

Optical Properties of Materials

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September 25, 2003

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Part I

Coneventions and Definitions

- Note that in this entire document f_e , f_h and f_{photon} are not necessarily thermal distributions unless specified.
- $W_{ab,monochromatic}$ represents the stimulated emission transition rate (**no of transitions per unit time per unit volume**) between two states of a discrete state system when irradiated with a monochromatic light.
- $W_{ab,total,monochromatic}$ represents the stimulated emission rate between all the states that can afford to participate when a continuous state system is irradiated with a monochromatic light. Note that $W_{ab,total,monochromatic} = \int_{E_{joint}} W_{ab,monochromatic}$ where I do not need to include dE_{joint} explicitly because I can simply replace $f_e f_h \rightarrow f_e f_h g_{joint} dE_{joint}$ and $W_{ab,monochromatic}$ is still interpreted as stimulated emission rate per unit time per unit volume but from any one set of states in the energy band dE_{joint} .
- $W_{ab,total}$ represents the stimulated emission rate between all the states when a continuous state system is irradiated with a generic spectrum of light. Note that $W_{ab,total} = \int_{\omega} W_{ab,total,monochromatic}$ where I do not need to include $d\omega$ explicitly because I can simply replace $n_{photon} \rightarrow f_{photon} g_{photon} d\omega$ and $W_{ab,monochromatic}$ is still interpreted as stimulated emission rate per unit time per unit volume from any one set of states in the energy band dE_{joint} but now stimulated by any one optical mode in the frequency range $d\omega$.

- I might drop the subscripts ab on and off whenever they are understood to be there.

Part II

Macroscopic Electromagnetic Characterization at Optical Frequencies

1 Refraction and Absorption

Fundamental physics behind both absorption and refraction (as well as other linear optical processes) is that the oscillating electric field mixes different energy eigen states. If we are looking at molecules or atoms, this would mean that localized electron cloud changes its shape with time. This leads to polarization which is related to refraction. This also changes the steady state amplitude of the system being in any one state. This is related to balance between absorption and stimulated emission processes. In molecules or atoms, this might also mean a steady state change in the shape of the electron cloud and that would mean static dipole moment. As we would see in the following discussion in details, this second process of absorption or static dipole moment would become significant only if frequencies are closely matched. Many a times, we are not as much interested in steady state amplitude as we are in knowing the rate of change of this steady state amplitude if perturbation is switched on at certain time. Conditional rate of change of amplitude (given that one state is occupied and one is empty) is constant and equal for both up and down transitions. This quantum mechanically calculated rate can then easily be used to write classical rate equations.

This shows that classical Kramers-Kronig relation which relates absorption and refraction, fundamentally originates from the mixing of energy eigen states due to electromagnetic perturbation.

2 Absorption and Material Loss

Sometimes usage of terms lossy and absorbing materials become very confusing. For example one can argue that absorbing material is not necessarily a lossy material. Let us think of a semiconductor. When light is incident on it – photons are absorbed and carriers are excited. But in steady state equal number of carriers relax back (lets assume optical relaxation) and emit equal number of photons back. So from energy point of view nothing is lost and material is not really lossy. **But this not the usual sense in which term “lossy” is used.** In usual sense of the word a semiconductor is a lossy material (above its bandgap). We generally think of only one optical mode. Lets think of a monochromatic plane wave incident on a sample. Photons would be absorbed from this mode but would be re-emitted in all directions (photo luminescence is usually angularly uniform). Hence as far as we are only concerned with once optical mode, photons are

getting lost from that mode and hence material is lossy.

There can be other types of losses as well – something that is loss even from total number of photons perspective. For example if excited carriers relaxes back by emitting energy in lattice vibrations.

Mathematically **both these** effects of losses are modeled as an oscillator damping coefficient, an optical decay lifetime or the spontaneous emission linewidth (all of these represent same physics that an oscillator is actually coupled to many different modes – if it couples to only one mode it would never decay and there is no loss and no linewidth). One can associate different linewidths (time constants) with different mechanisms of loss – but phenomenological they are all equivalent.

3 Conductivity or Permittivity?

3.1 General Discussion

One needs to distinguish between DC conductivity/permittivity and the AC conductivity/permittivity. For DC one needs to specify both the parameters. For any $\omega > 0$ any one of the parameters is sufficient. But still, at least for low frequencies (compared to bandgap energy) one still talks separately about permittivity and conductivity. Permittivity is supposed to represent the dipole moment due to oscillation of carriers in completely filled bands (or so called bound carriers) and conductivity is supposed to represent the dipole moment due to the oscillations (note we are talking about AC !) of carriers of partially filled bands (or so called free carriers). Note that, strictly speaking, in quantum mechanical picture, its not really possible to distinguish between the two effects. Polarization comes because of the intermixing of valance band states with the conduction band states. Smaller the band gap (compared to the frequency) more the mixing and more the polarization and bigger the permittivity. Quantum mechanically, both conductivity and permittivity falls off naturally from the same derivation. Both of them are calculated through the same physics (calculating the expectation of dipole etc) and both contains the same information. For example one does not need to differentiate between j_{free} and j_{bound} . One can simply write $j = i\epsilon_{eq}\omega E = \sigma_{eq}E$ ¹. For semiconductors probably its still possible to distinguish between the two. For example we can make experiments on an undoped semiconductor and measure the effects of bound charges and then repeat the experiment with dopings. But still near the band to band transition edges, I guess, one always has to talk about the “net” permittivity OR “net” conductivity due to all effects. Usually such high frequencies fall under optical regions and its more conventional to simply work out Maxwell’s equations with “net” permittivity forgetting everything about the conductivity.

Lets take a simple example. Suppose we are looking at a finitely conducting metal (and no band to band absorption). We know that such a material is lossy and absorbs. It is very common to include this effect by defining a complex permittivity function $\epsilon_{eq} = \epsilon_0 - i\frac{\sigma}{\omega}$ ². From

¹In $\exp(i\omega t)$ convention. If opposite convention is used then one would use $j = -i\epsilon_{eq}\omega E = \sigma_{eq}E$.

²In $\exp(i\omega t)$ convention. If opposite convention is used then one would use $j = -i\epsilon_{eq}\omega E = \sigma_{eq}E$ with $\epsilon_{eq} = \epsilon_0 + i\frac{\sigma}{\omega}$.

classical electromagnetic perspective this is just a mathematical convenience. One would claim that absorption is actually an artifact of ohmic losses and in theoretical accurate sense only real permittivity makes sense. Imaginary part is there only to make the mathematics easier and to include the effects of ohmic losses in more convenient fashion.

