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Lecture - 18 Optical Joint Density of States

So, today we will discuss the concept of optical joint density of states

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So, before that we will recall what we had studied in the last class. That is we discussed about radiative and non radiative recombinations, radiative and non radiative transitions. As the name indicates, radiative transition involves emission or absorption of a photon, emission or absorption, emission or absorption of a photon. And non radiative transition does not involve emission or absorption of a photon.

It is quite clear when we look at this, that an electron it sits in the conduction band. If it is makes a downward transition to the valence band, the difference in energy is given in the form of h nu. So, this is E 2 this is E 1. E 1 is an energy level in the valence band, and E 2 is some energy level in the conduction band. So, it involves emission of a photon or it could be incident photon leading to a transition of a electron from the valence band to the conduction band.

In the case of non radiative transitions, the energy difference is given in the form of phonons. The energy difference is this is usually the dominant forces in the case of indirect band gap semiconductors. So, for example, if I show an indirect band gap semiconductor like this, whatever be the process of excitation, whether it is optical process of excitation or current injection, it essentially leads to injection of carriers into this band which then come down by thermalization and accumulate at the bottom of the band. Similarly, here whatever hole generated wherever it is generated, whether a hole is generated here or here or here it will start moving to the top because the top of the band corresponds to low energy for holes or electrons moved on to lower levels and holes accumulate here.

Now, if an electron wants to make recombination with hole, then it has to make an oblique transition and as we have seen by this is not permitted by the case election rule. Case election rule requires that, the transition need to be vertical. That is delta k should be nearly equal to zero. But this not permissible by Case election rule, however as we have seen phonons can have large momenta because the momenta is the momentum is given by h cross k, which is equal to h cross into 2 phi by lambda here. So, this is lambda of phonons, lambda of phonons are the same order as that of electrons and therefore, these this difference in delta k.

So, please see this axis is k so, the difference delta k here is made up by phonons. There also another class of transitions which are all phonons assisted variations, phonon assisted, phonon assisted radiative transition. In this case, an oblique transition, an oblique transition can also lead to the emission of photon but it will be assisted by a phonon, a one or more than one phonons. This is called phonon assisted radiative transition. It can be the energy difference can be given out and momentum difference can be made out by number of phonons participating and there is also possibility of one photon plus phonons leading to this transition. Which is called phonon assisted radiative transition.

The energy difference is primarily made up of on photon but, the momentum difference is primarily made up of on phonons and that is called phonon assisted radiative transition. So, keeping in this in mind let us discuss the topic of optical joint density of states. Now what is the need for defining optical joint density of states. We have seen density of states. We had a reasonably detailed discussion on density of states, tell us the number of states available for unique volume and if you recall, that our objective here is now to realize sources and detectors. We are interested in emission and absorption,

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Emission and absorption means we want to see, what is the number of transitions or number of emissions because number of emissions will tell us number of photons emitted and therefore, we can estimate what is the power that is emitted. So, number of emissions per unit volume, number of emissions per unit volume is given by the number of density, the density of states multiplied by the probability of occupation. What is this, let me recall what we had seen.

The carrier density of electrons in the conduction band was given by, density of states rho c of E into probability of an occupation. You recall this n of E and n the carrier concentration was equal to integrated over this, so integrated over this. This was total number of carriers or carrier concentration. Equal to n of E into this. So n of E is equal to density of states multiplied by probability of occupations. Similarly, p of E p was given by p of E d E, which was equal to rho p of E into one minus f of E.

