Optics + Semiconductors: How do we start?

1. Classical treatment of charge in an optical (electric) field – oscillator model

2. Quantum mechanical treatment of an atom in a classical field

3. Semiconductors: bands instead discrete levels

4. Nanostructures (quantum wells, quantum wires, quantum dots)

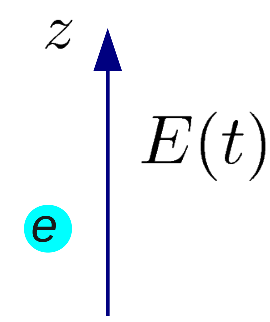
Rich optical properties due to many body environment

Role of lattice vibrations (phonons), Coulomb interactions, confinement, etc.

1. Classical treatment of charge in an optical field:
The Lorentz oscillator model

Lorentz Oscillator Model

- Classical treatment of a bound electron in an electric field



$$m_0 \frac{d^2 x}{dt^2} = -m_0 \omega_0^2 x - 2 m_0 \gamma \frac{dx}{dt} - eE(t)$$

Harmonic potential

Damping

$$= E_0 \cos(\omega t)$$
$$= \mathrm{Re}[E_0 e^{-i\omega t}]$$

- Ansatz $\quad x(t) = x(\omega) e^{-i\omega t}$

$$m_0(\omega^2 + i2\gamma\omega - \omega_0^2) x(\omega) = eE(\omega)$$

- Polarization $\quad P = n_0 d = -n_0 e x$

$$P(\omega) = -\frac{n_0 e^2}{m_0} \frac{1}{\omega^2 + i2\gamma\omega - \omega_0^2} E(\omega)$$

Lorentz Oscillator Model

- Optical susceptibility $\chi(\omega) = P(\omega)/E(\omega)$

$$\boxed{\chi(\omega) = -\frac{n_0 e^2}{2m_0\omega_0'}\left(\frac{1}{\omega - \omega_0' + i\gamma} - \frac{1}{\omega + \omega_0' + i\gamma}\right)}$$

$$\omega_0' = \sqrt{\omega_0^2 - \gamma^2}$$

- Optical dielectric function

$$D(\omega) = E(\omega) + 4\pi P(\omega) = [1 + 4\pi\chi(\omega)]E(\omega) = \epsilon(\omega)E(\omega)$$

$$\boxed{\epsilon(\omega) = 1 - \frac{\omega_{pl}^2}{2\omega_0'}\left(\frac{1}{\omega - \omega_0' + i\gamma} - \frac{1}{\omega + \omega_0' + i\gamma}\right)}$$

$$\omega_{pl} = \sqrt{\frac{4\pi n_0 e^2}{m_0}}$$

Plasma frequency

Causality

- Poles $\omega = \pm\omega_0' - i\gamma$

$$\chi(\omega) = -\frac{n_0 e^2}{2m_0\omega_0'}\left(\frac{1}{\omega - \omega_0' + i\gamma} - \frac{1}{\omega + \omega_0' + i\gamma}\right)$$

- Polarization at time t can only be created by electric fields E(t'), t'<t

$$P(t) = \int_{-\infty}^{t} \chi(t,t')E(t')dt' = \int_{-\infty}^{t} \chi(t-t')E(t')dt' = \int_{0}^{\infty} \chi(\tau)E(t-\tau)d\tau$$

$$\tau = t - t'$$

$$\overset{F.T.}{\Rightarrow} P(\omega) = \int_0^\infty d\tau \chi(\tau) e^{i\omega\tau} \int_{-\infty}^{\infty} dt E(t-\tau) e^{i\omega(t-\tau)}$$

$$\Rightarrow P(\omega) = \chi(\omega)E(\omega)$$

where $\chi(\omega) = \int_0^\infty \chi(\tau) e^{i\omega\tau} d\tau$

Fourier Transform

$$f(\omega) = \int_{-\infty}^{\infty} dt f(t) e^{i\omega t}$$

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) e^{-i\omega t}$$

Electron Plasma Frequency

- Plasma frequency: eigenfrequency of electron plasma oscillations around the position of the ions

$$\omega_{pl} = \sqrt{\frac{4\pi n_0 e^2}{m_0}}$$

- Assume electron density n(r,t) on an ion background of density

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0 \qquad \nabla \cdot E = 4\pi\rho \qquad m_0 \frac{\partial \mathbf{v}}{\partial t} = -e\mathbf{E}$$

where $\rho = e[n_0 - n(\mathbf{r},t)]$ $\qquad \mathbf{j}(\mathbf{r},t) = -en(\mathbf{r},t)\mathbf{v}(\mathbf{r},t)$

- Around equilibrium

$$n = n_0 + \delta n_1 + O(\delta^2) \qquad \mathbf{v} = \delta \mathbf{v}_1 + O(\delta^2) \qquad \mathbf{E} = \delta \mathbf{E}_1 + O(\delta^2)$$

$$\frac{\partial n_1}{\partial t} + n_0 \nabla \cdot \mathbf{v}_1 = 0 \qquad \nabla \cdot E_1 = -4\pi e n_1 \qquad m_0 \frac{\partial \mathbf{v}_1}{\partial t} = -e\mathbf{E}_1$$