Lets also consider the opposite example. Suppose we are looking at an undoped intrinsic semiconductor. First, suppose energy of the incident photons is below the bandgap. Then material is lossless and non-absorbing. Permittivity is real and conductivity is zero. But still if we can measure the AC oscillations in charge density one would observe an AC current. We can describe these effects by simply writing $j = \sigma_{eq}E$ with $\sigma_{eq} = i\omega\epsilon$ (one would not include the polarization current separately then – this term is the polarization current). From classical perspective this is just a mathematical convenience. Lets now consider the case when the energy of incident photons is above bandgap. We know this material is absorbing (and lossy in above mentioned sense). From classical electromagnetics perspective one would model this effect as an imaginary part in permittivity (this is seen by modeling atoms as oscillators and then calculate the polarizability of material – one would conclude that if oscillators are lossy then permittivity would have an imaginary part). And this would also show up as some effects in the polarization current measured. This effect can be modeled as a real part in conductivity (hence absorption now seems to appear as conventional transport phenomenon associated with real conductivity). Again from classical perspective this would simply be a mathematical trick.

But from quantum mechanical perspective this ambiguity is real. One can not actually decide which choice of parameter is more fundamental. In both examples there is state transitions involved and hence conventional absorption involved. Also in both examples there is oscillations of conduction electrons involved and hence conventional transport is involved.

Note that ϵ by conventional definition does not include the effects of oscillations of free carriers. So, including both polarization and free current, I can write $j = \sigma E + i\epsilon\omega E$. Whereas σ includes only the effects due to the motion of free carriers. Hence, $\sigma_{eq} = (\sigma_R - \omega\epsilon_I) + i(\sigma_I + \omega\epsilon_R)$. So we can conclude that equivalent conductivity is made of two parts - 1) one that comes simply because of the motion of the free carriers and 2) one that comes from the motion of bound charges (from ϵ). If one is simply going to measure total current then there is no way one can figure out the origin of the current. Note that the imaginary part of ϵ creates a real part in σ and vice versa. (Real ϵ implies that velocity is 90° out of phase with electric field and hence an imaginary conductivity.) Every added imaginary part in ϵ would cause a real part in current.

Now suppose we define ϵ to include all effects whatever possible. For example calculate ϵ from reflectivity measurements. In that case $\sigma_{eq} = i\omega\epsilon_{eq} = (-\omega\epsilon_{eq,I}) + i(\omega\epsilon_{eq,R})$. Usually this would be done by writing $\epsilon_{eq} = \epsilon' - i\epsilon'' - i\frac{\sigma}{\omega}$, where σ can be complex and is calculated assuming there is no band to band transitions and includes only the effects of free charges. Hence just knowing the ϵ we can calculate the current.

Sometimes one can make a distinction if current is because of free carrier or because of bound carriers. But this is possible only as long as rate of band to band transitions can be neglected (quantum mechanical mixing is OK as long as rate of transitions is zero). Otherwise a bound carrier can become a free carrier and we can not distinguish the two. Whenever such transitions can not be ignored, hence, the usual convention is not to try to make a distinction. And as a consequence only one of the two parameters - permittivity and conductivity - needs to

be specified including all effects. For example mixing of states from two bands is something that causes the polarization effect. And hence a real part in ϵ and an imaginary part in σ_{eq} . If material is conductive then we would also have a real part in conductivity and an imaginary part in permittivity. Note that we still do not have any band to band transition rate. Till this point one can distinguish which portion of current is coming from free carriers and which is coming from bound carriers. Now suppose band to band transitions are also possible (suppose we have increased the frequency such that these transitions get switched ON). Now this would appear as if polarization effect is retarded by some type of frictional forces (we discussed this above – band to band transitions show up as losses in oscillator) then we would also have an imaginary part in ϵ and a real part in σ_{eq} . Now there is no way one can make sure if observed current is free carrier current or bound carrier current.

Final conclusion is this. Write σ by ignoring band to band transitions and including only the effects of free carriers. Then write an expression for $\epsilon_{eq} = \epsilon' - i\epsilon'' - i\frac{\sigma}{\omega}$. Now if want to calculate the total current simply use $j = i\epsilon_{eq}\omega E$. If want to calculate polarization, simply use $P = \epsilon_{eq}(\epsilon_{eq} - 1)E$. (Note that quantum mechanically it not possible to say that only bound charges polarizes. All kinds of charges can create polarization. Note dipole moment is $P = Nez$. So we have polarization even from free carriers).

3.2 Neutral Free Electron Gas (plasma)

Using the Drude's theory of conduction one can obtain $\sigma_{eq} = \sigma_{free} = \sigma_0/(1 - i\omega\tau)$. The same information can also be written as $\epsilon_{eq} = \epsilon_0 - i\frac{\sigma_0}{\omega(1 - i\omega\tau)}$. And one can either use $j = \sigma E$ or $j = i\epsilon_{eq}\omega E$ but not both. Any of these expression would include currents due to all the charges whether free or bound or displacement (for this particular case of free gas there are no bound charge current).

Part III

Optical Processes in Semiconductors

4 Direct Band to Band Radiative Recombination

From the conservation of wave-vector (its not conservation of momentum, strictly) direct band to band transition would always be radiative. Conservation of energy comes out of Fermi's Golden rule whereas conservation of k comes from the fact that $H_{k,k'} = 0$ if $k \neq k'$. The last statement comes out only when we are working with dipole approximation and assumes that wavefunctions with slowly varying envelopes.

Our aim is to predict the transition rate between the conduction band and valance band. Explicitly, we want to calculate, under any given conditions, on an average (ensemble averaging) how many number of electrons from conduction band would fall into the valance band within infinitesimal small time interval or vice versa how many number of electrons would jump from

valance band to conduction band in that small time interval. Averaging is a combination of Quantum Mechanical and Statistical averaging. Also note that because only possibilities are either 0 transition or 1 transition, the **probability of transition** (event space is a set of system in the ensemble and we observe whether transition happened in each system in the ensemble) in an infinitesimal time is same as the **average number of transitions** in infinitesimal time. Its good to note the terminology and usage of terms and realize that both are one and same thing. These two terms are very frequently used interchangeably in the literature. On similar lines, only for Fermi distribution, we can use the terms “probability of finding an electron” and “average number of electrons” interchangeably. For Bosons we have to use average number of particles.

