition rate if we want to know how many transitions happen per unit time. So, again for that I would just like to rewrite that expression what of the probability of transition in a slightly elaborate form to see what is coming. So, first we will do for a finite time, so that means I am looking for a transition happening not at a very large time, but at a some arbitrary time *T*. So, that means the expression for the probability of transition which we had like that, I will first do the temporal integrals up to *T*. So, both the time integrals in dt and dt prime, I am going to do up to 0 to *T*. This integration we have done previously and we know that this integral gives me a *sin* square integral divided by its argument. So, sin^2 of $\Delta E/\hbar + \Delta E/\hbar_0$ times $T/2$ divided by $\Delta E/\hbar + \Delta E/\hbar_0/2$. This is whole square is the integral of the double integral of this kind gives you. Remember, we have two big double integrals of this kind. First double integral is of the first term over here and the second double integral is the second exponential which is appearing in the expression over here. So, these two things put together will give me two sin^2 kind of terms. Out of this first sin^2 which comes with a positive arguments meaning $\Delta E/\hbar + \Delta E/\hbar_0$ We have seen it before in *T* much-much larger than the internal time scale in this case, which is the argument of sign becomes much-much greater than 1. In that case, it forms a representation of a delta function as in the previous week's discussion we have learned.





On the other hand

$$\int_0^T dt\, e^{(\frac{\Delta E}{\hbar}-\omega_{k_0})t}\int_0^{T'} dt'\, e^{-i(\frac{\Delta E}{\hbar}-\omega_{k_0})t'}\left(\sin\left(\frac{\frac{i(\frac{\Delta E}{\hbar}-\omega_{k_0})T/2}{(\frac{\Delta E}{\hbar}-\omega_{k_0})}}{2}\right)\right)^2$$

$$\underbrace{\frac{\sin(\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})T/2)}{\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})}}_{\pi\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})}\frac{\sin(\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})T/2)}{\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})}$$

$$T \gg \left(\frac{\Delta E}{\hbar}-\omega_{k_0}\right)^{-1}$$

$$\delta(x-a)f(x)=\delta(x-a)f(a)$$

$$\delta\left(\frac{1}{2}\left(\frac{\Delta E}{\hbar}-\omega_{k_0}\right)\right)\frac{\sin(\frac{\Delta E}{\hbar}-\omega_{k_0})T/2}{\frac{1}{2}(\frac{\Delta E}{\hbar}-\omega_{k_0})}$$

