Session 14

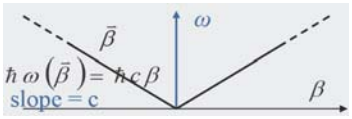
Note Title 11/13/2008

We discussed that photon emission/absorption process is much easier to understand in terms of a multi-particle electron-photon picture.

N−1 photon	N photon	N+1 photon
		$\varepsilon_2+(N+1)\hbar\omega$
	$\varepsilon_2+(N)\hbar\omega$	$\varepsilon_1+(N+1)\hbar\omega$
$\varepsilon_2+(N-1)\hbar\omega$	$\varepsilon_1+(N)\hbar\omega$	
$\varepsilon_1+(N-1)\hbar\omega$		

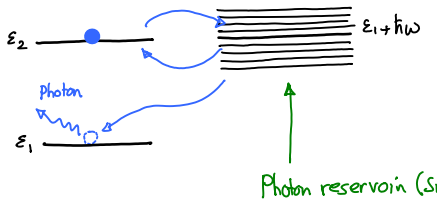
1 Photon state means having 1 photon at that frequency.
N photon state means having N photons at that frequency.
Note: for photons there is no exclusion principle.

Let's consider plane wave for the photon such as $\mathrm{Cos}(\vec{\beta}\cdot\vec{r}-\omega t)$.
Here β is the photon wavevector similar to k for the electron.
But here ω is a linear function of ω: $\omega = c\beta$ where
c is speed of light. (Compare with free electron $\omega = \frac{\hbar}{2m}k^2$)



Since β is continous (so is the frequency ω), the 1-level picture changes as:

This affects the photon emission from excited states.



→ This can be viewed similar to dissipation into a contact. So we want to calculate the rate at which the electron escapes when it's put in a state.

So we can use our Green's function formalism to derive the radiative lifetime of an electron. For the self-energy we have: $\Sigma = \tau g \tau^\dagger$ and to find the lifetime: $\frac{\hbar}{\tau_r} = \Gamma_1 = \tau a \tau^\dagger$. This is like transition from $|2,0\ \text{Photon}\rangle \to |1,1\ \text{Photon}\rangle$ where radiative lifetime is like another self-energy. τ_r is the escape rate of an electron from one state to another. So the broadening of the 0-photon state is:

$$\Gamma_1 = \tau a \tau^\dagger = \sum_{\beta} |\tau(\vec{\beta})|^2 \underbrace{2\pi\delta(E-\varepsilon_1-\hbar\omega)}_{\text{Photon reservoir spectral function}}$$

If we apply priodic boundary, we can convert the sum into integral:

$$\frac{\hbar}{\tau_r} = \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{\beta^2 d\beta \sin\theta\, d\theta d\phi}{8\pi^3} V |\tau(\beta)|^2 \times 2\pi\delta(\varepsilon_2-\varepsilon_1-\hbar\omega) \qquad (V \text{ is the volume})$$

$\beta = \frac{\omega}{c} \Rightarrow$

$$= \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{\omega^2 d\omega \sin\theta\, d\theta d\phi}{8\pi^3 c^3} V |\tau(\beta)|^2 \times 2\pi\delta(\varepsilon_2-\varepsilon_1-\hbar\omega)$$

$$= \int_0^\pi \int_0^{2\pi} \frac{\sin\theta\, d\theta d\phi}{8\pi^3 c^3} |\tau(\beta)|^2 \left(\frac{\varepsilon_2-\varepsilon_1}{\hbar}\right)^2 \times 2\pi V$$

we need to insert $\mathcal{T}$ now. $\mathcal{T}$ is the coupling between 0-photon and 1-photon state. So we must consider the potential that an electron feels due to one photon. The electric field of a single photon is:

Polarization vector

$$\vec{E} = \hat{v} E_0 \sin(\vec{\beta}\cdot\vec{r} - \omega t) \quad \text{where } \omega = c\beta$$

We want to relate E_0 in terms of photon energy. For this consider one photon with energy $\hbar\omega$. From electromagnetics, the total energy of one photon consists two part of electric and magnetic:

The average energy per unit volume: $$\frac{\mathcal{E}_{total}}{V} = \mathcal{E}_E^2 + \mathcal{E}_M^2 = \frac{1}{4}\epsilon_0 E_0^2 + \frac{1}{4}\frac{1}{\mu_0} B_0^2$$