Before we can calculate the “rate laws”, we need to experimentally determine the “mechanism” of process. For example an irreducible one step process would proceed with “first order” rate law and there would be simple linear dependence on photon and carrier concentrations (as the direct band to band recombination). Whereas for two step process it might depend on concentrations of photons and carriers in complicated manner (as recombination through the RG centers). Note that to claim that one-step process follow first order rate law we do not actually need any chemistry-style kinetic theory arguments involving capture area etc (although, such theories were developed in initial days and they are still frequently used in device literature). For example if we know that the absorption of a photon or the stimulated emission of a photon is an one-step process then we would proceed as follows to obtain the rate laws in sound quantum mechanical manner (spontaneous emission is a bit tricky and we would consider it latter). We would argue using stimulated emission but the arguments are exactly same for absorption also.

The important assumptions that we are going to make are

- independent particle approximation and
- non-excitonic modeling

4.0.1 Independent Particle Approximation

Independent particle approximation basically neglects the interaction between particles. By ‘interaction’ we do not mean anti-symmetry and symmetry requirements of Fermi or Bose particles (which is equivalent to say that just by using Slater determinant etc does not mean that we are including the effects of interactions other than anti-symmetry and symmetry requirements). These are also kind of ‘interactions’. But these can easily be taken care of if we just use multi-particle formulations without actually including the particle-particle interaction. Use of multi particle basis states (Slater determinant etc) while still ignoring interaction, one can explain many things (like spontaneous emission, adhoc inclusion of particle statistics terms in transitions rate calculations etc) in an elegant way. All though this is not usually done in many text books.

The inclusion of inter-particle interaction in solid state is really very difficult task. First of all we need to know the **multi particle eigen energy states** (perturbation theory can give me the ‘perturbation’ provided I know perturbing hamiltonian. But still I need to start with eigen energy states I think in the Fermi’s Golden rule, I have to have energy eigen states. Otherwise how would I get energy conservation ? In that case multiparticle basis states have to be an energy eigen state

(Check Mukul ??). In the presence of inter particle interactions its very difficult to calculate the true states of definite energy. Secondly we need to know the **perturbation hamiltonian** in order to calculate the transition rates between two states assuming one is occupied and other is vacant. I am not sure if the perturbing hamiltonian would still be same in the presence of inter particle interactions (Check Mukul ???) . I don't think so. Thirdly we need to know the **thermal probability distribution** of finding the system in any one of these states. Now if I know the energy of each of the multiparticle states then its not difficult to obtain the probability distribution among all multi-particle states. Thats simply going to be the Boltzman distribution (in multi particle form). Fourthly we need to add up all the transition rates to calculate the net transition rate from valance band to conduction band. For this we need to know the density of states. Now calculating the **multi-particle density of states** is again a very difficult task. Combining all these together, we realize that independent particle approximation is just indispensible in solid state device physics.

4.0.2 Multi Particle Scheme

If we ignore inter-particle interaction, we can do the solid state physics in multi-particle formulation in a rather elegant fashion. In occupation number representation any 'one' of the basis states for spanning the multi-particle hilbert space can be written as $|1, 0, 1, 0, \dots\rangle$ where each entry represents a single particle energy eigen state (or it can also be any other single-particle basis state) when other particles are removed from the system. (Note that the complete multi-particle state is just a 'basis' and may not be an multi-particle 'energy eigen state'. But if inter-particle interaction is negligible then they also turn out to be multi-particle energy eigen states.) Now the QM state of any such multi-particle system can be written as linear supperposition of such basis states. Now when we are doing quantum statistical mechanics, we had claimed that 'statistical uncertainty' and 'quantum mchanical uncertainties' are indistinguishable. So let us assume that there are only statistical uncertainties (does this statement assumes that multi-particle basis state has to be an energy state ? I dont know for sure (check MUKUL????) – but I think not. Statistical mechanics I guess can be applied in any basis and energy basis shoud not have any fundamental precedence. But in any case we have to have energy eigen states in order to use Fermi's Golden rule. So we have to abondon particle-interactions). What I mean is that the state is not a linear superposition of multiparticle basis states. It is in one of the basis states but thermodynamics perturbs the system and makes it swim among various multi-particle basis states. And now I want to know what are the statistical probability distribution of finding the system in one of these basis states ? This can easily be obtained in the form of multi-particle Boltzman distribution. For the time being, suppose thermodynamics can tell me this. I would not really use this. We would finally need much common single-particle fermi distribution only. How do I calculate R-G rates knowing all this ? Perturbation theory (with annihilation and creation operators) can tell me the 'transition probability' from $|1, ?, ?, ? \dots, 0, ?, ? \dots\rangle$ to $|0, ?, ?, ? \dots, 1, ?, ? \dots\rangle$ provided I can write down the perturbation hamiltonian. Now since there is only 'statistical uncertainty' whether system was in this initial state or not – I can simply multiply the transition probability by the thermodynamic occupation probability of this initial state and that would give me the actual probability of transition that one expects to observe in an experimental measurement. One point

to be noted here is that I can change the ? marks in the above states and transition probability donot change. That should be obvious. But for proving that one needs to do perturbation theory. Now another important point is that we need to all the transition rates to obtain the net transiion rate from conduction band to valance band. For this I need density of states. Again I would not need multi particle density of states straight away. We can finally use our single particle states DOS only.

Now occupation probability of $\sum_i |1, ?, ?, ? \dots, 0, ?, ? \dots\rangle$ where summation is over all unknowns is simply given as occupation probability of electron times the occupation probability of hole (for this also we need independent particle approximation (Check Mukul ???)). Since transition rate for any of such states is constant, that can be taken out of the summation. So the total transition probabilty between any two such (single-particle ?????) states would be transition probability between any 'one' set of such multi-particle state (referred as conditional probability) times the electron occupation probability times the hole occupation probability. Thats the basic approach we are going to follow. Now below I am describing the actual perturbation theory concepts.

4.0.3 Perturbation Theory

Visulaize that one 'empty' valance band state and one 'full' conduction band state (for calculating conditional probability) is existing in the background of photons of 'right' frequency but whatsoever intensity. (Note, firstly, that this means a multi-particle state in which there is '1' for some single particle state and a '0' for some valance band state. Secondly, we are working in the photon picture because although for predicting rate laws for absorbtion and stimulated emission its really not necessary to quantize the radiation, but we need to do it for spontaneous emission). Now if keep the radiation on for some time t_0 then we can calculate the evolution of the state of the electron in the conduction band. The state at time t_0 would be written as the linear combination of all the stationary states including the valance band states also. So if we make an experiment after t_0 then there would be some probability that the original conduction band electron would be found into the valance band. Physically what it means is – for example if the transition probability is 80% between two states and if we have 100 exactly simmlar “set of states” in the valance-conduction band such that the time evolution of each of them is independent of each other then we should expect that on an average after time t_0 80 electrons would be found in the valance band. So we can add the probability of transition between each set of states to get the total number of transitions. Another point to note is that this probability of transition is given by Fermi's golden Rule and is found to be propotional to time t_0 . Hence one can devide by t_0 to obtain the total number of transitions per unit time that is one can speak about the uniform “transition rate”. Note that the “transition rate” just depend on the “matrix elements” between the two state and donot depend on occupation probabilities. Although they might depend on the photon densities (equivalent of concentrations) or on other properties of the perturbation like frequency of radiation because that decides which particular energy states would be involved or the amplitude of the perturbation. Now after this, just using the simple rules of probability (actually physics here is not that simple – actually its wrong quantum mechanically) we can say that probability of transition from certain conduction band state to certain valance band state in time

