

## In This Lecture:

- **Semiconductor Linear Optics: General Absorption, Emission Expressions**

# The Electromagnetic Field [SI Units in action]

As you know, the machinery of QM works with *potentials*:



$$\vec{E}(\vec{r}, t) = -\frac{\partial \vec{A}(\vec{r}, t)}{\partial t} - \vec{\nabla} \phi(\vec{r}, t),$$

$$\vec{B}(\vec{r}, t) = \vec{\nabla} \times \vec{A}(\vec{r}, t).$$

We shall work in the Coulomb gauge:

$$\vec{\nabla} \cdot \vec{A}(\vec{r}, t) = 0,$$

$$\phi(\vec{r}, t) = \frac{1}{4\pi\epsilon} \int d^3r' \frac{\rho(\vec{r}', t)}{|\vec{r} - \vec{r}'|}.$$

However, the effect of the optical (EM) field is to cause certain transitions (interband, intraband) creating at most e-h pairs, therefore the *local* charge neutrality is always preserved,

$$\text{i.e., } \rho(\vec{r}, t) = 0 \Rightarrow \phi(\vec{r}, t) = 0.$$

$$\text{So, } \vec{E}(\vec{r}, t) = -\frac{\partial \vec{A}(\vec{r}, t)}{\partial t}.$$

Assume a monochromatic planewave EM field:

$$\vec{A}(\vec{r}, t) = \hat{e} A_0 \cos(\vec{k}_{op} \cdot \vec{r} - \omega t) \Rightarrow \vec{E}(\vec{r}, t) = -\hat{e} \omega A_0 \sin(\vec{k}_{op} \cdot \vec{r} - \omega t).$$

The associated optical intensity is given by:

$$I = \left\langle \left\langle \vec{S}(\vec{r}, t) \right\rangle \right\rangle = \left\langle \left\langle \frac{\vec{E} \times \vec{B}}{\mu_0} \right\rangle \right\rangle = \frac{n_r c \epsilon_0 \omega^2 A_0^2}{2}.$$



In the presence of EM field the canonical momentum operator,  $\vec{p} = -i\hbar\vec{\nabla}$  of an electron ( $e < 0$ ) is replaced by the kinetic momentum,  $\vec{p} \rightarrow \vec{p} - e\vec{A}$ , so that,

$$H = \frac{1}{2m_0} (\vec{p} - e\vec{A})^2 + e\phi + V(\vec{r}),$$

$$= \frac{p^2}{2m_0} - \frac{e}{2m_0} (\vec{p} \cdot \vec{A} + \vec{A} \cdot \vec{p}) + \frac{e^2}{2m_0} A^2 + e\phi + V(\vec{r}),$$

Local charge neutrality +  
Coulomb Gauge

Note that,  $\frac{e}{2m_0} \vec{p} \cdot \vec{A} = e \frac{\vec{A} \cdot \vec{p}}{2m_0} - i \frac{e\hbar}{2m_0} \vec{\nabla} \cdot \vec{A}$ ,

Coulomb Gauge

$$H = \frac{p^2}{2m_0} - \frac{e}{m_0} \vec{A} \cdot \vec{p} + \frac{e^2}{2m_0} A^2 + V(\vec{r}),$$

Compare their typical  
relative magnitudes


For most practical optical field intensities:  $|e\vec{A}| \ll |\vec{p}| \approx \frac{\hbar\pi}{a_0}$ ,

so that  $\frac{eA}{p} \sim 10^{-5}$  for a 1 W/cm<sup>2</sup> photon density of a 1 eV energy illumination.

Thus neglecting the  $A^2$  term leaves us with

$$H = \underbrace{\frac{p^2}{2m_0} + V(\vec{r})}_{H_0} - \underbrace{\frac{e}{m_0} \vec{A} \cdot \vec{p}}_{H'(t)},$$

Radiation perturbation  
(time-dependent)



The nicety of the radiation perturbation is that the matrix elements of the perturbation already takes part in the  $\vec{k} \cdot \vec{p}$  band structure techniques.

**Terminology:** The result we have obtained is also termed as the so-called **velocity gauge**. An alternative expression follows in the next page. However, in the rest of our analysis we shall carry on from the expression on this page.