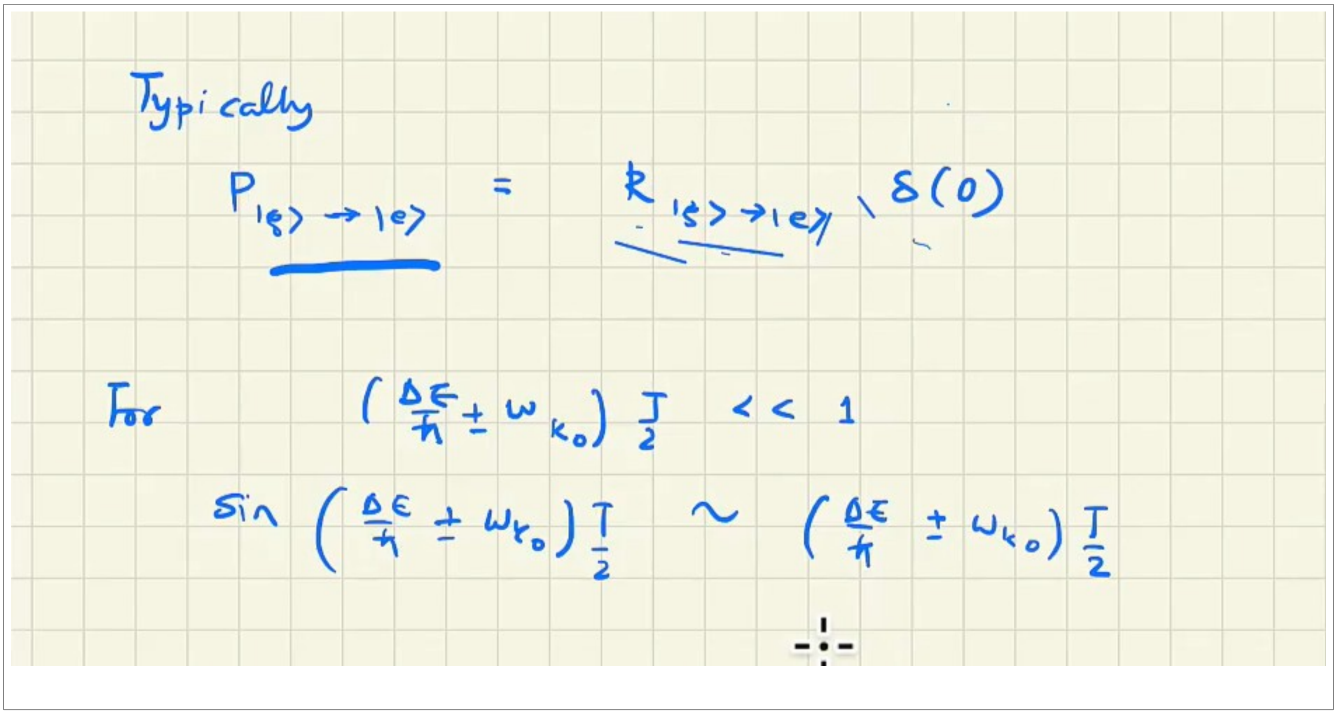
$$Since\ \frac{\sin x}{x}\rightarrow\wedge x\rightarrow 0\rightarrow T$$

$$\underbrace{\frac{P_{|g\rangle\rightarrow|e\rangle}}{\langle 1_{k_0}|1_{k_0}\rangle}=\underbrace{\frac{|\langle e|m|g\rangle|^2}{(2\pi)^3 4\hbar^2\omega_{k_0}}}_{Rate\ of\ transition}\pi\left(\delta\frac{\frac{\Delta E}{\hbar}-\omega_{k_0}}{2}\right)T}_{Time\ duration}$$

$$\frac{R_{|g\rangle\rightarrow|e\rangle}}{\langle 1_{k_0}|1_{k_0}\rangle}=\frac{|\langle e|m|g\rangle|^2}{(2\pi)^3 2\hbar^2\omega_{k_0}}\left(\delta\frac{\frac{\Delta E}{\hbar}-\omega_{k_0}}{2}\right)$$