t_0 is that the probability that conduction band state is filled times the probability that the valance band state is empty times the probability of transition in time t_0 . We can then add up all such probabilities to get the total number of transitions in time t_0 and then we can divide by time to get the total transition rate. Note that this summation would actually be done by multiplying by the joint state density and then integrating over all possible transition. (In case we work with delta functions, concept of joint state density becomes useful). To summarize, matrix elements gives conditional transition rate between any two states, multiply with occupation densities to get the transition rate between those states, multiply by joint density of states and integrate to get total transition rate between two bands and then multiply by time to get total number of transition.

There are a few points to note here.

- (a) First is that probably from our rudimentary chemistry-type of kinetic rate law we would have expected that the rate of transition should also be proportional to the number of photons or the density of photons etc. This actually is correct ! We look at the above arguments carefully the amplitude of the electromagnetic perturbation is hidden there in the matrix element of transition which would finally get squared in the process of calculating probability. Note that the number of photons is proportional to the square of the field amplitude !
- (b) Finally, we can relate the above transitions probabilities to the absorption (through photon supported band to band transitions, we can have absorption through conduction or through losses in polarization all these should also be included in a generic theory) coefficients, in case of absorption. Absorption coefficient is the probability of absorption of a photon per unit length. That is the number of photons absorbed per unit volume per unit time (this is exactly the above total transition rate) divided by number of photons incident per unit area (which is related to the intensity).
- Relation between absorption and refraction. See previous section.

4.1 Recombination Generation in Single Particle Approach

4.1.1 Notation

- $W_{ab,monochromatic}$ represents the stimulated emission transition rate (**no of transitions per unit time per unit volume**) between two states of a discrete state system when irradiated with a monochromatic light.
- $W_{ab,total,monochromatic}$ represents the stimulated emission rate between all the states that can afford to participate when a continuous state system is irradiated with a monochromatic light. Note that $W_{ab,total,monochromatic} = \int_{E_{joint}} W_{ab,monochromatic}$ where I do not need to include dE_{joint} explicitly because I can simply replace $f_e f_h \rightarrow f_e f_h g_{joint} dE_{joint}$ and $W_{ab,monochromatic}$ is still interpreted as stimulated emission rate per unit time per unit volume but from any one set of states in the energy band dE_{joint} .

- $W_{ab,total}$ represents the stimulated emission rate between all the states when a continuous state system is irradiated with a generic spectrum of light. Note that $W_{ab,total} = \int_{\omega} W_{ab,total,monochromatic}$ where I do not need to include $d\omega$ explicitly because I can simply replace $n_{photon} \rightarrow f_{photon}g_{photon}d\omega$ and $W_{ab,monochromatic}$ is still interpreted as stimulated emission rate per unit time per unit volume from any one set of states in the energy band dE_{joint} but now stimulated by any one optical mode in the frequency range $d\omega$.
- I might drop the subscripts ab on and off whenever they are understood to be there.

4.1.2 Einstien's A, B Coefficients Arguments

These arguments are completely alternative. All that we are going to argue can easily be proved in quantum mechanical perturbation theory. Still I think Einstein's A, B coefficients arguments are very intuitive and are very powerful. This is the reason we are starting the discussions from here.

Einstien's A and B coefficient proves that without a spontaneous emission phenomenon its impossible to achieve thermal equilibrium with known distribution laws. When we irradiate a discrete state system with a monochromatic radiation, we write the transition rates (**number of transitions per unit volume per unit time** that is $W_{ab,total,mono}$) between two specific discrete levels as a constant (A_{spont} , A_{stim} and B_{abs} , which only depends on state overlap integrals, freq etc) times photon density n_{photon} (except in the case of A_{spont}) times f_e times f_h^3 . One should note that A_{spont} , A_{stim} and B_{abs} coefficients do not depend on temperature and remains same even in non-equilibrium situations (this was an assertion in Einstien's argument, but nowadays we can justify thorough perturbation theory done below). So the temperature dependance can come from the holes, electron and photon densities only. Now in equilibrium:-

$$A_{spont}f_e f_h g_{joint} dE_{joint} + A_{stim}(f_e f_h g_{joint} dE_{joint}) f_{photon} g_{photon} d\omega = B_{abs}((1 - f_e)(1 - f_h) g_{joint} dE_{joint}) f_{photon} g_{photon} d\omega$$

$$A_{spont} + A_{stim} f_{photon} g_{photon} d\omega = B_{abs}((1 - f_e)(1 - f_h)/(f_e f_h)) f_{photon} g_{photon} d\omega$$

$$f_e = \frac{1}{1 + \exp(E_2 - E_f)/KT}$$

$$f_h = \frac{\exp(E_1 - E_f)/KT}{1 + \exp(E_1 - E_f)/KT}$$

³Note that in case we have a continuous radiation spectrum or a continuous state distribution, we can simply replace $f_e f_h \rightarrow f_e f_h g_{joint} dE_{joint}$ and $n_{photon} \rightarrow f_{photon} g_{photon} d\omega$ to obtain the transition rates from a bunch of closely spaced levels due to photons in a bunch of closely spaced modes. So one does not need to bother. Just assume discrete system and go ahead.

$$\frac{(1-f_e)(1-f_h)}{f_e f_h} = \exp(E_2 - E_1)/KT$$

$$A_{spont} + A_{stim} f_{photon} g_{photon} d\omega = B_{abs} (\exp(E_2 - E_1)/KT) f_{photon} g_{photon} d\omega$$

$$f_{photon} g_{photon} d\omega = \frac{A_{spont}}{B_{abs} \exp(E_2 - E_1)/KT - A_{stim}}$$

$$f_{photon} = \frac{1}{\exp(\hbar\omega)/KT - 1}$$

The only way we can make the multiplying coefficients to be temperature independent is by forcing the following relationship among them:-

$$A_{spont} = A_{stim} g_{photon} d\omega \quad (1)$$

$$B_{abs} = A_{stim} \quad (2)$$

Where g_{photon} is the optical mode density⁴. So we can write

$$W_{total,mono,spont}/W_{total,mono,stim} = (A_{spont} f_e f_h g_{joint} dE_{joint}) / (A_{stim} (f_e f_h g_{joint} dE_{joint}) f_{photon} g_{photon} d\omega)$$