The probability of occupation of holes is 1 minus f of E d. If you keep this at the background, then if I consider, let us consider a radiation which is incident of energy h nu and consider the level E 1 here and a level E 2. A level e 2 in the conduction band. For a given photon of energy h nu or frequency nu, if you fix e 2 e 1 is automatically fixed, by the condition that h nu equal to e 2 minus E 1. An emission or absorption

involves, for example absorption, absorption involves an electrons state in the E 1 at E 1 in the valence band and vacant state E 2 the conduction band. Similarly, if you are looking at the emission then this involves, an electron sitting here at some other value, let us say E 2 dash and a vacant state at E 1 dash. This would to, emission of a photon of energy h nu dash

So, emission and absorption process simultaneously involves, the a state in the valence band and a states in the conduction band and therefore, any process involves states in the valence band and a states in the conduction band. Normally, in this case we had density of states in the conduction band, density of states in the valence band because whole concentration does not depend on this. Whole concentration depends on the density of the states in the valence band but in photon interactions, you have one state here and we state here and therefore, we define an optical joint density of states, which simultaneously takes care of the number of states for a given energy h nu, please see. If an incident energy h nu photon of energy h nu is incident if you fix E 2 E 1 is fixed.

Because the difference has to be same. I am considering only allowed transition, I am not considering oblique transitions. We consider the allowed transitions or those transitions which follow the case election rule. So, when E 2 is fixed E 1 also fixed and then it is possible when, we define a joint density of states. Let me proceed with the derivation, then it will become clear to you that the joint density of states does not depend on the actual value of E 2 and E 1 it always depends on E 2 minus E 1. So, we will just see the derivation and then it will become clear. So, the need for defining an optical joint density of states is because the transition involves states in the valence band and conduction band and there can be several combinations of E 2 and E 1 which will be equal to h nu. We see this is E versus k, E versus k. k is a vector, depending on the direction of propagation of electron beam that E k diagram continuously changes.

If you are taking a direction $1 \ 0 \ 0$ the E k diagram will be slightly different. If you are following along $1 \ 1$ direction then E k diagram will be slightly different. Which means, for a given energy h nu there are several pairs of E 2 minus E 1 and therefore, there is a density of states that is number of states, number of pairs of states available for a photon of energy h nu to interact and this is given by the density of states.

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So, we will see it become more clear as we proceed further. So, E 2 is equal to E c plus h cross square k square by 2 m c. This is the parabolic approximation, which is valid near the bottom of the band parabolic approximation and E 1 equal to E v minus h cross square k square divided by two m v. We already have this. So E 2 minus E 1, h nu is equal to E 2 minus E 1 is equal to E c minus E v, E c minus E v is E g plus h cross square k square divided by 2 into 1 over m c plus 1 over m v. This is actually, one over m r this where m r is the reduced mass. So, we can write h nu is equal to E g plus h cross square, k square divided by twice m r, where m r is the reduced mass. 1 over m c plus 1 over m v equal to 1 over m r. So, let me remove this and therefore, from this expression

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We have k square is equal to k square is equal to h nu minus E g here, so h nu minus E g into two m r by h cross square. Twice m r by h cross square. So, k square is equal to h nu minus E g. Is this okay? And if you substitute in the expression we had E 2 is equal to E c plus h cross square k square by 2 m c. If you substitute for k square from here, we have E c E 2 minus E c plus h cross square by 2 m c. Let me write it fully, 2 m c into this 1 substitute here. So, for there is k square. k square is here, while substitute 2 m r by h cross square into h nu minus E g. I have substituted for.

So, E 2 is equal to E c plus m r by m c into h nu minus E g. What do we see? For every value of E 2, there is a value of nu. Nu and E 2 there is no E 1 in this because E 2 E 1 automatically gets fixed once you say h nu and therefore, there is a one to one correspondence. This is a constant, these all are constants only E 2 is any energy level here. Which means E 2 is a variable and nu is a variable and therefore, there is a one to one correspondence between E 2 and nu. Exactly like this you can also write in terms of E 1 and you see that the there is a one to one correspondence between E 1 and nu.