## Electric Dipole Approximation (Length Gauge)

Note that the Hamiltonian as expressed in the previous page depends on the specific gauge (Coulomb) we have chosen. Another form for the radiation perturbation that is in common use is given by:

$$H'(t) = -e\vec{r} \cdot \vec{E}(\vec{r}, t) \quad \text{.....} \rightarrow \text{Electric dipole approximation}$$

It can be shown that in the long wavelength of the EM wave ( $k_{op}$  small) the electric dipole approximation agrees with the  $\mathbf{A} \cdot \mathbf{p}$  results. As a matter of fact, even though  $\mathbf{r}$  operator becomes problematic for infinite solids, it can be handled and moreover, the  $\mathbf{r} \cdot \mathbf{E}$  expression has its own virtues from computational perspectives of the linear and nonlinear susceptibilities; see, for instance Aversa-Sipe PRB 52 14636 (1995).

## Absorption, Spontaneous/Stimulated Emission

Due to time-dependent perturbation, we need to make use of Fermi's golden rule. The resultant transition rate among the unperturbed initial/final states is given by

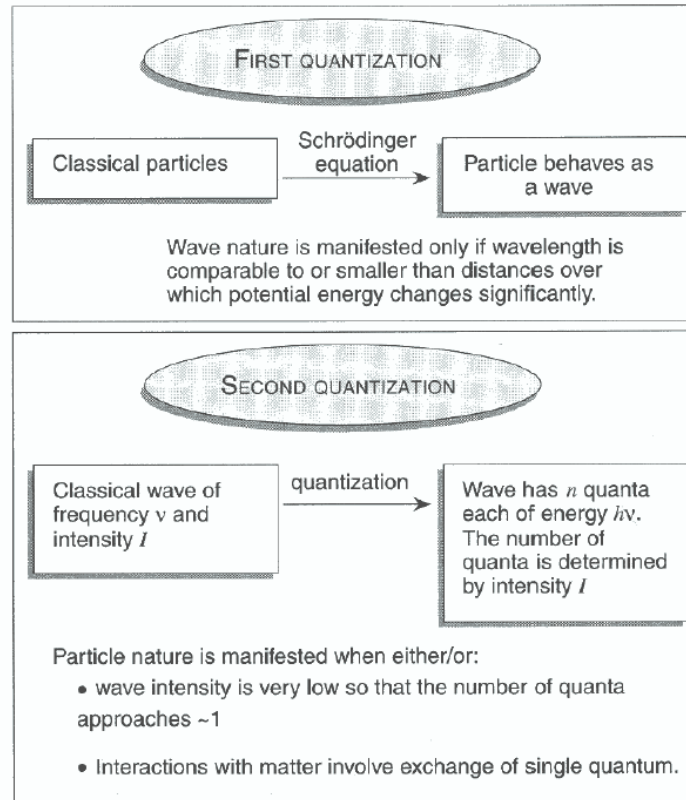
$$W(i) = \frac{2\pi}{\hbar} \sum_f |\langle f | H' | i \rangle|^2 \delta(E_f - E_i \mp \hbar\omega) \quad H' = -\frac{e}{m_0} \vec{A} \cdot \vec{p}$$

We need to switch (temporarily) from our semiclassical approach to the photon picture; (i.e., second quantized EM field). The aim is to capture the stimulated/spontaneous emission processes.

Interestingly, the relation between absorption and stim/spon emission was first proposed by Einstein w/o even invoking standard QM, leading to Einstein's  $A$  and  $B$  coefficients; see Chuang for this alternative route.

$$\begin{array}{ccc} & \leftarrow \langle i \rangle = |k_i, n_{ph}\rangle & \rightarrow \\ \text{Absorption: } |f\rangle = |k_f, n_{ph} - 1\rangle, & & \text{Emission: } |f\rangle = |k_f, n_{ph} + 1\rangle \end{array}$$

# Second Quantization



**Figure 6.13:** A conceptual picture of first and second quantization. The second quantization allows us to describe classical waves as quantum mechanical particles.