Which means

$$W_{total,mono,spont}/W_{total,mono,stim} = 1/f_{photon} \quad (3)$$

The left side gives me the ratios of two types of total monocromatic rate of transition (per unit time per unit volume) when a bunch of closely spaced levels are interacting with a bunch closely spaced optical mode. Right hand side tells me that this ratio has to be equal to the number of photons (just a number) present in any one of these modes (not necessarily equilibrium Boson distribution because relations between coefficients are supposed to remain same even in non-equilibrium). Also one can write

$$W_{total,mono,stim}/W_{total,mono,abs} = \frac{f_e f_h}{(1-f_e)(1-f_h)} \quad (4)$$

The usual practice is to write down absorbtion rate in terms of a experimentally measured parameter known as “empty” absorbtion coefficient α_0 and then use (4) to obtain the stimulated emission rate and then use (3) to obtain the spontaneous emission rate. Or otherwise one can also obtain the absorbtion rate theoretically using Fermi’s Golden Rule. $W_{total,mono,abs} = (\frac{2\pi}{\hbar} |H_{ba}|^2) (g_{joint}) (1-f_e)(1-f_h)$. Where $H_{ba} = -\frac{eA_0}{2m_0} p_{cv}$ with $k_e = k_h + k_{op}$ under slowly varying envelop approximation. Fermi-Dirac factors (or generally speaking occupation number in non-equilibrium situations) fall off naturally in multiparticle theory but in single particle theory we have to throw them manually.

⁴ For a special case of free space the density of optical modes is $g_{photon} = \frac{8\pi\nu^3 E^2}{c^3 \hbar^3} = (\frac{1}{2\pi^2}) (\frac{2}{\hbar\omega}) (\frac{\omega}{c/n_r})^3$.

4.1.3 Absorbtion (Generation) Rate Calculations from α_0

Usually, one measures the absorbtion coefficient α (in the units of per unit length) or the “empty absorbtion coefficient α_0 ” and then relate the absorbtion rate (in the units of per unit volume per unit time) to that coefficient. Since, accurate first principle modeling of optical properties can be rather involved, this approach provides a good mixture of experimental data with theoretical insight.

Absorption Coefficient Absorbtion coefficient α is defined as the coefficient in the equation

$$\frac{dn_{photon}}{dz} = -\alpha n_{photon}$$

(Its the average number of photons absorbed per unit length per photon present in the direction of propagation). α_0 is defined as

$$\alpha \equiv \alpha_0(1 - f_e)(1 - f_h)$$

The absorption coefficient (α) can also be related imaginary component of permitivity or the refractive index. Think of a uniform plane wave propagating along z direction in an homogeneous absorbing material. Classical wave equation accepts a solution of the form $\exp(j(\omega t - k_z z))$. Note that k_z can in general be a complex number. Let $k_z = k_{z,r} + jk_{z,i}$ where only that solution has been chosen which has $k_{z,i} < 0$ (so that forward propagating wave is only allowed to be a decaying wave – no gain material allowed). Then the time averaged flux of power at any cross-section would vary from cross-section to cross-section as $\exp(2k_{z,i}z)$. Now since number of photons and time averaged flux of power at any cross-section are directly propotional, one concludes that $-2k_{z,i} = \alpha$. Moreover, $k_z = \sqrt{\omega^2 \mu(\epsilon_r + j\epsilon_i)} = \omega \sqrt{\mu \epsilon_0}(n_r + jn_i)$ where n is the refractive index. One should be careful that n_i needs to be a negative number (assuming μ is real number)⁵. If the material so non magnetic then we have

$$\alpha = -\frac{2\omega n_i}{c}$$

For direct bandgap semiconductors, just above the bandgap, $1/\alpha \approx 1\mu m$.

Absorption Rate The absorption coefficient can easily be related to our absorbtion rate $W_{ab,total,monochromatic}$ which represents the number of absorbing transitions between any two states of the system that can afford to be involved per unit time, per unit vlume when system is irradiated by a monocromatic light. Look at an infinitesimally small volume of a semiconductor. Assume that beam of

⁵Remember, we started with the convention of $\exp(j(\omega t - k_z z))$, this leads to the requirement that $k_{z,i}$ needs to be negative and that finally requires that n_i needs to be negative. There is huge amount of literature that starts with a convention of $\exp(j(-\omega t + k_z z))$, which requires $k_{z,i}$ and n_i to be positive numbers. Such considerations also set requirements on sign of imaginary part of permitive as well depending upon the convention chosen for the time harmonic dependence. Since $n_r > 0$, it follows that the sign of imaginary part of permitivity follows exactly same convention as that of n_i .

photons is propagating in z direction. Inside the volume (had there be no inflow-outflow)

$$\frac{\partial n_{photon}}{\partial t} = W_{total,mono}$$

But for maintaining the steady state

$$n_{photon}(z + dz/2)(c/n_r)dxdy - n_{photon}(z - dz/2)(c/n_r)dxdy = -\frac{\partial n_{photon}dxdydz}{\partial t}$$

$$\frac{\partial n_{photon}}{\partial z} \frac{c}{n_r} = -\frac{\partial n_{photon}}{\partial t} = -W_{total,mono}$$

$$W_{total,mono} = \alpha n_{photon}c/n_r = \alpha_0(1 - f_e)(1 - f_h)n_{photon}c/n_r$$

Note that $n_{photon}c/n_r$ is the number of photons incident per unit time per unit area across any cross-section. This number can be related to more directly observable parameters like intensity of light or electric field strength. Note that power incident per unit area is related to Poynting vector, which is energy flow density vector by $I = \frac{1}{2}Re\{E \times H^*\}$. For a plane wave solution, $E = E_0 \exp(j(k_z z - \omega t))$ one has $H = \frac{E}{\eta}$ where $\eta = \sqrt{\frac{\mu}{\epsilon}} = \frac{1}{c\epsilon_0(n_r + jn_i)}$. Hence

$$\frac{I}{\hbar\omega} = \frac{E_0^2 \exp(-2k_z,iz) c\epsilon_0 n_r}{2\hbar\omega} = \frac{n_{photon}c}{n_r}$$

