Quantum Technology and Quantum Phenomena in Macroscopic Systems
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Lecture – 29
Derivation of Fermi-Golden Rule

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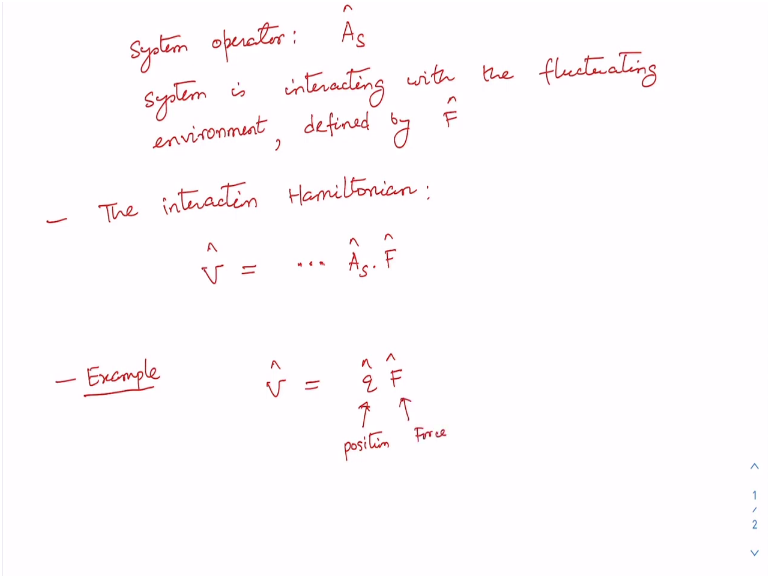

Hello, welcome to this supplementary lecture in this lecture we are going to derive the Fermi Golden Rule. This rule we have discussed in lecture 21 but I did not tell you how to derive it if you are curious to know the derivation, please go through this particular lecture otherwise you can skip it. You know that the Fermi Golden Rule is one of the most important formulas in quantum mechanics which has vast application ranging from atomic physics to nuclear physics to condensed matter physics.

In lecture 21 I have written down the Fermi Golden Rule as follows: this is basically the probability of transition from the state i to state f in the system and this is given by this particular formula we are going from the state i to state f in the system and A s is the system operator this is the matrix element of the system operator then we take the mod square we have here 1 by h cross square.

This transition is happening due to the interaction with the environment or some external agency denoted by given by this operator f or the fluctuating operator or it is also called the noise operator and this is this particular quantity is the spectrum of the noise or the fluctuating bath operator. And it is evaluated at the frequency omega which is the difference in the initial energy state of the system and the final energy of the system divided by h cross.

So, this is what we are going to derive here this spectrum is basically the Fourier transform of the correlator and I will explain everything in this lecture. So, this is what I have minus infinity to the plus infinity dt. Let us derive it. Say we have a system with two energy levels denoted by this ket i and ket f. The system is described by system operator A s and it is interacting with the fluctuating environment.

Let me see the system is interacting with the fluctuating environment and let me assume that the system is getting connected to one of the variables in the environment which is denoted by the operator say F cap right. Then the interaction Hamiltonian in this case would be interaction Hamiltonian we can write as V is equal to the system operator dot F and these three dots I have just left it.

So, that we can take the dimensions into account because ultimately this interaction Hamiltonian should have the dimension of energy. So, for dimensional consideration let us say we have depending on the system we are going to fill it up. But overall, the form of the Hamiltonian is going to be of this type. To give an example we know that if we have a say quantum harmonic oscillator interacting with the bath or environment we can write down the interaction as V is equal to q into F.