When second-quantized, the vector potential's amplitude becomes:

$$A_0 = \sqrt{\frac{\hbar}{2\omega\epsilon V}} (b^\dagger + b)$$

Photon creation/annihilation operators;  
monochromatic (mode index suppressed)

**Properties:**

$$b^\dagger |n_{ph}\rangle = \sqrt{n_{ph} + 1} |n_{ph} + 1\rangle,$$

$$b |n_{ph}\rangle = \sqrt{n_{ph}} |n_{ph} - 1\rangle$$

Absorption:

$$\begin{aligned} \langle i | \bar{A} \cdot \bar{\nabla} | f \rangle &= \sqrt{\frac{\hbar}{2\omega\epsilon}} \langle k_f, n_{ph} - 1 | (b^\dagger + b) \hat{e} \cdot \bar{\nabla} | k_i, n_{ph} \rangle \\ &= \sqrt{\frac{\hbar n_{ph}}{2\omega\epsilon}} \langle k_f | \hat{e} \cdot \bar{\nabla} | k_i \rangle \end{aligned}$$

Emission:

$$\begin{aligned} \langle i | \bar{A} \cdot \bar{\nabla} | f \rangle &= \sqrt{\frac{\hbar}{2\omega\epsilon}} \langle k_f, n_{ph} + 1 | (b^\dagger + b) \hat{e} \cdot \bar{\nabla} | k_i, n_{ph} \rangle \\ &= \sqrt{\frac{\hbar(n_{ph} + 1)}{2\omega\epsilon}} \langle k_f | \hat{e} \cdot \bar{\nabla} | k_i \rangle \end{aligned}$$

From now on we shall treat absorption and emission separately because of the different settings of the processes.

For the absorption, assume an incoming photon with momentum  $\hbar k_{op}$  and energy  $\hbar\omega$  to be absorbed by the se/c via all possible initial/final states as long as energy/momentum conservations are satisfied.

$$W_{abs} = \frac{2\pi}{\hbar} \frac{e^2}{m_0^2} \left( \frac{\hbar n_{ph}}{2\omega\mathcal{E}} \right) \sum_{\text{initial/final electron states}} \left| \int \psi_f^* \hat{e} \cdot \vec{p} e^{i\vec{k}_{op} \cdot \vec{r}} \psi_i d^3r \right|^2 \delta(E_i - E_f + \hbar\omega)$$

Absorption rate per unit volume of se/c
Joint DOS
Polarization dependence of absorption is in this matrix element

# Absorption Rate $\rightarrow$ Absorption Coefficient

Start with the continuity equation for photons:

$$\frac{dn_{ph}}{dt} = \underbrace{\frac{\partial n_{ph}}{\partial t}}_{\substack{\text{Assume only absorption} \\ \text{to be dominant} \\ \frac{\partial n_{ph}}{\partial t} = W_{abs}}} + \underbrace{\vec{\nabla} \cdot \vec{J}_{ph}}_{\substack{\text{Assume 1D (say, along } x) \\ \text{propagation (plane wave)} \\ \frac{\partial (vn_{ph})}{\partial x}}}$$

In the steady state  $d/dt \rightarrow 0$  and the form that defines the absorption coefficient  $\alpha$  is given by

$$n_{ph}(x) = n_0 e^{-\alpha x}$$

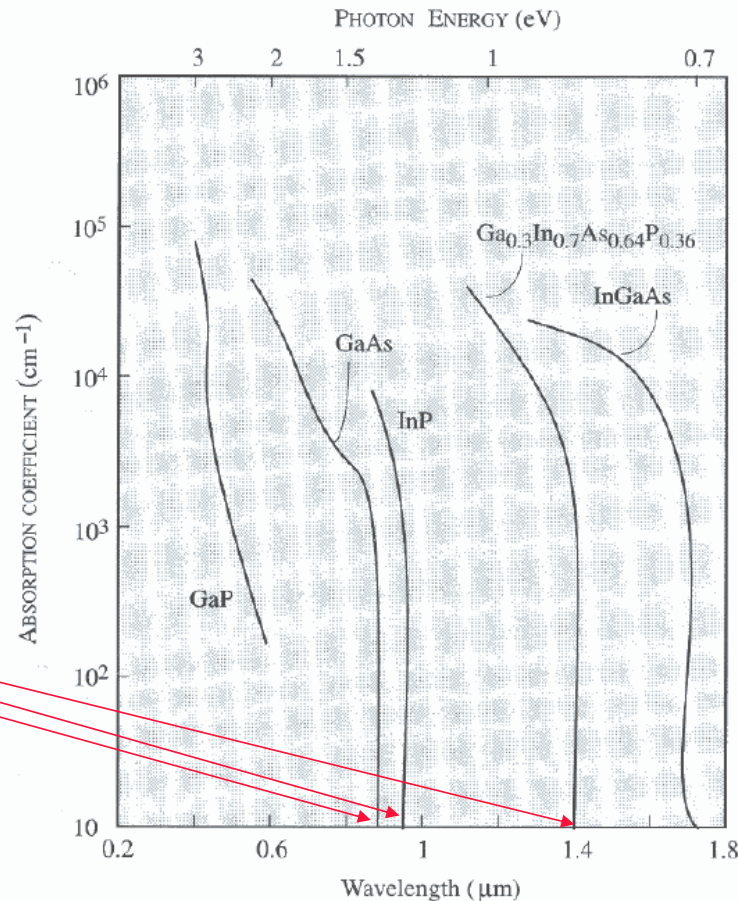
Inserting this form into the continuity equation yields:

$$W_{abs} = \alpha \underbrace{vn_{ph}}_{\substack{\text{speed of light in this se/c}}} \quad \text{or} \quad \alpha = \frac{W_{abs}}{vn_{ph}}$$

# Absorption Coefficient of Some se/c

It is the absorption coefficient that is provided in the literature

Photons with an energy higher than the bandgap are strongly absorbed causing interband transitions of the VB electrons



## Kramers-Kronig Relations (KKR)

- KKR is based on the principle of **causality**: the response to an applied field such as the polarization (effect) cannot precede the applied field (cause)
- Mathematically, it follows from the integral representation of the step function (Heaviside fn) over the complex plane

Complex Dielectric Function

$$\epsilon(\omega) = \epsilon'(\omega) + i\epsilon''(\omega)$$

Real and imaginary parts of diel. fn. are not independent!

$$\epsilon'(\omega) - \epsilon_0 = \frac{2}{\pi} P \left( \int_0^{\infty} \frac{\omega' \epsilon''(\omega')}{\omega'^2 - \omega^2} d\omega' \right),$$

$$\epsilon''(\omega) = -\frac{2\omega}{\pi} P \left( \int_0^{\infty} \frac{\epsilon'(\omega') - \epsilon_0}{\omega'^2 - \omega^2} d\omega' \right)$$

can also be written as Hilbert transform pairs

For a non-magnetic ( $\mu_0$ ) homogeneous isotropic medium (such as bulk cubic xtal) the wave vector of an EM wave is given by:

$$k(\omega) = \beta + i\alpha$$

$$k(\omega) = \omega \sqrt{\mu_0 \epsilon(\omega)}$$

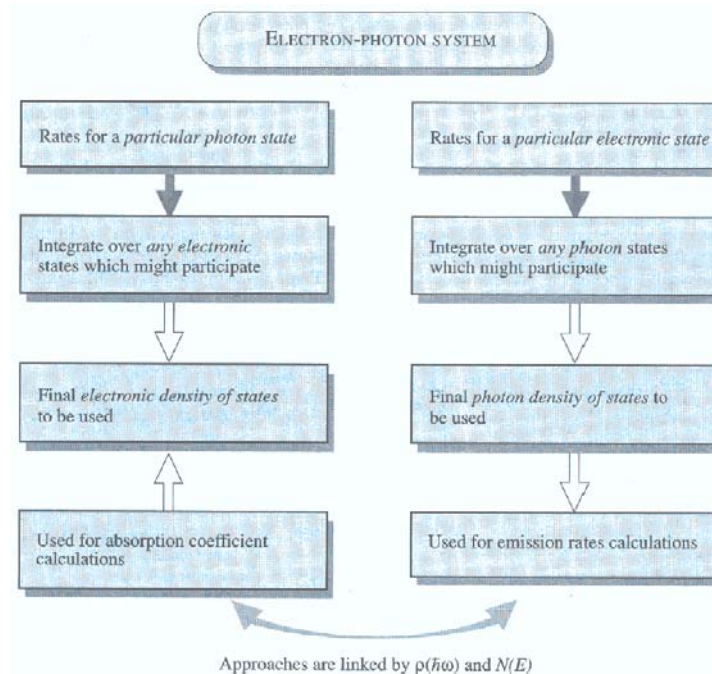
$$k(\omega) = \frac{\omega}{c} \sqrt{\epsilon_r(\omega)}; \text{ where } \epsilon_r = \epsilon / \epsilon_0$$

$$\beta^2 - \alpha^2 = \left(\frac{\omega}{c}\right)^2 \epsilon'_r$$

$$2\alpha\beta = \left(\frac{\omega}{c}\right)^2 \epsilon''_r \implies \text{Absorption coef. is proportional to the imaginary part of the diel. fn. which in turn effects on the index of refraction through the KKR}$$

## Absorption vs Emission Rates

In the absorption expression, if we are considering the rate at which a photon is absorbed, this involves summing over any possible electronic levels, as long as the energy conservation is obeyed. One may instead, be interested in the problem where a single electron with (xtal) momentum  $k_i$  is scattered into a final state with momentum  $k_f$ . In this case the final states sum would be over all photon states that can cause such transitions and would involve photon density of states. These two approaches are illustrated in the following figure.