Hence,

$$W_{total,mono} = \frac{\epsilon_0 n_i n_r E_0^2 \exp(-2k_z,iz)}{\hbar}$$

4.1.4 Absorbtion (Generation) Rate Calculations from First Principles

Or otherwise one can also calculate the absorbtion coefficient or the absorbtion rate in non-excitonic model using Fermi's Golden Rule. So one can write the abosorbtion rate as

$$W_{ab,mono} = \left(\frac{2\pi}{\hbar} |H_{ba}|^2 \delta\right) (1 - f_e)(1 - f_h)$$

Here, H_{ba} is the perturbation Hamiltonian (time independent part) matrix element between initial and final states. One usually works with a electric dipole Hamiltonian which can either be write as

$$H(t) = q\vec{E}_0 \cdot \vec{r}(2\cos(\omega t))$$

where oscillating electric field perturbation is taken as

$$\vec{E} = 2\vec{E}_0 \cos(\omega t)$$

And time independent part is taken to be

$$H = q\vec{E}_0 \cdot \vec{r}$$

Here q is a positive number. Other way of writing the same Hamiltonian is $-\frac{q}{m_0}\vec{A}\cdot\vec{p}$. Now if are considering discrete state systems like atoms or quantum dots, delta function is not at all acceptable because it gives infinite transition rates. Theoretically, discrepancy comes because states are not really states-of-definite energy (they surely are changing, particles are jumping! Hence one needs to include homogeneous broadening of linewidth). Secondly, there are other thermodynamic processes that disturbs at least the phase of the states while they are evolving (inhomogeneous broadening of linewidth). To get rid of this one can actually define the lifetime of states and the linewidth of accompanying radiation replacing delta function. Linewidth can be either homogeneous or inhomogeneous. But in semiconductors we can get rid of this in another way. We neglect linewidths. But remember we have infinitesimally small number of states between E_{joint} and $E_{joint} + dE_{joint}$ per unit volume. So if dE_{joint} goes to zero actual number of states also go to zero. In this way one can take care of infinities. Suppose our aim is to calculate the total transition rates between all possible set of states interacting with a monochromatic light. First of all we need to calculate the joint DOS - number of allowed transitions between E_{joint} and $E_{joint} + dE_{joint}$. For both conduction and valance bands we have the same DOS in k -space. Also assuming $k_c = k_v + k_{op} \approx k_v$ we can conclude only vertical transitions are possible. In order to take the help of delta function sitting over there we should count the number of such vertical transitions in an infinitesimally small transition energy band. This is called joint density of states. But we want DOS in $E_c - E_v$ space. One can write $E_c - E_v$ as a function of k . If both the bands are parabolic then $E_c - E_v$ would also be parabolic but with a “reduced” effective mass of $\frac{1}{m_{eff}^*} = \frac{1}{m_e^*} + \frac{1}{m_h^*}$. So joint DOS would still look “same” just with a different effective mass. Now one can integrate $W_{ab,monochromatic}g_{joint}$ over the entire $E_b - E_a$ space and get the total transition rate due to monochromatic light (note that we donot need worry about matching frequency with bandgap because delta function is sitting over there!). Hence we can write, assuming H_{ba} is same for all the states (It can be proved using Kane’s Band Theory (check MUKUL ???))

$$W_{total,mono} = \frac{2\pi}{\hbar} |H_{ba}|^2 g_{joint}(E_{ab})(1 - f_e)(1 - f_h)$$

which is same expression which we had previously written in terms of absorbtion coefficient:-

$$W_{total,mono} = \frac{cn_{photon}}{n_r} \alpha_0(E_{ab})(1 - f_e)(1 - f_h) \quad (5)$$

So,

$$\alpha_0 = \frac{2\pi}{\hbar} |H_{ba}|^2 g_{joint}(E_{ab}) \left(\frac{n_r}{cn_{photon}} \right) \quad (6)$$

This also tells us that experimentally measured $\alpha_0(\hbar\omega)$ should actually go as $A_0^2 g_{joint}/n_{photon}$. One usually keep the amplitude of electromagnetic wave as a constant and check what is the decay rate of intensity with distance. In that case the photon flux would not be constant from frequency to frequency because the quanta of energy is increasing linearly with frequency. That means number of photons should reduce linearly with frequency. If you keep flux of photons to be same from frequency to frequency then A_0^2 would reduce linearly with frequency. So the actual dependance should look like $g_{joint}/\omega \approx g_{joint}$. So it goes approximately as square root

dependence. How about α ? $(1 - f_e)(1 - f_h)$ dependence actually suppresses the absorption of light near the band gap energies (**Burstein-Moss shift in absorption edge**). At higher energies we do not have any carriers in both the bands and α becomes approximately same as α . Also

$$W_{ab,total} = \int c/n_r \alpha_0(E_{ab})(1 - f_e)(1 - f_h) g_{photon} f_{photon} d\omega$$

4.1.5 Stimulated Emission (Recombination) Calculations

Using (4) one can easily obtain the rate of stimulated emission as :-

$$W_{total,mono} = \frac{cn_{photon}}{n_r} \alpha_0(E_{ab})(f_e f_h) \quad (7)$$

and

$$W_{ab,total} = \int \frac{cg_{photon} f_{photon} d\omega}{n_r} \alpha_0(E_{ab})(f_e f_h)$$

Where α_0 is either experimentally measured or is given by (6). Now this integral in general is not easy in high carrier densities or low temperature regimes. But whenever we can use Boltzman distribution (even in non-equilibrium), it can be simplified to a great extent. $f_e \approx \exp((E_{fe} - E_b)/KT)$ and $f_h \approx \exp((E_a - E_{fh})/KT)$. So $f_e f_h \approx \exp(E_a - E_b + E_{fe} - E_{fh})/KT$. Now we would get rid off delta function and we would get $W_{ab,total,mono} = cn_{photon}/n_r \alpha_0(E_{ab}) \exp((E_{ab} - \Delta E_f)/KT)$. Also note that $n \approx N_c \exp(E_{fe} - E_c)/KT$ and $p \approx N_v \exp(E_v - E_{fh})/KT$, so $np/(N_c N_v) \approx \exp(E_g - \Delta E_f)/KT$.

$$W_{ab,total,monochromatic} = \frac{cn_{photon}}{n_r} \alpha_0(E_{ab}) \left(\frac{np}{N_c N_v} \right) = G_{th}(\omega) np \quad (8)$$