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This means that, rho of E 2 d E 2 must be equal to rho of nu d v. There is a one to one correspondence between nu and E 2 therefore, the number of states between E 2 and E 2 plus d E 2, rho E 2 d E 2 is the number of states between E 2 and d E 2. This rho is actually rho c, conduction band density of states. Rho c of E 2 is d E 2 is equal to rho nu d nu. What is rho nu and d nu? Is the number of states, the number of states for photons, for photons of energy of energy between, between h nu and h nu plus delta nu h nu plus d nu to interact with to interact with, rho nu d nu is the number of states per unit volume per unit volume. Number of states is include per unit volume because you remember this was per unit volume, per unit volume of the material, per unit volume. Number of states per unit volume available for the photons to interact to interact means what to emit or absorb.

If photons are incident then if photons are incident with the frequencies between nu and nu plus d nu, nu plus d nu then the number of states available for these photons to interact per unit volume is given by rho nu d nu and this rho nu d nu is related to rho of E 2 and d E 2 because of this one to one relation and therefore, our interest is to get rho nu. Why we are interested in rho nu because once you know the density of states available for interaction, interaction means emission or absorption in this case. So, number of states available for interaction multiplied by the probability of that interaction, probability of emission or probability of absorption will give you total number of emissions or total number of absorptions per unit volume. So, that is our interest to find out how many photons are unit emitted, or unit volume of the material and then of course, if you multiply by the rate constant it will give you rate of emission. Finally, we are interested in the rates of emissions and absorptions. So, optical joint density of states the advantage of this is it simultaneously takes care of number of states in the valence band and the conduction band. It does not know which is E 1 and which is E 2 it knows that if h nu is this energy gap, how many pairs are possible where are those pairs corresponding to which, the energy difference is?

So, how many states are available for a photon of energy h nu to interact with? That is given by optical joint density of states. In many books literature, they also write this as c v because rho c is for the conduction band rho v is for the valence band and this is c v or some books also write this as rho o p optical. So, but, we can just drop that v, I do not think we have any other place where we have rho nu and therefore, I would simply keep as rho nu d nu. Rho nu d nu is the number of states per unit volume for photons of energy between h nu and h nu plus d nu to interact with.

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And therefore, to simplify this therefore, rho of nu is equal to rho c of E 2 multiplied by d E 2 by d nu. We can simplify this further rho E 2, we know the expression for rho E 2 that is equal to I will write it here, 1 over 2 phi square into 2 m c by h cross square to the power 3 by 2 recall the definition of rho c of E 2 into E minus E c E 2 minus E c to the power half. This was the first term rho c of E 2 multiplied by d E 2 by d nu. What is d E

2 by d nu? d E 2 by d nu, this is a constant, this is a constant, so we simply have h into m r by m c. So, multiplied by, so, let me erase this into h into m r by m c.

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This simplifies further, 1 2 phi from this we can take with this and say h cross. 2 phi from here I bring here h by 2 phi h cross 1 h cross this is h cross square to the power 3 by 2 is h cross q and it cancelled so I am left with 1 divided by phi h cross square into 2 m c to the power 3 by 2 there is one m c here. Is there something else that I missed? This is alright. m c to the power 3 by 2. What have I missed? d E 2 by d nu, I should have a term m r by m c, m r by m c here. Wait a minute, a rho of nu is equal to rho E 2 into d E 2 by d nu. So d E 2 by. There was a, was there a power half here h nu minus E g? Did I missed something? One over phi h square that is correct. This is correct. What have I written is correct. There is nothing wrong okay. Is perfectly fine. Perfectly fine. I want to substitute for E 2 minus E c.

I just now erased that. I am sorry. So, E 2 minus E c E 2 was equal to E 2 plus E c and then plus m r by m c so this is equal to m r by m c into h nu minus E g. E 2 minus E c. So, E 2 minus E c to the power half equal to this multiplied by the power half ,half and, and for this term here I want to substitute this. Is that alright? There is no confusion I suppose. That for this also I wanted to substitute E 2 minus E c to the power half. Is this so? I will let me write all of this 1 over phi h cross square 2 m c to the power 3 by 2.