## Continue with the Emission Rate

The rate of an electron  $\hbar k_i$  to emit any photon and reach a state with momentum  $\hbar k_f$  is given by

$$W_{em} = \frac{2\pi e^2}{\hbar m_0^2} \left( \frac{\hbar(n_{ph} + 1)}{2\omega\mathcal{E}} \right) \sum_{\text{photon states}} \left| \int \psi_f^* \hat{e} \cdot \bar{p} e^{-i\bar{k}_{op} \cdot \bar{r}} \psi_i d^3r \right|^2 \delta(E_i - E_f - \hbar\omega)$$

Notice that the emission term can be rewritten as stimulated and spontaneous emission terms as

$$W_{em} = W_{st} + W_{spon}$$

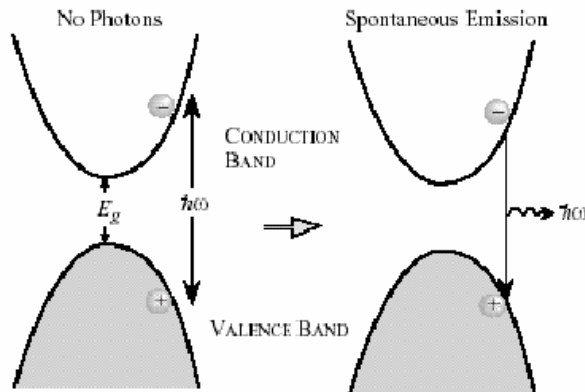
$$W_{st} = \frac{2\pi e^2}{\hbar m_0^2} \frac{\hbar n_{ph}}{2\omega\mathcal{E}} \sum_{\text{photon states}} \left| \int \psi_f^* \hat{e} \cdot \bar{p} e^{-i\bar{k}_{op} \cdot \bar{r}} \psi_i d^3r \right|^2 \delta(E_i - E_f - \hbar\omega)$$

$$W_{spon} = \frac{2\pi e^2}{\hbar m_0^2} \frac{\hbar}{2\omega\mathcal{E}} \sum_{\text{photon states}} \left| \int \psi_f^* e^{-i\bar{k}_{op} \cdot \bar{r}} \psi_i d^3r \right|^2 \delta(E_i - E_f - \hbar\omega)$$

# Spontaneous vs Stimulated Emission

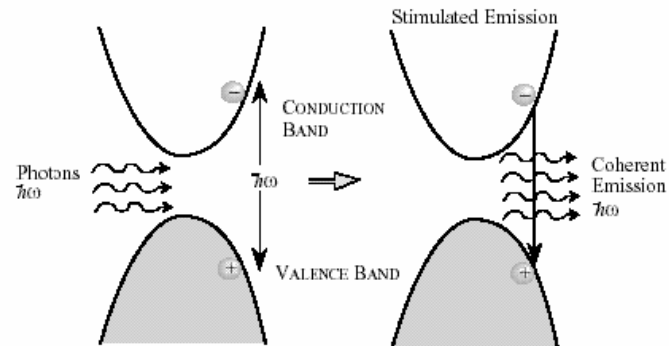
The stimulated emission is due to the initial photons present in the system and the emitted photons maintain phase coherence with the initial photons. The spontaneous emission comes from the perturbations due to the vacuum state (i.e.,  $n_{ph} = 0$ ) energy fluctuations and the emitted photons are incoherent with no phase relationship. The difference between these two kinds of processes is the key to understanding the differences between a light emitting diode and the laser diode

## Spontaneous em.



- SPONTANEOUS EMISSION: Responsible for light emission in LEDs
- Electron-hole recombination in the absence of photons
  - Outcoming photons are incoherent, i.e. have random phases
  - Electron-hole recombination lifetime is limited by  $\sim 1$  ns

## Stimulated em.



STIMULATED EMISSION: Responsible for light emission in laser diodes

- Electron-hole recombination in the presence of other photons
- Photons produced are coherent, i.e. have the same phase
- Electron-hole recombination lifetime is

$$\frac{1}{\tau_{stim}} = \frac{n_{ph}}{\tau_{spont}}$$

$n_{ph}$ : photon number