Since the electric and magnetic parts are equal $\rightarrow$ $\mathcal{E}_{total} = V\frac{\epsilon_0}{2}E_0^2 = \frac{V}{2\mu_0}B_0^2 = \hbar\omega \rightarrow E_0 = \sqrt{\frac{2\hbar\omega}{\epsilon_0 V}}$

The vector potential can now be calculated from the well known relation: $\vec{E} = -\frac{\partial A}{\partial t}$ if $\vec{A} = A_0\hat{v}\cos(\beta\cdot r - \omega t) \rightarrow \vec{E} = -\hat{v}\underbrace{A_0\omega}_{E_0}\sin(\beta r - \omega t)$

$\rightarrow A_0 = \frac{E_0}{\omega} = \sqrt{\frac{2\hbar}{\omega\epsilon_0 V}}$ The vector potential created by a photon cannot be directly added to the Hamiltonian as a scalar potential v: $H = \frac{p^2}{2m} + V + \cancel{A}$. The EM vector potential $\vec{A}$ must be added to $\vec{p}$ which is a vector:

$H = \frac{(\vec{P} + e\vec{A})^2}{2m}$ To find the coupling we need to find how much H is changed by adding a photon:

$H = \frac{1}{2m}(\vec{P}+e\vec{A})\cdot(\vec{P}+e\vec{A}) = \frac{p^2}{2m} + \frac{e}{2m}(\vec{A}\cdot\vec{P} + \vec{P}\cdot\vec{A}) + \frac{e^2}{2m}\vec{A}\cdot\vec{A}$ Since A due to a photon is small, we can ignore quadratic term: $\vec{A}\cdot\vec{A} \simeq 0$

Note: $\vec{P}\cdot(\vec{A}\varphi) = -i\hbar\vec{\nabla}\cdot(\vec{A}\varphi) = -i\hbar\varphi\underbrace{\vec{\nabla}\cdot\vec{A}}_{=0} - i\hbar\vec{A}\cdot\vec{\nabla}\varphi = \vec{A}\cdot(-i\hbar\vec{\nabla}\varphi) = \vec{A}\cdot(P\varphi) \Rightarrow \vec{A}\cdot\vec{P} = \vec{P}\cdot\vec{A} \Rightarrow H = \frac{p^2}{2m} + \frac{e}{m}(\vec{A}\cdot\vec{P})$

$\vec{A} = \hat{v}A_0\cos(\vec{\beta}\cdot\vec{r} - \omega t) \rightarrow H = \frac{p^2}{2m} + \frac{e}{m}(\vec{A}\cdot\vec{P}) = \frac{p^2}{2m} + \frac{eA_0}{2m}\vec{P}\cdot\hat{v}\left(\underbrace{e^{i\beta\cdot r}e^{-i\omega t}}_{\text{absorption}} + \underbrace{e^{-i\beta\cdot r}e^{i\omega t}}_{\text{emission}}\right)$ $\quad i\hbar\frac{\partial}{\partial t}\{\psi\} = H\{\psi\} \rightarrow$

$$i\hbar\frac{\partial}{\partial t}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix} = \begin{bmatrix}\mathcal{E}_1 & K_{em}\\ K_{abs} & \mathcal{E}_2\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$$

For the matrix element $K_{abs/em}$, we have $K_{abs/em} = \langle 1|\frac{e}{m}\vec{A}\cdot\vec{P}|2\rangle = \frac{eA_0}{2m}\int d^3r\,\varphi_1^*(\vec{P}\cdot\hat{v}\,e^{\pm i\vec{\beta}\cdot\vec{r}})\varphi_2$

$e^{\pm i\vec{\beta}\cdot\vec{r}}$ is often ignored when we are at the atomic scale as φ changes on the scale of Angstrom but $\vec{\beta}$ changes only on the scale of micron.

$$\rightarrow K_{abs/em} = \frac{eA_0}{2m}\hat{v}\cdot\underbrace{\int d^3r\,\varphi_1^*\vec{P}\varphi_2}_{\vec{P}} = \frac{eA_0}{2m}\hat{v}\cdot\vec{P}$$

Example Emission from the degenerate hydrogen $2S, 2p_x, 2p_y, 2p_z$ levels to $1s$ level.