Here and into this h is already taken so m r by m c into all of this m r by m c to the power half into h nu minus E g to the power half. It is a simple algebra you can do yourself but, I thought I will finish it. So, now you can see m c to the power 3 by 2 cancels with m c to the power 3 by 2 but, m r to the power 3 by 2 will remain. So, the final answer will be 1 over phi h cross square into twice m r to the power 3 by 2 into h nu minus E g to the power half. This is expression for rho of nu.

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So, let me erase all this unwanted things and directly write the expression. So rho of nu here is equal to 1 over phi h cross square 2 m r to the power 3 by 2, into h nu minus E g to the power half. Is it okay? This is a simple algebra. Therefore, how does rho nu vary? If I want to plot rho of nu versus E. So, rho of nu versus E, for normally we plot E here we will plot E there also. Please see this, for h nu greater than E g it up to E g there is because this expression, all the expressions are valid for h nu greater than E g any emission or absorption takes place, we are looking at inter band transitions .There are also intra band processes. We will discuss it little later.

Now we are looking at inter band transitions which are possible for h nu greater than E g therefore, from E g starts as h nu minus E g to the power half, variation of rho nu. We have a mathematical expression for rho nu. This is very important because next we will multiply by the probability of occupation, probability of emission and probability of absorption and we will get an expression for gain co-efficient which will contain all this

terms. That is why we need this derivation. So, optical joint density of states tells us the number of states available for photons to interact with it simultaneously takes care of states in the valence band and the conduction band. So, in all optical processes it is the joint density of states which are important. In electronic processes we always deal conduction band and valence band separately but, photon emission and absorption involves a state in the valence band and state in the conduction band simultaneously and therefore, we need to take optical joint density of states.

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So, let us go to probability of, because if we multiplied this by the probability of emission we will get number of emissions. If you multiply by probability of absorptions we will get number of absorption. So, probability of, probabilities of emission and absorption.

Probabilities of emission and absorption. So, all the while you see that we are discussing with E k diagram. One of early class I have said. Everything can be seen from the E k diagram. The normal band and energy band diagram does not tell you anything and I am considering direct band gap semiconductors and we are looking at vertical transitions. That is allowed transitions other effects we are not taking at the moment. We will see that we will have to take those into a account to explain actually practically absorbed spectrum. So, probability of emission. Let us, for emission you need an electron sitting in

state E 2 which makes a downward transition and therefore, you need a whole or a vacant state at E 1.

So, this is emission. What is the probability of emission? Probability of emission therefore, requires probability of emission of a photon of energy h nu equal to E 2 minus E 1 requires that the state E 2 is occupied by an electron and the state E 1 is a vacant state in the valence band which is a whole. Which means this is probability of occupation of whole. The probability of emission. Therefore, probability of emission f of E is a product of the probability of occupation of electron here and probability of occupation of whole. So, that is equal to f of E 2. This f is the Fermi function, you can write this as p if you wish we can write this as p probability because f we may so, p of e this is Fermi function. f of E 2 into, into one minus f of E. Exactly like that probability of emission will be given by for probability of absorption is given by if, if you have a state here electrons are sitting at the energy E 1 dash and if you have a vacant state here that E 2 dash then the photons get absorbed.

So, the probability of occurrence of this processor, probability of absorption is probability of occupation f of E 1 dash and here 1 minus f of E 2 dash. I have shown two different energy levels otherwise it is f of E 1 into this. Let us see graphically because therefore, the net probability of net emission will depend on which is greater. If probability of emission is greater than the probability of absorption then you will have net emission and vice versa and therefore, which one is greater of the two or which one can be greater of the two and which how can you make one greater than the other. If I want to realize this source, I need probability of emission greater than probability of absorption.