And here q is the position operator of the harmonic oscillator and F is the force exerted on the oscillator due to coupling to a bath right. So, this is position and this is force.
So, in this case dimensionally everything falls in place. So, this I am talking about a quantum harmonic oscillator interacting with the environment all right.
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In Heisenberg picture

$$\langle \hat{A} \rangle = \langle \psi(t) | \hat{A} | \psi(t) \rangle$$

$$= \langle \psi(0) | \underbrace{e^{i/\hbar \, \hat{H} t} \, \hat{A} \, e^{-i/\hbar \, \hat{H} t}}_{\hat{A}_H(t)} | \psi(0) \rangle$$

$$\hat{A}_H(t) = \underset{\substack{\uparrow \\ e^{i/\hbar \, \hat{H} t}}}{\hat{U}^{\dagger}(t)} \, \hat{A} \, \underset{\substack{\uparrow \\ e^{-i/\hbar \, \hat{H} t}}}{\hat{U}(t)}$$

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So, the full Hamiltonian for the harmonic oscillator and the bath in this case would be H is equal to H 0 is the bare Hamiltonian that means when the harmonic oscillator is not interacting with the environment and this is the interaction part of the Hamiltonian and here H 0 would be h cross omega a dagger a actually we also write plus half but because plus half part is anyway constant then we generally neglect it.

And also, we have the Hamiltonian due to the bath or the environment and then we have this V term here right interaction term. I hope you get the idea here why in general we can write the interaction Hamiltonian for a system and environment in this particular form. Let us go further. So, you know whenever interactions are involved it is always better to work in the so-called interaction picture.

So, we will now do everything in the so-called interaction picture in earlier classes. So, far I have talked about the Schrodinger picture as well as the Heisenberg picture. Some of you already know about the interaction picture but still let me quickly give you a small introduction to it. Just recall that in Schrodinger picture we had the wave function or the state vector is depend on time explicitly while the operator do not and the time evolution of the state vector is given by the so-called Schrodinger equation.

So, this is what all of us know this is the Schrodinger equation and from here I can write that this psi of t the state vector it is going to evolve as per this equation. So, here you have this evolution operator U of t and if you have started from the state vector at time t is equal to 0 is this one. So, and this evolution operator U of t is equal to e to the power minus i by h cross H of t.

In the Heisenberg picture I am just reminding you what we have learned so far regarding the various representations of quantum mechanics this is the Heisenberg picture or Heisenberg representation. In Heisenberg representation the state vector do not depend on time and this time dependence is taken into account in the operators if you recall we have this expectation value of the operator A.

We can write it in the Schrodinger picture as psi of t A of psi of t and then I can just writing the evolution operator I can write here it in this form psi of 0 e to the power i by h cross H of t A e to the power minus i by h cross H of t psi of 0 and here you see if I define this as the operator then this time dependence is taken into the operator here and this is the so-called Heisenberg picture.

And in Heisenberg picture the operator is represented by here you have say U dagger t A U of t and U dagger t as you can make it out U dagger t is equal to e to the power i by h cross H into t and U t is e to the power minus i by h cross H into t.

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$$\hat{H} = H_0 + V$$

$$e^{i/\hbar\, \hat{H}_0 t}\left(\hat{H}_0 + \hat{V}\right)$$

$$= e^{i/\hbar\, \hat{H}_0 t}\, \hat{H}_0 + \underbrace{e^{i/\hbar\, \hat{H}_0 t}\, \hat{V}\, e^{-i/\hbar\, H_0 t}}\ \underbrace{e^{i/\hbar\, H_0 t}}$$

Define:

$$\boxed{\hat{V}_I(t) = e^{i/\hbar\, \hat{H}_0 t}\, \hat{V}\, e^{-i/\hbar\, \hat{H}_0 t}}$$

Then, $$e^{i/\hbar\, \hat{H}_0 t}\, \hat{H} = \hat{H}_0\, e^{i/\hbar\, \hat{H}_0 t} + \hat{V}_I\, e^{i/\hbar\, \hat{H}_0 t}$$

Now let us discuss Interaction picture as the name suggests in Interaction picture quantum phenomena are described with Hamiltonians that depend explicitly on time. Here both operators and the state vector both state vectors and operators evolve in time. The total

Hamiltonian for the system and bath or the environment is H is equal to H 0 plus V in Interaction picture we will write it.