$$\varphi_{1s} = \frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0};\quad \varphi_{2s} = \frac{1}{\sqrt{32\pi a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0};\quad \varphi_{2p_x} = \frac{1}{\sqrt{16\pi a_0^3}}\left(\frac{x}{a_0}\right)e^{-x/2a_0},\quad \varphi_{2p_y} = \frac{1}{\sqrt{16\pi a_0^3}}\left(\frac{y}{a_0}\right)e^{-y/2a_0},\quad \varphi_{2p_z} = \frac{1}{\sqrt{16\pi a_0^3}}\left(\frac{z}{a_0}\right)e^{-z/2a_0}$$

$\vec{P}$ for $2S \rightarrow 1S$ is: $\vec{P} = \int d\vec{r}\,\varphi_{1s}^*(-i\hbar\nabla)\varphi_{2s} = -i\hbar\int dr\,\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\left(\frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\cancel{\frac{\partial}{\partial\theta}}^{0}\hat{\theta} + \frac{1}{r\sin\theta}\cancel{\frac{\partial}{\partial\varphi}}^{0}\hat{\varphi}\right)\frac{1}{\sqrt{32\pi a_0^3}}\left(2-\frac{r}{a_0}\right)e^{-r/2a_0}$

$= \hat{r} \times \text{Const.}$ which is isotropic.

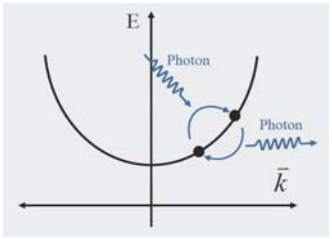
For $2p_x \rightarrow 1S$: $\vec{P} = \int d\vec{r}\,\frac{1}{\sqrt{\pi a_0^3}}e^{-r/a_0}\left(\hat{x}\frac{\partial}{\partial x} + \hat{y}\frac{\partial}{\partial y} + \hat{z}\frac{\partial}{\partial z}\right)\frac{1}{\sqrt{16\pi a_0^3}}\left(\frac{x}{a_0}\right)e^{-x/2a_0} = \hat{x} \times \text{Const.}$ which is polarized in $\hat{x}$ direction.

Thus:

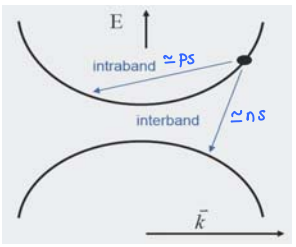
Transition	$\vec{P}$	
$2S \rightarrow 1S$	$\hat{r}$	isotropic. Emits in all directions.
$2p_x \rightarrow 1S$	$\hat{x}$	emits in the (y,z) plane
$2p_y \rightarrow 1S$	$\hat{y}$	emits in the (x,z) plane
$2p_z \rightarrow 1S$	$\hat{z}$	emits in the (x,y) plane

In a real Hydrogen atom, an electron spreads out uniformly amongst the $2p_x, 2p_y$ and $2p_z$. This results in isotropic emission. Also note that s and p are not actually degenerate because there is a coupling between the $1s$ and $(2p_x, 2p_y, 2p_z)$ levels whose resulting self energy creates a small energy shift between the s and p levels.

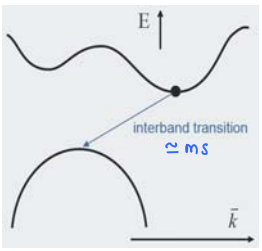
We can also investigate transitions between two extended states inside an energy band. These are often called intraband transitions.



Transitions



In Silicon



In a simple form of assuming plain wave initial and final wavefunction we have:

$$K_{abs/em} = \int d\vec{r}\; e^{\mp i\vec{\beta}.\vec{r}}\; e^{-i\vec{k}'.\vec{r}}\; x\,(\vec{p}.\hat{v})\, e^{i\vec{k}.\vec{r}}$$ which is non-zero iff $k-k'\pm\beta=0$ (because $\int e^{i(\vec{k}-\vec{k}'\pm\vec{\beta}).\vec{r}}\, dr$ is zero otherwise)

Also from broadening $\Gamma = \frac{\hbar}{\tau_r} = \sum |K|^2 \delta(\mathcal{E}_k - \mathcal{E}_{k'} \pm \hbar\omega_\beta)$ the delta function is non-zero if: $\mathcal{E}_{k'} = \mathcal{E}_k \pm \hbar\omega_{\vec{\beta}}$

For emission $\mathcal{E}_{k'} = \mathcal{E}_k - \hbar\omega_\beta$ and for absorption $\mathcal{E}_{k'} = \mathcal{E}_k + \hbar\omega_\beta$.