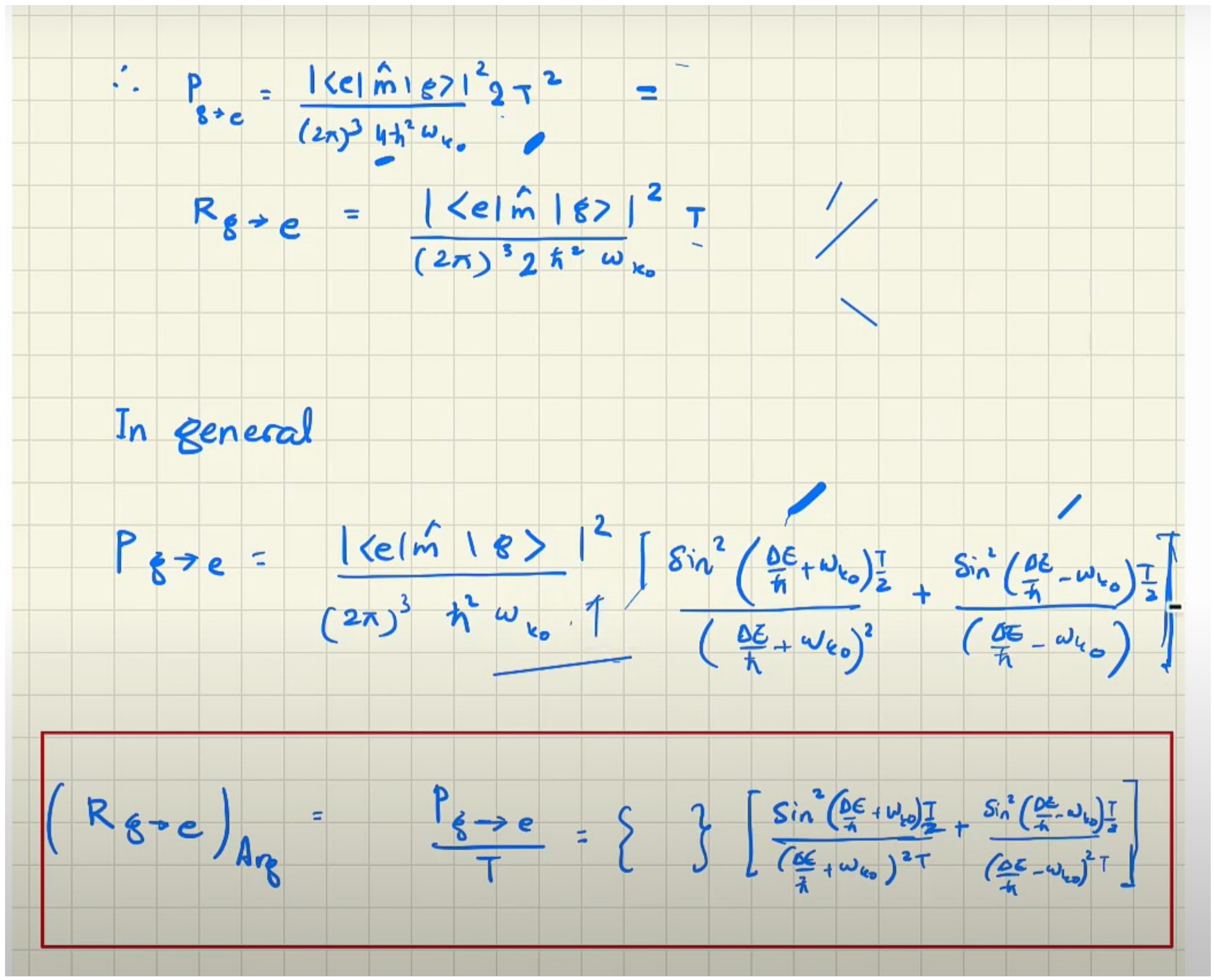
And therefore, it will land up to a vanishingly small value. It will approach a delta function if *T* goes to infinity, but as we know we are will not take it to infinity literally but it will be just a very large time. That means it will approach a delta function, it will not become a delta function, but it will go as close to a delta function as you increase the *T*. That means the contribution from the first double integral goes down if you wait for larger and larger time. So, therefore the first integral is going down with time. So, this is a decaying function of *T*. The second integral is what we should be careful about and there we will see what happens if I just look do this integral in the same form which we have done. Again the integral structure is very similar only thing is changing in the expression is the argument of the exponential which is $\Delta E/\hbar - \Delta E/\hbar_0$. Previously it was a + $\Delta E/\hbar_0$. So, everything will go as smoothly as it was going for the first double integral. This time also I will get a sin^2 upon some argument square. Only change is that the argument of *sin* has picked up a – term in between, $\Delta E/\hbar - \Delta E/\hbar_0$. And the denominator is also that. Now, previously we would have done the same thing just like we did and we could argue that it is also a square of a delta function. This time the argument of delta function is this thing, $\Delta E/\hbar - \Delta E/\hbar_0$ in the limit T tending to infinity. That means it will approach towards a delta of that argument. So, I do not want to do that at this stage explicitly because I want to know the rate. So, I would want to see how does it grow in time. So, what I do, I take this square function and split the two terms, I write it two times, *sin* of $\Delta E/\hbar - \Delta E/\hbar_0$ times d/2 divided by its argument and another such term. So, square has been written as the same quantity twice. Now out of this let us think of the first term over here. I know under large time limit, large time this time will mean T times this whole argument should be much much greater than 1. That means T should be much much greater than $\Delta E/\hbar$ + – – $\Delta E/\hbar_0$ to the power – 1. So, in that limit the first one again will try to approach the delta function as this here we have argued. So this I will do but I will leave alone the second sign pair I would first do the large time limit of the first thing and then I will try to see using that what do I learn about the product in one way if I just kill the T dependency completely by taking the speed much much greater than this quantity in both the terms then there is no information of T left, I just get the limiting value of the function. But I just want to know in this case how does it go in time. So, I will do the limiting case of T for the first term and I will see the effect of that limiting T value onto the second term. So, I just want to use the property of delta function to make assessment about that object.