This suffix V of I t and here H 0 is independent of time independent of time and the state vector in the Interaction picture is defined as by this state vector psi of a suffix I is put there too just to show that it is different from the Schrodinger state vector psi of t by this rotation e to the power i by h cross H 0 t all right. Now as you know that this psi of t is this part is governed by the Schrodinger equation, we have i h cross d psi of t dt is equal to H into psi of t operating on psi of t.

Let us derive a Schrodinger like equation for the state vector psi I in the Interaction picture. To do that let me take the time derivative of this and multiply it by i h cross. So, from here I can have i h cross d psi i of t dt that would be equal to I have to take the time derivative this side and also I have to multiply by i h cross and if I do that let me do it you will have e to the power i by h cross H 0 t d psi of t dt plus i by h cross H 0 e to the power i by h cross H 0 into t and we have here psi of t okay.

So, if I just do the manipulation what I am going to have here is i h cross d psi i t dt that would be equal to you will have here if I multiply this and this I will have minus H 0 this is psi I of t and this part from this part I will have e to the power i by h cross H 0 t this is the I just using the Schrodinger equation here. So, I will have H of psi of t I hope you are getting it.

So, let us look at this particular part now if I let us look at e to the power i by h cross H 0 t h here H is equal to H 0 into + V. So, right in the Schrodinger picture this is what I have then e to the power i by h cross H naught t I just put H 0 + V here and if i open it up i will get e to the power i by h cross H naught t H 0 plus e to the power i by h cross H naught t V. Now here I write e to the power - i by h cross H naught t and e to the power + i by h cross H naught t and this is identity. So, i can do that.

Now if we define an interaction term in the Interaction picture as V of I t that is as e to the power this whole thing I am going to define that is e to the power i by h cross H naught t V e to the power minus i by h cross H naught t. So, if I define it this way then I have this term e to the power i by h cross H naught t H. This I can write as H naught e to the power i by h cross H naught t + V I e to the power i by h cross H naught t.

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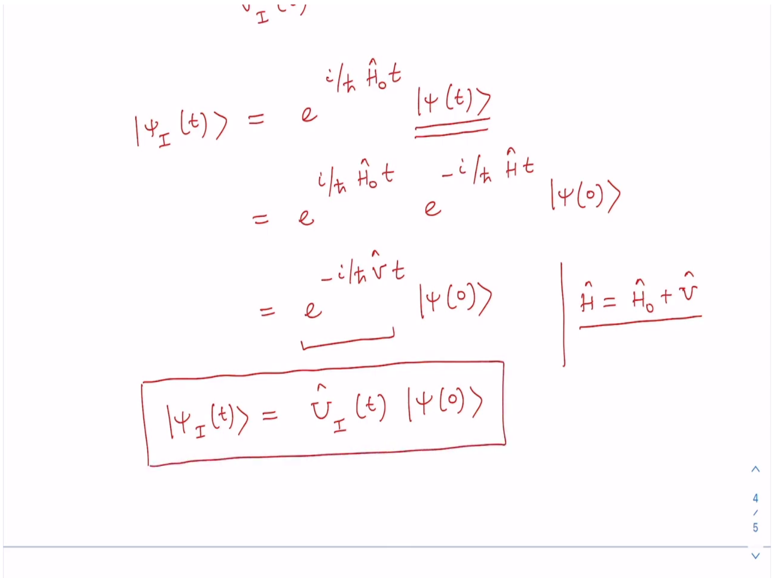

As you can clearly see if you are following this derivation right now therefore, we can write i h cross d psi of t in the interaction picture I have it as if I actually put everything there okay let me put it here I have H 0. So, right this is what I have if I write everything now including whatever we have so far derived then you will get H naught psi i of t plus H 0 e to the power i by h cross H naught t psi of t which is you know this part is psi of I t.