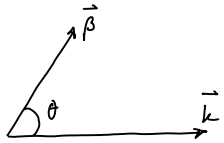
Interband transitions usually take nanoseconds whereas intraband transitions could take picoseconds. In Silicon, however, interband transitions take as long as a millisecond. This is basically because the photon wavevector $\vec{\beta}$ required to satisfy $\vec{k}_f = \vec{k} - \vec{\beta}$ is very large. Since $\vec{\beta}$ is often very small for light the coupling between non-vertical transition is weak and hence τ is large. Note that vertical transitions are not allowed in Silicon because the valance band is filled directly below the bottom of the conduction band edge.

Intraband transition lifetimes are defined as:

$$\text{Emission:}\quad \Gamma = \frac{\hbar}{\tau} = \sum_\beta \left[(N_\beta + 1) 2\pi |K|^2 \delta\left(\mathcal{E}(\vec{k}) - \mathcal{E}(\vec{k}-\vec{\beta}) - \hbar\omega(\vec{\beta})\right)\right]$$

$$\text{Absorption:}\quad \Gamma = \frac{\hbar}{\tau} = \sum_\beta \left[(N_\beta) 2\pi |K|^2 \delta\left(\mathcal{E}(\vec{k}) - \mathcal{E}(\vec{k}+\vec{\beta}) + \hbar\omega(\vec{\beta})\right)\right]$$

For emission we require: $\mathcal{E}(\vec{k}) - \mathcal{E}(\vec{k}-\vec{\beta}) - \hbar\omega(\vec{\beta}) = 0 \Rightarrow \frac{\hbar^2}{2m}k^2 - \frac{\hbar^2}{2m}\underbrace{(k^2+\beta^2-2k\beta\cos\theta)}_{(\vec{k}-\vec{\beta}).(\vec{k}-\vec{\beta})} - \hbar c\beta = 0$



$$\rightarrow \cos\theta = \frac{\hbar c\beta + \hbar\beta^2/2m}{\hbar^2 k\beta/m} = \underbrace{\frac{c}{\hbar k/m}}_{\text{electron velocity}} + \frac{\beta}{2k}$$ (photon/phonon velocity)

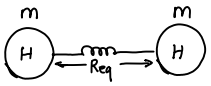
$\rightarrow$ Since $\cos\theta \le 1$ emission is possible only if the electron velocity $\frac{\hbar k}{m}$ exceeds the photon/phonon velocity.

Usually this is called Cerenkov radiation. $\cos\theta$ gives the cerenkov cone for phonons/photons. This is exactly the same as the sonic boom produced by jets.

Same result can be obtained for absorption, with only a sign change results.

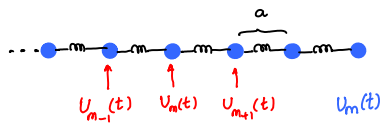
Phonons

Phonons are the lattice vibrations which propagate through a solid or molecule (sound). For example Hydrogen molecules vibrate around an equilibrium bond distance, R_{eq}, with an intensity proportional to temperature similar to a spring mass system.



$\rightarrow$ Resonant frequency: $\omega = \sqrt{\frac{k}{m}}$

Phonons are the quantized energy exchanged between vibrating masses. We can extend this to the infinite 1-D lattice of the form:



$U_m(t)$ is the displacement of the m^{th} atom from its equilibrium position at time t.