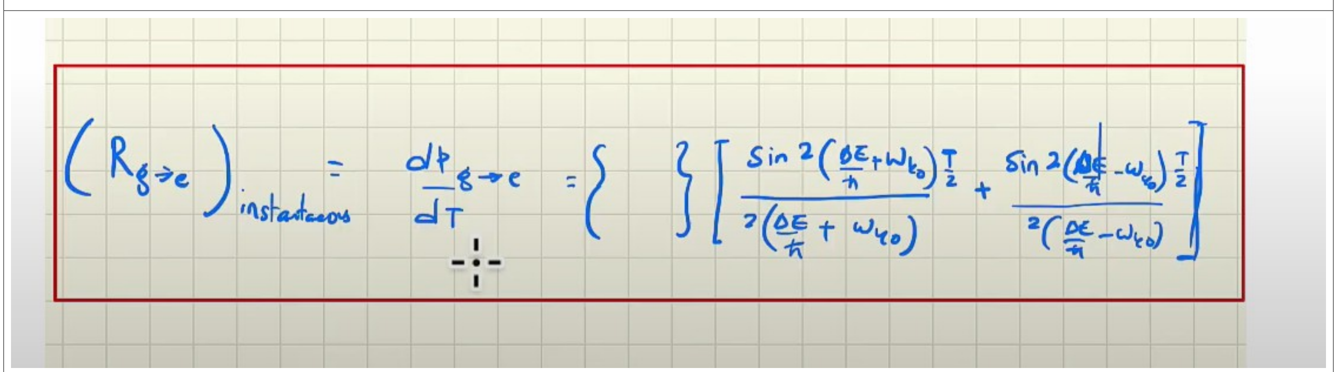
Now you see our structure is pi over times a delta of some quantity $\Delta E/\hbar - \Delta E/\hbar_0$. So, let us call this x. So, I have a delta of x and then *sin* x ty2 divided by that x. So, 1/2 times $\Delta E/\hbar - \Delta E/\hbar_0$, I am going to call it x later. So, I have a delta of x *sin* x times T divided by x. Now, for delta functions we know there is this property of multiplication. If I have a delta function of this kind, delta x – a, suppose a is 0 then delta x fx, then this is also equal to delta x – a f a for any regular function. So, that means the argument of the delta function can be flipped So, this function over here we can think that this remains a regular function as the T tends to infinity. into the argument of the function f if it is a regular function multiplying that. So, therefore I can use this property that this x tending to 0 will try to put the argument of this function also to 0. So, I need to compute let us call this quantity 1 over 2 times $\Delta E/\hbar - \Delta E/\hbar_0$ as x. So, ultimately I am looking for *sin* x times T divided by x and the limit x tending to 0. And that I know *sin* x times T divided by x limit x tending to 0 just gives me t. So, therefore this delta function multiplying this *sin*e functions and limit that the argument of delta function vanishes will just give me a T dependency. So, you see at late time probability of transitions keeps increasing with T. If the first delta function is non-zero, if the frequency of the photon matches then that means the probability of transition will keep going in time. So, overall I have a expression for probability of transition of an atom from ground to cytodipthate which is this factor times capital D. And therefore, I can see that it looks like there is a rate of transition which is independent of time and then there are multiplying that with a time duration for which I am looking for probability of transition to happen. They are not getting excited at a different rate at a different time. It is independent of T. And therefore, a time independent rate of transition can be defined as a prefactor of capability. So, this is how we can define the probability of transition and the rate of transition of an atom given any long time duration probability. So, I have this rate, this rate will turn on, it will become only non-zero when the frequency matches. This $\Delta E/\hbar$ not matches this $\Delta E/$x bar. Here I have not put the normalization factor, but you are free to do that. I am just assuming that the states are normalized and then I am working with this rate.