So, therefore this particular term and this particular term get cancelled out but we have also this term V of I e to the power i by h cross H naught t psi of t and this part is again nothing but psi I of t. So, therefore what we ultimately get is in the Interaction picture we get a Schrodinger kind of a equation actually this is the Schrodinger equation in the Interaction picture. So, this is equal to V I of t psi I of t.

So, what you see here that the evolution of this state vector in the Interaction picture is completely determined by this interaction part of the Hamiltonian. So, to summarize in Interaction picture the state vector is denoted as psi I of t is equal to e to the power i by h cross H naught into t psi of t and the operator describing the interaction is given by V of I t is equal to e to the power i by h cross H naught t V e to the power minus i by h cross H naught t.

There is a very useful form which we are going to utilize next regarding this state vector in the Interaction picture psi of I t I can write it as, as per the definition we have e to the power i by h cross H naught t psi of t but you know that this is actually it is evolving from say this is the state vectors Schrodinger state vector at a given time t whose evolution already we know and that evolves as per the Schrodinger equation and we here we will have it as e to the power -i by h cross H that is the total Hamiltonian H of t into psi operated on psi of 0.

This we know from here we can write because H is equal to this is Schrodinger operator total Hamiltonian of the system that is H 0 plus the interaction term in the Schrodinger picture. So, utilizing this we can easily see that we will have e to the power minus i by h cross V of t V into t okay psi of 0. This one is actually the unitary operator in the Interaction picture U I of t psi of 0.

So, this particular form is very useful and we are going to exploit it in our derivation of the Fermi Golden Rule.

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$$|\psi_I(t)\rangle = |\psi(0)\rangle + \frac{1}{i\hbar}\int_0^t dt'\, \hat{V}_I(t')\left\{|\psi(0)\rangle + \frac{1}{i\hbar}\int_0^{t'} dt''\, \hat{V}_I(t'')\, |\psi_I(t'')\rangle\right\}$$

$$= |\psi(0)\rangle + \frac{1}{i\hbar}\int_0^t dt'\, \hat{V}_I(t')\, |\psi(0)\rangle + \cancel{\frac{1}{(i\hbar)^2}\int_0^t\int_0^{t'} dt'\, dt''}\, \hat{V}_I(t')\, \hat{V}_I(t'')\, |\psi_I(t'')\rangle$$

$$\boxed{|\psi_I(t)\rangle = |\psi(0)\rangle + \frac{1}{i\hbar}\int_0^t dt'\, \hat{V}_I(t')\, |\psi}$$

Now, after having all the background let us proceed to derive the Fermi Golden Rule. The probability amplitude that the system is found to be in the state. Let me write here the probability amplitude that the system is found in the state say ket f at time t is given as we are going from the state i to state f. So, this is the amplitude we can write it as a f i of t is equal to we are in an arbitrary state psi of t and then we go to the state f right.

So, this is the probability amplitude. So, a fi I can write it as the scalar product of this f and psi of t which I can write because I know how this state vector evolves and this is equal to e to the power minus i by h cross h of t, I am now in the Schrodinger we are not talking about any interaction picture or Heisenberg picture here this simple quantum mechanics we are using here.

Your familiar quantum mechanics at this stage and this I can write further as in this form I can because this Hamiltonian is H is equal to as you know it is equal to H 0 plus the interaction. So, let me write it as f e to the power minus i by h cross H 0 of into t e to the power minus i by h cross V of V into t and we have here psi of 0 all right. Now therefore I can write it as a fi in terms of unitary operators I can write it as f this is this is actually U 0 unitary operator U 0 t.

And this already we defined that is your unitary operator in the interaction picture psi I of t psi of 0. Now U 0 of t that is the evolution operator if it operates on the state vector f ket f which is e to the power minus i by h cross H 0 t f, f is the system of state we know that when this eigenvalue equation H 0 operator when it operates on the state vector f. So, we get the energy E f corresponding to the state vector f. So, this is basically an eigen state.