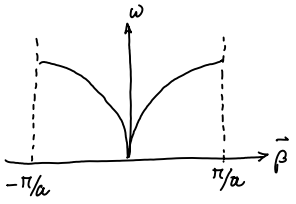
$$m\frac{d^2U_m}{dt^2} = k(U_{m+1}-U_m) - k(U_m-U_{m-1})$$ Assuming periodic form like sine and cosine solutions for $U_m(t)$ we have: $\frac{d^2U_m(t)}{dt^2} = -\omega^2 U_m$

Or $-\omega^2 U_m = \frac{k}{m}(U_{m+1} - 2U_m + U_{m-1})$ We can write this in a matrix form:

$$\omega^2\begin{bmatrix}U_1\\U_2\\U_3\\\vdots\end{bmatrix} = \frac{k}{m}\begin{bmatrix}2 & -1 & & & -1\\ -1 & 2 & -1 & 0 & \\ & -1 & 2 & -1 & \\ & 0 & \ddots & \ddots & \ddots\\ -1 & & & & \end{bmatrix}\begin{bmatrix}U_1\\U_2\\U_3\\\vdots\end{bmatrix}$$

Taking advantage of matrix periodicity for phonon $\vec{\beta}$, we may use the ansatz: $U_m = U_0 e^{\pm i\beta a}$

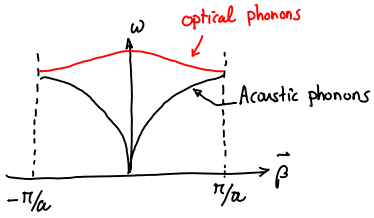
$$\rightarrow \omega^2 = \frac{2k}{m}(1-\cos\beta a) = 2\left(\frac{2k}{m}\right)\sin^2\left(\frac{\beta a}{2}\right) \rightarrow \omega = \sqrt{\frac{k}{m}}\,2\sin\frac{\beta a}{2}$$



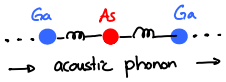
Around the origin the dispersion curve is often approximated linearly:

$$\omega = \sqrt{\frac{k}{m}}\,a\beta$$

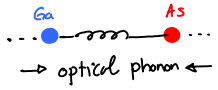
This is called acoustic phonon. In semiconductors another phonon brach may also exist which is called optical phonon. The reason it is called optical phonon is because if we shine light on the material, these phonons are excited.



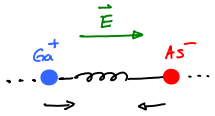
Acoustic phonons propagate in one direction



Optical phonons propagate in opposite direction



This is because at presence of electric field $\vec{E}$ of a photon, which is almost uniform on an atomic scale, positive and negative ions respond oppositely:

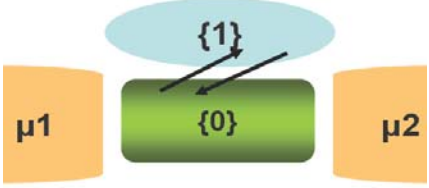


Scattering viewed as a contact

We can view the incoherent process as an additional contact. For example for the case of scattering with phonons, the channel remains at equilibrium where no phonon is generated in the channel. Instead they are generated in this additional contact. This is a virtual contact, hence, doesn't have a meaningful Fermi function. But we assume a chemical potential μ_s and impose the condition that there must not be a net current between the channel and this virtual contact.

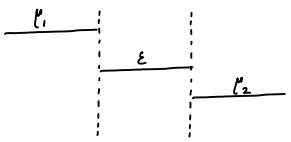
Note:

Coherent transport: electron transport in the channel doesn't affect anything in the channel, such as no phonon is emitted or absorbed. Impurity scattering is an example as the impurity ion doesn't vibrate or get deflected when it scatters an electron.



Incoherent transport: The surrounding is affected by the electron transport. In other words the state of the system changes by electron transport.

We now investigate current flow through a device having multiple contacts.



One level device: $I_1 = \int dE\, D(E) \frac{\gamma_1}{\hbar} (f_1 - N)$

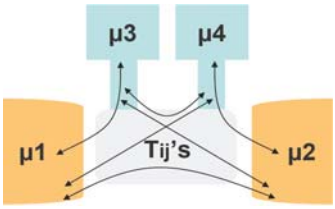
Multi-level device: $I_1 = \int dE \left\{ \text{Trace}[\Gamma_1 A] f_1 - \text{Trace}[\Gamma_1 G^n] \right\} = \int dE\, I_1(E)$

We may also write the current using the transmission as: $I(E) = \text{Trace}\left(\Gamma_i G \Gamma_j G^\dagger\right)(f_i - f_j)$

Büttiker introduced the following relation for the current in multiple contact devices: $I_i = \sum_j T_{ij}(E)(f_i - f_j)$