Its important to remeber that $G_{th}(\omega)$ depends on the state overlap integral (p_{cv}) which is supposed to be same for all states in small infinitesimal energy band (this also takes care of strength of optical mode interaction with states), number of photons in that mode (A_0^2) and density of states ($g_{joint}/N_c/N_v$) at that transition energies. [Normalized interaction - p_{cv} , strength of radiation - n_{photon} and normalized DOS profile - $g_{joint}/N_c/N_v$]. This is the form that is very frequently used in device literature. Now if we have a spectrum of light incident then we can again integrate the above expression to obtain $W_{ab,total} = \int W_{ab,total,monochromatic}$. Note that as far as Maxwell distribution is valid we can again take out np factor. So we can write

$$W_{ab,total} = G_{th} np$$

where $G_{th} = \int G_{th}(\omega)$. Where we are integrating over a distribution of photons among electromagnetic modes. **Just remember that all of above three factors can change with energy and the integration should take care of all three. After integrating out things G_{th} would only depend on the photon deistribution and over all properties of band (p_{cv} 's and DOS at various energies).** Note that under degenrate carrier distributions (for example in lasers or high doping or low temperatures) one can not use above expression. In the limmiting non-equilibrium situation at $T = 0K$ (for exmaple a highly injected lasser at absolute zero) we would

have $f_e = 1$ and $f_h = 1$ both upto a fixed level. In this case $W_{ab,total} = G_{th}n = G_{th}p$. And this rate would be higher than the previous expression. So we can conclude that with temperature optical recombination-generation rate reduces provided photon density is kept constant (spontaneous would surely reduce, for example).

4.1.6 Spontaneous Emission (Recombination) Calculations

Using (4) and (3) one can obtain an expression for spontaneous emission as :-

$$W_{total,mono} = \frac{cg_{photon}d\omega}{n_r} \alpha_0(E_{ab})(f_e f_h) \quad (9)$$

Where α_0 is either experimentally calculated or is given by 6.

From which one can easily calculate the total, monochromatic spontaneous emission rate if we know the density of modes. For the special case of free space optical modes we have :-

$$g_{photon} = \frac{8\pi n_r^3 E^2}{c^3 h^3} = \left(\frac{1}{2\pi^2}\right) \left(\frac{2}{\hbar\omega}\right) \left(\frac{\omega}{c/n_r}\right)^3$$

One side remark. Suppose I put the semiconductor inside a cavity in equilibrium at some temperature. At any frequency, I can calculate the spontaneous emission rate. Moreover the absorption and stimulated transition rate densities depends on the properties of the system and the temperature (through carrier densities). So there should be unique photon densities in each frequency so that absorption can become equal to the emission at each frequency. This is precisely the Planck's radiation law.

4.1.7 Gain Coefficient and Lasing Condition

Gain coefficient is simply the negative of "net" absorption coefficient ignoring spontaneous emission. $g = \frac{W_{total,mono,stim} - W_{total,mono,abs}}{n_{photon}c/n_r}$. One can simply prove that for g to be positive, one has to have $f_e + f_h > 1$ which in turn implies that for transparency we must have $E_{fn} - E_{fh} = \hbar\omega$ (under quasi-equilibrium assumption). Now its actually very difficult to invert a semiconductor and achieve $f_e + f_h = 1$ or equivalently to push the hole quasi fermi level into the valance band. The reason is that the hole effective mass is much higher and hence it has much higher density of states. So even for very high hole densities the value of f_h remains very small.

5 Indirect band to band radiative+non-radiative recombination

Such process invariably involve phonons. This process is highly unlikely. In indirect band semiconductors more dominant processes are through RG centers. At $1.42eV$ photon wavelength is $0.87\mu >> a$ and hence $2\pi/\lambda \ll k$. So it has to be a three particle process.

5.1 Band to shallow impurity-trap spontaneous radiative recombination

Usually the larger step is radiative. It actually is going to be a two step process. But if the second phonon involving step is very small its probability can always be assumed one. So it can be approximated by above techniques. Using the similar arguments as above $\tau = n_i^2 / G_{th} / N_{impurity}$. Shallow donor/acceptor levels might act as RG center at low temperatures. But even at room temperatures they are highly inefficient RG centers.

5.2 Single level recombination generation center

'Trap' or 'RG center' is a synonymously used term for any kind of impurity that creates energy states near the mid gap. This can be both donor type or acceptor type (for donor type $n_T = N_T - N_T^+$ and $p_T = N_T^+$ and for acceptor type $n_T = N_T^-$ and $p_T = N_T - N_T^-$). Crystal defects can also act as traps. RG through RG center is always non-radiative because of momentum conservation and because of the fact to photon carries very little momentum. (probably electrons in the trap states donot have appropriate momentum classically they are not moving rather gets trapped, so only phonons can help this process) Multiple phonons are involved but still its not a multi-particle process otherwise the rate would be extremely small. It is supposed to be a cascade process. In which electron is first trapped into a much higher ionized state of the trap with single phonon. Later on it spirals down giving out energy as many other small phonons.

Its a two step process, as first electron capture and subsequently hole capture takes place. Similarly emission is also two step process. Each of these step is an elementary irreducible step. So just using the similar arguments (no chemical rate laws required .. just use probability arguments) each of these steps can be written as first order rate laws. This can be obtained through similar QM arguments only replacing photons by phonons. For example an electron emission rate can be written as $e_p n_T p$. The net electron recombination rate $r_n = c_n n p_T - e_n n_T$. Number of empty states in conduction band has been incorporated into e_n . Units of c_n would be $cm^{-3}s^{-1}$ whereas the units of e_n are s^{-1} . And the $r_p = c_p p n_T - e_p p_T$. Where the emission coefficient would include the phonon density and should be temperature dependent. One can then enforce the detail balance condition at thermal equilibrium. In equilibrium $r_n = r_p = 0$. So using this condition we can eliminate two of the coefficients out of the four c_p , c_n , e_p and e_n . These two equations can be used to replace $e_p = c_p p_1$ and $e_n = c_n n_1$. Where n_1 , p_1 is the equilibrium concentration when Fermi level is at the place of the trap level. Since RG center Now r_n and r_p can be written in terms of n_0 , p_0 , n_{T0} and p_{T0} . Note that we know n_{T0} etc from the Fermi Dirac-type distribution function. Now we make an **assumption** that c_p , etc coefficient remain same even in the non equilibrium but n_T would definitely change. Strictly this is the only assumption involved. Actually, there should not be any doubt that this constant should not depend on the carrier densities etc and hence should remain same even in non-equilibrium. Hence, it shouldn't really be called an assumption and should be strictly correct. Non-equilibrium n_T is not given by the Fermi-Dirac type distribution. People usually make an additional assumption of non-degenerate doping to simplify expressions. Then at steady state $r_n = r_p$ gives us non-equilibrium

n_T . Finally we obtain, for **non-degenerate semiconductors**,

$$r_n = r_p = \frac{np - n_i^2}{\tau_p(n + n_1) + \tau_n(p + p_1)}$$

. Where $\tau_n = 1/c_n/N_T$ and $\tau_p = 1/c_p/N_T$ are called the minority lifetimes because its implications under simplified conditions discussed below.