So, using this from basic quantum mechanics we know that I can write it as e to the power minus i by h cross E f t ket f okay. So, therefore I can write from here I can write a fi the amplitude as e to the power i by h cross E ft f and this part you know that this is your state vector in the Interaction picture that is psi I of t. So, you see the connection how I am entering into the Interaction picture now, all right.

Now going further because we have this Schrodinger type equation in the Interaction picture actually that is the Schrodinger equation in the Interaction picture is this governed by this operator V of I t psi I of t the solution of this equation we can write we can write it in a series like this psi of I t is equal to if I take the derivative difference here integrate it I will get psi I of 0 okay plus 1 by i h cross integration 0 to t say dt dash V I t dash psi I t dash.

Using this we can construct a series solution as follows I can write psi I of t is equal to psi of 0 because psi I of 0 and psi of 0 it is actually one and the same thing, they are similar in the Schrodinger picture as well as in the interaction picture at time t is equal to 0. So, we have next term as 1 by i h cross integration 0 to t dt dash V I t dash this one I can replace in this form psi I of 0 which is psi of 0.

So, let me just write psi of 0 it is psi of 0 plus 1 by I h cross 0 to t dash d t double dash V I t double dash psi I t double dash okay. This I can write as psi of 0 plus 1 by i h cross integration 0 to t dt dash V I t dash psi of 0 plus 1 by i h cross square 0 to t 0 to t dash dt dt double dash dt dash dt double dash V I t dash V I t double dash psi i t double dash. Actually, you can go on and on we can make a series.

But we are interested in determining the transition between the two energy states of the system at very short time limit and to do that we ignore this particular term as per the time dependent first order perturbation theory. And we write psi of I t is equal to psi of 0 plus 1 by i h cross 0 to t dt dash V I t dash psi of 0. So, this is the solution we keep it.

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$$\hat{V}_I(t) = e^{i/\hbar H_0 t}\,\hat{V}\,e^{-i/\hbar \hat{H}_0 t}, \quad \hat{V} = \hat{A}_s \hat{F}$$

$$a_{fi} = e^{i/\hbar E_f t}\,\frac{1}{i\hbar}\int_0^t dt' \langle f|\,e^{i/\hbar \hat{H}_0 t'}\,\hat{A}_s\,e^{-i/\hbar \hat{H}_0 t'}\,|i\rangle .$$

$$\underline{\underline{\langle k|\hat{F}(t')|j\rangle}}$$

$$\left(\text{Assuming that } \hat{F} \text{ is not affected by } \hat{U}_0(t) = e^{-i/\hbar \hat{H}_0 t}\right)$$

Let us take the initial states of bath and system to be separable initial state of the system plus bath let us say psi of 0 and system at time t is equal to 0 and the bath or the environment at time t is equal to 0 are separable. In fact, let us say system is in the state ket i and the bath or the environment is in the state ket j which I can write in combined form as i j. So, this is our initial state of the combined system plus bath.

Also assume that we will assume that system bath interaction system bath interaction to be very weak interaction to be very weak and bath is so large or the environment is so large that they remain system plus bath remains separable throughout the evolution remain separable throughout the evolution that is the reason we are interested in very short time limit.

In this time limit we can consider them to be separable and this approximation is known as Born approximation. So, under this Born approximation we can very well apply the first order perturbation theory in our case. Now the probability amplitude that the interaction causes a transition from the state ket i to ket f in the system that probability transition amplitude or probability amplitude for i to f is already we know that is a fi t is equal to e to the power i by h cross this already we have written E f t.

We are going from the state psi I of t to f that is the system state to be correct more rigorously let us assume that the final bath state is in the ket state k that is the final bath state. Then we can then write because we know the expression for psi I already. So, I can write a fi this amplitude I can write as e to the power i by h cross E f t f k and here I have psi of 0 + 1 by i h cross integration 0 to t dt dash V I t dash psi of 0.