So, you see this rate will turn on only when The frequency of the photon exactly matches the energy gap and the rate at long time average, at long time limits the rate is uniform.

It is constant rate excitation keeps on going and particles keep getting excited during their higher excited state with a uniform rate. Typically for long time averages most of the times you will always obtain this structure. That delta, there is some rate multiplying *δ(0)*. Remember, one way of writing the 2 sin^2 term was delta of this quantity whole square. Previously, we had the same quantity I had written as a mod square of that and that is why the *T* was equivalent to delta of 0. So, in long time averages either you will get a *T* or you will get a *δ(0)* multiplying some finite quantity and that is how typically for long time averages the rates are read off. That we try to write down the probability of transition as a some common factors times some uniformly increasing function *δ(0)* , some the duration of operation of the function The interaction is on between 0 to *T* and that 0 to *T* is virtually the *δ(0)*. In long time limit *T* becomes very large which is as good as infinity and that is what this *δ(0)* is typically. For small time durations on the other hand if I am looking for transitions happening very instantaneously meaning once the interaction becomes I do not wait for long enough. and wait for shorter time scale compared to the internal time scales. That means this time $\Delta E/\hbar + \Delta E/\hbar_0$ for the first term and $-\Delta E/\hbar_0$ for the second integral term times $T/2$ should be much much smaller than 1. Remember in the exponentials, the integrals of exponentials we are giving me this sign or that sign over here. So, these two signs come with their own arguments the short time scale limit will be this argument of both the signs are much smaller than 1. So, that is what we are using as a short time scale duration discussion that $\Delta E/\hbar + -\Delta E/\hbar_0$ that should be much smaller than 1. In that case, sign with a small argument can also be approximated at the leading order as the argument itself. Sign x for small x is good to a good degree can be approximated by x itself. So, that is what we can do, we can say that wherever I see a sign in the time scales where this assumption holds, I can approximate the sign by their arguments. So, therefore, the transition probability what we had written previously will just be becoming T^2 because you see that both the signs either it will pick up $\Delta E/\hbar + \Delta E/\hbar_0 T/2$ as a numerator factor or $\Delta E/\hbar - \Delta E/\hbar_0 T/2$ as a numerator factor. And in both the cases they will cancel each other with the denominator. So, you see sign can be forgotten because the argument itself replaces sign. You see everything cancels out only *T* survives from the first term and similarly everything cancels out only *T* survives from the second term. So, ultimately the full probability which is sum of these two exponentials, I will get a T^2 from the first term, another T^2 from the second term. So, ultimately for short time scales I would get an answer which would be twice of T^2. So, there should be a two factor over here which I have missed. So, twice of T^2 should be the case of the transition probability and the rate can be obtained by just dividing this quantity by t. Just like previously I can write the whole thing as a common factor which is one *T* I can supply in and one *T* I can keep out. So, that means twice of *T* times the whole factor times a *T* I can write as a full probability that means rate can be read out as the coefficient of the t left out. It will be twice of *T* times this whole factor divided by $4h^2$ which was here which now with the help of that 2 can be converted into $2\hbar^2$. So, ultimately for short time scales, we can see that the probability of transition scales linearly. It increases linearly in time for short duration and then it adopts its *sin*usoidal forms. So, in general time scale, I have this sin^2 expressions. So, I have a sin^2 over here and another sin^2 over here. These two terms together determine me the full probability of transition. Its asymptotic limits we have seen that its asymptotic structure for short time scales is this. For long time scale also we found out that the probability now becomes proportional to t. So, there is a difference In the late time limit, the probability becomes proportional to *T* and rate is proportional to *T* to the power 0. That means the rate is time independent. While in the early time scales, probability is proportional to T^2 and the rate is proportional to t. So, there are two asymptotic limits in which the rates behave very differently and probabilities scale differently with respect to time. In between time scales, the full *sin*e function and its denominator should make appearance and I cannot use in either of the approximation. The full expression matches on these two expressions what we learned in the asymptotic limits. So, this is my full expression for probability of transition at finite time t. Again, I can think divide and multiply the whole thing by *T* and then the factor *T* which is outside and division by *T* in the denominator, I can use these two things to define for us a rate. So, I have multiplied and divided by *T* and then the whole three factor of *T* can be defined to be the rate of transition. That is one definition under which a rate of transitions can be looked at. However, this is more like a average rate because I have obtained the total probability of transition and then divided it completely with the total time duration of operation. This is giving me average rate, total transition divided by total time. However, there could have been an instantaneous transition rate as well because I have now an expression of probability as a function of t. So, forget about this multiplication and division. Then I have just some *sin*usoidal functions of *T* which is dictating the probabilities change over time. That means I can also define an instantaneous rate locally at this point how the transition rate is shaping up that I can define as *dp/dt*. So, *dp/dt* would be just the derivative of this quantity, *p/T* is just the division by d of this quantity. So, *dp/dt* would be just the derivative of this quantity, *p/T* is just the division by d of this quantity.