- **Note that lifetime is dependent on capture/emission coefficients and is inversely proportional to the trap density. And the defects/trap density is almost proportional to the doping density.** It remains constant till some doping density and after that simply increases linearly with doping density. Since the impurity density greatly depends on processing steps, usually its very difficult to predict the lifetime and varies from process to process. For τ sensitive devices people try to externally put measured amount of impurity (usually gold in Si) to control values of τ . On the other hand if very low recombination rate is needed then many “gettering” steps should be included. **The standard values of τ falls in three ranges - ms , 10 μ s and ns. Third values is obtained by diffusing Au in Si. Second values is typical value encountered. And long lifetimes as ms are obtained with very careful processing only.**
- Temperature dependence should be inbuilt in life time through emission/capture coefficients. (In classical theory life time is written as the reciprocal of capture area times thermal average velocity times trap density. So, it seems that the temperature dependence is actually coming through the thermal average velocity. So we would expect that as temperature increases the lifetime would reduce and relaxation rate would become faster. (More phonons - quantum mechanically). There are other empirical models also for including the **temperature dependence** straight away in the time constant.)
- There one more important issue involved with the RG-centers. Although the relationship is derived for steady state condition, it can be used even for the **transient analysis**. This kind of argument assumes that we are actually working in quasi-steady state and actually time variation is a sequence of steady states in which $r_n = r_p$ at every moment of time. If such a case is not valid then one cannot simply obtain n_T from steady state rather one needs to simultaneously solve a differential equation $dn_T/dt = r_n(t) - r_p(t)$. It should be simultaneously solved with other time varying equations. Note that when voltages and electric field varies with time then the trap levels should remain equidistant from band edges and as voltage moves the Fermi level either comes closer or goes farther representing that the probability that trap levels are filled varies with the voltage. Now if the time variation is very slow then we can assume it passes through a series of steady states and can calculate n_T at each instance of time.

5.2.1 Low Level Injection

Assuming a) $\delta n, \delta p \ll n_0$ in n-type. b) N_T^+ is very small and electric field is almost zero so that $\delta n \approx \delta p$. c) $E_T = E_i$ (so that $n_1 = p_1 = n_i$). d) lifetimes don't differ much. Under these

assumptions $R = \delta n / \tau_n$ (for p-type material and $R = \delta p / \tau_p$ for n-type material. **Note that for a single material in steady state we can not have two lifetimes because we are assuming $\delta n \approx \delta p$. In steady state if one electron goes off then one hole also has to go (because $\frac{\partial n_T}{\partial t} = 0$). This also tells us that if electrons are being injected into an infinitesimal volume then holes also have to be injected from somewhere).**

5.2.2 High Level Injection

$\delta n \approx \delta p \gg n_0$ and rest all the assumptions stay :- $R = \delta n / (\tau_n + \tau_p) = \delta p / (\tau_n + \tau_p)$

5.2.3 RG depletion

$n \ll n_1$ and simultaneously $p \ll p_1$. Note that by definition $n_1 p_1 = n_i^2$ and hence for RG-depletion region we should have $n_1 p_1 \ll n_i^2$. Note that in usual pn junction depletion region we have $p_0 n_0 = n_i^2$ in equilibrium although $n, p \ll (N_d - N_a)$ and in forward bias actually $pn > n_i^2$. Only in reverse bias one can treat the pn junction depletion region as RG-depletion region. We can show that in such a case $R = -\frac{n_i}{\tau_n + \tau_p}$. Which is actually a generation rate because we are continuously extracting carriers out of the depletion region so the recombination rate would be smaller than the generation rate giving us the net generation rate.

6 Surface Recombination

Surface states comes because of the change of periodicity of the material. People also refer to these as coming because of dangling bonds. These states behaves in a simmlar fashion as bulk traps (RG center does). Only difference is that the surface traps are never single. Bulk states, because they originate from a single type of impurity are single levels. Whereas surface states are spread all over the band gap. Note that one very important assumption that we frequently make is that the states themselves are **non-interacting**. What that emans is that particle exchange in-between states is not happening. This assumption is quite practical because surface states are spatially spread over the surface. And scattering processes are usually instantaneous in both space and time. And hence the rates of transition from one band to any of the trap states are additive because inter trap transitions are not possible because of physical separations.

The only significant difference between the two cases are the units. Note that n and p are still measured as cm^{-3} but r_n and r_p (its not a good idea to write them as $\frac{\partial n}{\partial t}$!) etc are measured as $cm^{-2}s^{-1}$. Whereas n_T is measured as cm^{-2} . e_n and e_p are measured as s^{-1} and c_n and c_p are measured as cm^3s^{-1} as previously. **(So the only difference is r_n, r_p and n_T, p_T . Hence r_n and r_p would be equated to the injected “current”.)** For a single level we would obtain exactly synonymous expression for surface recombination rate though $1/c_n N_T$ and $1/c_p N_T$ are measured in s/cm so instead of writing them as τ we write them as $1/s$ whre as is **surface recombination “speed”**. So in simplified situation we would expect the surface recombination rate to be written as $s_n \delta n$ which is speed times density which is equivalent to particle “current” which can then be equated to surface current.

6.1 Low Level Injection/Flat Band (E=0)

We need low level injection to make $n \approx n_0$ and we need a flat band condition near the surface to make $n_0 = N_d$ and $p_0 = N_a$. So these are now a system/material constant independent of bias or device structure (in depletion region in pn junction in equilibrium $n = n_0$ but n_0 is dependent on device structure). Under low level injection/flat band condition we can show that the conventional expression becomes $s_p \delta p$ for n-type material where s_p is a system dependent parameter and does not depend on the level of injection and excess carrier concentrations or position of quasi fermi levels etc. Also if multiple levels are involved, we can integrate the expression taking δp out of the integral. So integral still remains a system constant.

6.2 Depleted Surface

When $n \ll n_1$ and $p \ll p_1$ then again we can write surface recombination rate as $s_p \delta p$ with s_p as a system parameter.

Again lifetime would be dependent on state density and temperature. Surface rates also depend on processing steps and surface orientations. Also, again transient situations have to be carefully handled.

7 Excitons

Excitons introduces another level. So radiation coming out would be little lower frequency.

8 Auger/Impact Ionization

Its carrier carrier interaction. Two carriers collides, one loses all energy and falls into valance band other becomes more energetic.

9 Tunneling

10 Polarons

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