This is what we have. By the way also we know that the initial condition that we have is psi of 0 is equal is i j and the initial ket state system ket state i and the final ket state f is orthogonal to each other this we know and because of that I can write a fi it is easy to see that I can write it simply e to the power i by h cross E f t 1 by i h cross integration 0 to t dt dash f k V I t dash i j.

Now this V I we know that V I t is equal to e to the power i by h cross H 0 t V this is the interaction term in the Hamiltonian in the Schrodinger representation minus i by h cross H 0 t where V is the as I said it is the interaction term in the Schrodinger representation and this is equal to it is the product of the system operator and the environment operator fluctuating environment operator say f.

And then I can write my amplitude probability amplitude a fi is equal to e to the power i by h cross E f t 1 by i h cross integration 0 to t dt dash here I will have f e to the power i by h cross H 0 t dash A s e to the power minus i by h cross H 0 t this i then I have k that is the final state of the bath operator. So, this is f is the bath operator at time t dash and this is the initial j is the initial state of the bath operator here we have assumed that this bath operator is not affected by the evolution operator U 0.

So, let me write here we are assuming because of Born approximation assuming that f by the bath operator is not affected by the evolution operator of the system which is U 0 t is equal to e to the power minus i by h cross H 0 t that is why I can write it separately like this.

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$$J = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \qquad |J| = 1$$

$$\int dt'\,dt'' \rightarrow \int dt_0\,d\tau$$

$$\gamma_{fi} = \frac{1}{\hbar^2} \left|\langle f|\hat{A}_s|i\rangle\right|^2 \int_0^t \int_0^t dt'dt''\, e^{-i\omega(t'-t'')} \langle F(t'')F(t')\rangle$$

$$\downarrow$$

$$\gamma_{fi} = \frac{1}{\hbar^2} \left|\langle f|\hat{A}_s|i\rangle\right|^2 \int_0^t dt_0 \int_{-t_0}^{t-t_0} d\tau\, e^{i\omega\tau} \langle \hat{F}(t_0+\tau)\,\hat{F}(t_0)\rangle$$

Now as e to the power minus i by h cross H 0 t when it operates on the ket state i we are going to get e to the power minus i by h cross E i the energy corresponding to the state ket i this we know from our elementary quantum mechanics. Similarly, we know that e to the power minus i by h cross H 0 t when it operates on ket f we are going to get e to the power minus i by h cross E f of t f ket f. So, using this we can write a fi at time t is equal to e to the power i by h cross E f of t 1 by i h cross integration 0 to t dt dash e to the power i by h cross E f minus E i t dash f A s i.

And then it is multiplied by this k f t dash j. If we now define omega as E i minus E f by h cross then we can write a fi the amplitude as e to the power i by h cross E f t 1 by i h cross integration 0 to t dt this e to the power minus i omega t dash f A s i and we have k f of t dash j all right. Now we are ready to calculate the transition probability we can now calculate transition probability between the system state ket i to ket f for this we have to sum over all the possible final bath state summing over all possible final bath states.

We can write the transition probability gamma f i is equal to sum over all the final bath state that is a f i mod square and if we now open it up a f i we know we will get 1 by h cross square integration dt dash dt double dash e to the power minus i omega t dash minus t double dash here I have f A s i mod square and sum over multiplied by sum over all the final bath state j F t double dash k k F t dash j okay.

Now you see that we know from our completeness condition that sum over k this k k is identity of its identity operator. So, therefore utilizing this we get gamma f i is equal to 1 by h cross square integration 0 to t 0 to say t dash dt dash dt double dash e to the power minus i omega t dash minus t double dash have here this is also there this f A s i mod square into j. Now this is this goes out. So, we will have j F t double dash F of t dash j.