How to make the probability of emission greater than probability of absorption? Let us see this but, first there are two cases here. Case one thermal equilibrium and case two will be quasi equilibrium. So, thermal equilibrium thermal equilibrium means a probability of occupation in the valence band and in the conduction band is simultaneously described by one single Fermi function at thermal equilibrium one Fermi function describes the probability of occupation of electrons in the valence band as well as in the conduction band. In quasi equilibrium you will require 2 different Fermi functions. One for the valence band and one for the conduction band.

So, let us see first case one. Thermal equilibrium, probability of f of E 2 p E is equal to f of E 2 into 1 minus f of E 1. Let us see graphically, what is this? So, we have this is E v, if we do not of E c, I am sorry and this is E v and if I want to plot a typical Fermi function, we have plotted this earlier also. So, this is f of E. This function is f of E. It is 0 at this end 0 and 1 here 1 and 0.5 is here, approximately so I go here and in this semiconductor E f remains here.

It need not be intrinsic or anything I have just taken some semiconductor and this is the valence band and this is the conduction band and the upper one is the conduction band. E 2 is some value here so E 2 is here and E 1 is some value here in the valence band. It could be closed to the edge so, it is some value there and some value here. What is f of E 2, f of E 2 is this at E 2 the value of the function here. So, it is this value here, which means it is simply this width. This width here, this magnitude may be 0.1 or 0.2. Whatever in my graph actually has you know numbers are extremely small but, in my graph it looks like say point because this is 0.5 and therefore, this has his 0.1 approximately.

This is f of E 2. Probability of emission is f of E 2 into 1 minus f of E 1. What is f of E 1? E 1 is here. So, this value here up to this, this value. Approximately 0.9 is f of E 1 1 minus f of E 1 is this difference here. Is this clear? Maybe I should have drawn anything big bigger figure but, I hope you can find out this is 1 minus f of E 1 this is f of E 2 so f of E 2 into f of E 1 is this, this product this number whatever it is multiplied by this. So, that is probability of emission. So, we have this into this and probability of absorption. Probability of absorption. Suppose I take E 1 and E 2, that I could have taken let me draw another graph it would be better rather than making complication there. So, this is E c and this is E v, here is the probability f of E and I draw a fresh probability function Fermi function yea and this is 1 this is 0.5.

I gave you a question in the minor to draw because I am drawing in front of you regularly. So, you should also make practice to draw. So, this is approximately 0.5 so E f is here. Fermi energy is here. So, we now have some value E 2 dash E 2 dash and some value E 1 dash. I could have, please remember I could have taken the same value E 2 and E 1.

Now, you see the probability of absorption f of is a product of f of E 1 which is this, this is f of E 1 because this function is f of E probability Fermi function therefore, at E 1 the value of the function is f of E 1. So, this is f of E 1. This value which is here is f of E 1 and one minus f of E 2 what is f of E 2 is here so E 2 is this that is this value 1 this is 1 therefore, this difference is 1 minus f of E 2 this one. is 1 minus f of E 2 dash. So, what do you see? do we need to do any mathematics here? No need of any mathematics. Probability of emission is f of E 2, a small quantity multiplied by a small quantity and p a probability of absorption is f of E 1, a big quantity multiplied by 1 minus f of E 2 dash another big quantity. So, it is obvious that p a is greater than p e or p a is in general much greater than p e because the numbers involved here or 0.0001 and this will be 0.9999.

So, the product here p a is much greater than p e. In fact, in thermal equilibrium it is impossible to have p a, p e greater than p a. That means, probability of emission is always less than probability of absorption. That means there is no semiconductor will emit on its own at thermal equilibrium. We have to do something, so that it can so, which means we have to move out to quasi equilibrium. We know how to get quasi equilibrium? There are different ways of pumping the semiconductor and the most convenient is using a p n junction. So, let us just see this in quasi equilibrium what happens. You can see that also graphically but, mathematically also you can see. So, in quasi equilibrium, let me draw the graphs.