For a 4 terminal device the transmission is a 4 by 4 matrix:

$$\begin{pmatrix} I_1 \\ I_2 \\ I_3 \\ I_4 \end{pmatrix} = \begin{pmatrix} (T_{12}+T_{13}+T_{14}) & -T_{12} & -T_{13} & -T_{14} \\ -T_{21} & (T_{21}+T_{23}+T_{24}) & -T_{23} & -T_{24} \\ -T_{31} & -T_{32} & (T_{31}+T_{32}+T_{34}) & -T_{34} \\ -T_{41} & -T_{42} & T_{43} & (T_{41}+T_{42}+T_{43}) \end{pmatrix} \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \end{pmatrix}$$

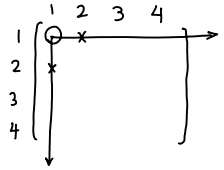


Because currents follow Kirchoff's law too, these are actually only three independent equations.

Since 3 & 4 are virtual contact $I_3 = I_4 = 0$. We can also set a reference for the voltage by choosing $\mu_2 = 0$

μ_1 is also given as the input voltage. Hence we are left with three equations and three unknows which are I_1, μ_3, and μ_4.

We can prove an interesting result on transmission matrix called the sum rule: Sum of all terms in row i or column i is $\text{Trace}(\Gamma_i A)$.



$\sum_j T_{ij} = \text{Trace}(\Gamma_i A)$

$\sum_j T_{ji} = \text{Trace}(\Gamma_i A)$

Note:

$G = (EI - H - \Sigma)^{-1}$ $\quad \Gamma = \Gamma_1 + \Gamma_2 + \Gamma_3 + \Gamma_4$

$A \equiv i(G - G^\dagger) = G\Gamma G^\dagger = G^\dagger \Gamma G$

(definition) (proved)

Proof: $T_{ij} = \text{Trace}\left(\Gamma_i G \Gamma_j G^\dagger\right)$

$$\sum_j T_{ij} = \sum_j \text{Trace}\left(\Gamma_i G \Gamma_j G^\dagger\right) = \text{Trace}\left(\Gamma_i \underbrace{G\Gamma G^\dagger}_{A}\right) = \text{Trace}(\Gamma_i A)$$

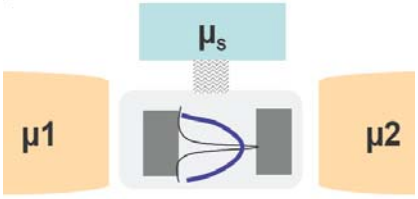
$$\sum_j T_{ji} = \sum_j \text{Trace}\left(\Gamma_j G \Gamma_i G^\dagger\right) = \text{Trace}\left(\Gamma G \Gamma_i G^\dagger\right) = \text{Trace}\left(\Gamma_i \underbrace{G\Gamma G^\dagger}_{A}\right) = \text{Trace}(\Gamma_i A)$$

Note that, however, $T_{12} \neq T_{21}$ in general. For instance a device in magnetic field is not symmetric for when the current changes direction.

In-scattering:

Consider a multiterminal device which has a chemical potential μ_s that adjusts itself such that there is no current across it: $\Gamma = \Gamma_1 + \Gamma_2 + \Gamma_s$ and $\Sigma = \Sigma_1 + \Sigma_2 + \Sigma_s$

To find the equation for current let's start with the electron density:



$$G^n(E) = (G\Gamma_1 G^\dagger) f_1 + (G\Gamma_2 G^\dagger) f_2 + (G\Gamma_s G^\dagger) f_s$$

In compact form: $G^n = G\Sigma^{in} G^\dagger$

$$\Sigma^{in} = \Gamma_1 f_1 + \Gamma_2 f_2 + \cancel{\Gamma_s f_s}$$

$\Sigma^{in}_s(E) = D_0 G^n(E)$ → we can modify this equation to compensate for the fact that electrons are coming in from higher energy and emit a photon. So: $\Sigma^{in}_s(E) = D_0 G^n(E + \hbar\omega)$

We can also include the absorption process to get: $\Sigma^{in}_s(E) = D_0(N+1) G^n(E + \hbar\omega) + D_0 N G^n(E - \hbar\omega)$