So, you can see that the average rate gives you a some expression with the *sine*^{2} divided by T in the denominator because this is how we have defined the average rate. Instantaneous rate would be taking the time derivative of the whole first expression here with respect to T. So, you will see that sin^2 will become 2sin of its argument and cos of its argument and then the whole $\Delta E/\hbar + \Delta E/\hbar_0/2$ will be thrown out that will cancel one power of the denominator

So, you can see that the time derivative of the sin^2 function gives me $sin\ 2\ \theta$ and the extra factors which come about under the derivative settles the denominator by decreasing its power by 1. You see average rate and instantaneous rates can be two different quantities average rate is just all the probability accumulated over all time duration and divided by total time of operation while instantaneous rate is just the local value at which the probability of transition happens at what rate the probability is changing So these two quantities can in principle be different. Unless we are interested in a very short scale change in probability, we should most of the time work with an average rate because these time scales over which probability changes significantly is much shorter than our observational time scales. We will be doing experiments with some apparatus that apparatus has a finite time resolution it cannot instantaneously measure all the changes it gives us a number every finite duration of time under that finite duration of time it is accumulating certain probability of excitation of atom at this time it was this much at for future time it is this much that is why it is giving me a series of this quantity rather than the local derivative quantity so local derivative is a mathematical concept in some sense which can be realized by very precise and very instantaneous detectors only. Any detector which is slightly open in its resolution in time mapping, how frequently it samples the atom, that is most likely measuring this average rate over the sampling time duration. Instantaneous rate can only be obtained by very fast detectors and that is what typically is not done. It is not impossible, but typically it is not achieved. in a simplistic lab setting. So, most of the times people do business with this average time duration discussion. And this gives rise to something called Fermi's golden rule as well, as we will see in the next class. In this class, we have just learned about the possible rates. Next class, we will see if there is a spread in the probability of excited states, there is a spread in the excited states, energy of the excited states. This structure of transition and rate also receives contribution from that spread as well. And that is very elegantly captured by the concept of Fermi's golden rule that we will see in the next class. So, I stop over here.