So, as you see this is basically the expectation value of the product of these two operators noise operators and this is actually called correlator and this, I can write it as an average the fluctuation operator or the bath operator evaluated at two different times t dash and F t and this is known as correlator this is called correlator. So, using this I can now write gamma f i transition probability as 1 by h cross square and let me take this out here f A s i mod square and then here integration 0 to t 0 to t double dash actually t dash dt dash dt double dash e to the power minus i omega t - t - t double dash.

And then we have this correlator evaluated at F t double dash F t dash we can express gamma f i in a more convenient form if we substitute t dash is equal to t 0 and t double dash is equal to t 0 plus tau that means I am going from the variable set t t double dash to the variable set t 0 tau and if you look at this expression here this transformation the Jacobian of transformation as you can see is 1 0 1 1 and because the determinant of the Jacobian of transformation is equal to 1.

So, therefore we can write this double integral dt dash dt double dash as dt 0 d tau. So, the expression gamma f i which we have as 1 by h cross square the matrix element for the system operator taking the mod square and we also have the limit of the integration double integration is 0 to t and 0 to t dt dash dt double dash e to the power minus i omega t dash minus t double dash f t double dash f t dash.

I think I made a mistake earlier in the limit here okay here this should be t okay and here it should be limited to t not t dash. So, please make that correction. Now with this change of variables this expression I can now write as gamma f i is equal to 1 by h cross square f A s i mod square integration limit I have here dt 0 and then I have d tau. Now you can easily check it here the limit would be from minus t 0 to t minus t 0.

And here the limit would be from 0 to t it is very easy to see and you will have e to the power i omega tau and we have this correlator here F t 0 plus tau F t 0.

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$$\gamma_{fi} = \frac{1}{\hbar^2} \left|\langle f|\hat{A}_s|i\rangle\right|^2 \int_{-\infty}^{\infty} d\tau\, e^{i\omega\tau} \langle \hat{F}(t_0+\tau)\hat{F}(t_0)\rangle$$

$$\downarrow$$

$$\boxed{\gamma_{fi} = \frac{1}{\hbar^2} \left|\langle f|\hat{A}_s|i\rangle\right|^2 \int_{-\infty}^{\infty} dt\, e^{i\omega t} \langle \hat{F}(t)\hat{F}(0)\rangle}$$

Now if the integration is taken over time long compared to the auto correlation time of the bath the limit on the second integral, I can take it or approximate it from minus infinity to plus infinity. And in that case, we will have gamma f i is equal to 1 by h cross square f A s i mod square 0 to t dt 0 and we will have minus infinity to plus infinity d tau e to the power i omega tau F t 0 plus tau F t 0.

And as you can see this is nothing but the Fourier transform of the correlator and therefore, we can write this expression as 1 by h cross square f A s i mod square and then this integration will give us t and this I can write simply as FF omega. And in fact, this is actually I have to make a small correction here this gamma f i is the transition probability but when I have written down the Fermi Golden Rule formula.

I wrote gamma f i that gamma f i in the Fermi Golden Rule formula denotes the rate of transition probability. So, rather than gamma f i so let me just write it as say capital gamma f i. So, this is the transition probability. So, accordingly you have to make correction everywhere wherever gamma f i is there you please make it capital gamma f i. And so what will have we have this, this is the transition probability.

And the transition rate of transition probability now let me denote it as gamma f i and then this is the transition probability divided by time this is the rate of transition probability or gamma f i then I can write it as 1 by h cross square f A s i mod square F F omega or let me write the full formula here now gamma f i is equal to 1 by h cross square modulus of f A s i then take the square.

And this is integration I have from minus infinity to plus infinity d tau e to the power i omega tau F t 0 plus tau F tau F t 0 actually many times t 0 is taken to be 0 because this is the reference time you can say. So, then more conveniently or the usual form that we have that is what also we have written in lecture 21 the gamma f i would be equal to 1 by h cross square f A s i mod square.

And integration minus infinity to plus infinity now let me take the liberty of writing it as dt and here i have e to the power i omega t F t and F 0. So, this is the required Fermi Golden Rule formula that we have derived now in this supplementary lecture.