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p E, p E probability of emission is equal to f of E 2 into 1 minus f of E 1 and p a so case two, now am discussing case two. So, case two quasi equilibrium p a is equal to probability of absorption is equal to f of E 1 into one minus f of E 2. One single function for thermal equilibrium but, for quasi equilibrium this is f c of E 2 a Fermi function for the conduction band and f v of E 1 this is f v of E 1 and this is f c of E 2. Recall the graphical picture, that we had one Fermi function like this and a second Fermi function like this. So, there were two Fermi functions this is f c of E for the conduction band and this is f v of E where is the Fermi energy if this is 0 and this is 1 then 0.5 is here so 0.5. Draw a vertical line. So, this intersect here. So, we have E f v the Fermi energy of E f v for the valence band sitting here E f v here and E f c is sitting here.

E f c, E f c is the Fermi energy corresponding to the conduction band function. This function and E f v is that, there are 2 Fermi functions. Now, you can immediately see that there is a possibility. There is a possibility. If we push this sufficiently high or if we push this sufficiently low there is a possibility of having. So, f c of E 2 into this. So, let us substitute mathematically and see what we get this? Therefore, p e p e equal to f c of E 2 that is 1 divided by E to the power E 2 minus E f c by k t plus 1. First term multiplied by 1 minus f of E 1. So, 1 minus f of E 1. I can take a common denominator. So, I get E to the power E f v by k t E minus E f v by k t divided by 1 plus E to the power of E minus E f v by k t. This is 1 minus f of E this is f of E 2 and this is f of E 1. 1 minus f of E 1. 1 minus this. So, then I multiplied by this 1 1 cancelled. So, I am left with only this term in the numerator. So this is p e of E write for p a of E.

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So p a of E is f v of E 1. So, instead of this you will get so we have p a of E p a is equal to probability of absorption, all of this is for nu p E of nu and p e of nu because E 2 minus e 1 in this expression is fixed in h nu so p a of nu is equal to f v. So, 1 divided by 1 plus E to the power E 1 minus E f v. Only thing is we need to add an suffix c or v, otherwise it is same Fermi function because we have 2 Fermi functions we have to add this, this into 1 minus f c of E 2. So, in the numerator I will get E minus E to the power E 2 minus E f c by k t divided by 1 plus E to the power E 2 minus E f c. I just jumped one step that is all. Solved. What do you see? The denominator is common, see the denominator is common. 1 plus this 1 plus here and this is here. 1 plus E 2 minus E f c is here denominator is common.

So, p e of nu and p a of nu. For p e of nu, we want p e of nu to be greater than p a of nu. When can this happen? In thermal equilibrium, it is not possible. When can this happen? When this numerator term is greater than this numerator term. Denominator is the same this numerator is greater than this numerator, which means it is E to the power therefore, this power is greater than this power. K t is also common that means E 1 minus E f v is greater than E 2 minus E f c. So implies E 1 minus E f v is greater than E 2 minus E f c. A very, very important condition which is now coming. So, I can take E 1 there so, I can take E f c here. It implies E f c minus E f v greater than E 2 minus E 1 and h nu is always greater than E g. This is the condition for emission to be greater than absorption. Probability of emission to be greater than probability of absorption. That is, the difference in the quants, quasi Fermi level must be greater than the band gap, the difference in the quasi Fermi levels must be greater than the band gap energy E g. This is a very important condition, this is equivalent condition to the condition of population inversion. In atomic systems you know when for amplifications to take place N 2 minus N 1 should be positive or N 2 should be greater than N 1 or N 2 minus N 1 should be greater than 0. If you have 2 atomic energy levels and N 2 is the number of atoms in the upper level and N 1, then if N 2 minus N 1 is greater than 0, then you can have amplifications. For net amplification. This we call population inversion in laser physics.

This is an equivalent condition, as we will see further for semiconductor lasers. In semiconductor lasers this is not the condition, in semiconductor lasers, this is the condition. That the difference between the quasi Fermi levels must be greater than it we will stop here for today and continue in the next class.