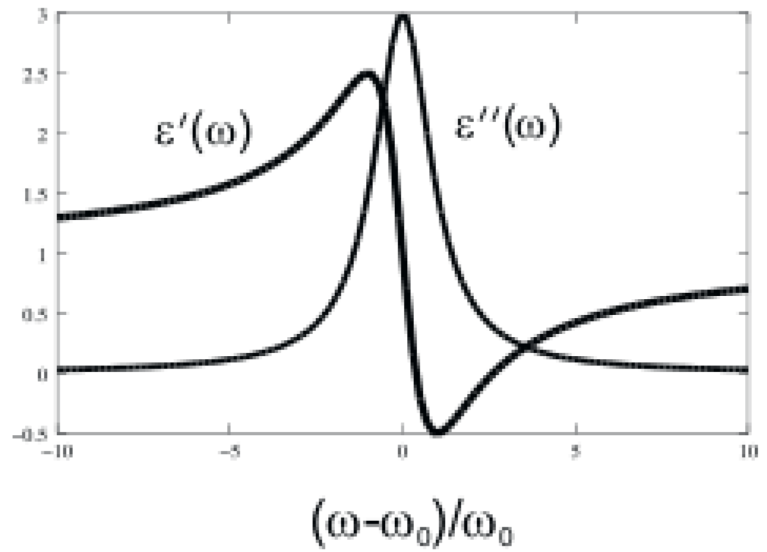
$$\frac{\partial^2 n_1}{\partial t^2} - \frac{e n_0}{m_0} \nabla \cdot \mathbf{E}_1 = 0 \Rightarrow \frac{\partial^2 n_1}{\partial t^2} + \underbrace{\frac{4\pi e^2 n_0}{m_0}}_{\omega_{pl}^2} n_1 = 0$$

Re & Im parts of dielectric function

- For $\omega_0 \gg \gamma$ i.e. $\omega_0' \approx \omega_0$

$$\epsilon(\omega) = 1 - \frac{\omega_{pl}^2}{2\omega_0} \frac{1}{\omega - \omega_0 + i\gamma} = \epsilon'(\omega) + i\epsilon''(\omega)$$

$$\epsilon'(\omega) - 1 = -\frac{\omega_{pl}^2}{2\omega_0} \frac{\omega - \omega_0}{(\omega - \omega_0)^2 + \gamma^2} \qquad \epsilon''(\omega) = \frac{\omega_{pl}^2}{2\omega_0} \frac{\gamma}{(\omega - \omega_0)^2 + \gamma^2}$$



Absorption & Refraction

- Maxwell equations in a medium (no ρ, no j)

$$\nabla \times \mathbf{H}(\mathbf{r},t) = \frac{1}{c}\frac{\partial}{\partial t}\mathbf{D}(\mathbf{r},t) \qquad \nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial}{\partial t}\mathbf{B}(\mathbf{r},t)$$

- For optical frequencies, $\mathbf{B} = \mathbf{H}$

$$\nabla \times \nabla \times \mathbf{E}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial}{\partial t}\nabla \times \mathbf{H}(\mathbf{r},t) = -\frac{1}{c^2}\frac{\partial}{\partial t^2}\mathbf{D}(\mathbf{r},t)$$

$$\nabla(\nabla \cdot \mathbf{E}(\mathbf{r},t)) - \nabla^2\mathbf{E}(\mathbf{r},t) - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\mathbf{D}(\mathbf{r},t) = 0$$

- F.T.

$$\nabla^2\mathbf{E}(\mathbf{r},\omega) + \frac{\omega^2}{c^2}\epsilon'(\omega)\mathbf{E}(\mathbf{r},\omega) + i\frac{\omega^2}{c^2}\epsilon''(\omega)\mathbf{E}(\mathbf{r},\omega) = 0$$

$$E(\mathbf{r},\omega) = E_0(\omega)e^{i[k(\omega)+i\kappa(\omega)]z}$$

Extinction coefficient

Wavenumber

We get

$$[k(\omega) + i\kappa(\omega)]^2 = \frac{\omega^2}{c^2}[\epsilon'(\omega) + i\epsilon''(\omega)]$$

Absorption & Refraction

- We get $$k^2(\omega) - \kappa^2(\omega) = \frac{\omega^2}{c^2}\epsilon'(\omega) \qquad 2\kappa(\omega)k(\omega) = \frac{\omega^2}{c^2}\epsilon''(\omega)$$
- Index of refraction

$$n(\omega) = \frac{k(\omega)}{k_0} = k(\omega)\frac{c}{\omega}$$

- Absorption coefficient

$$\alpha(\omega) = 2\kappa(\omega)$$

$$n(\omega) = \sqrt{\frac{1}{2}\left[\epsilon'(\omega) + \sqrt{\epsilon'^2(\omega) + \epsilon''^2(\omega)}\right]}$$

$$\alpha(\omega) = \frac{\omega}{n(\omega)c}\epsilon''(\omega)$$

- For $|\epsilon'| \gg |\epsilon''|$ $$n(\omega) \approx \sqrt{\epsilon'(\omega)}$$

and weakly dependent n(ω) $$\alpha(\omega) \approx \frac{\omega}{n_b c}\epsilon''(\omega) = \frac{4\pi\omega}{n_b c}\chi''(\omega)$$

Conclusion

- Optical response determined by dielectic function

$$\epsilon(\omega) = 1 - \frac{\omega_{pl}^2}{2\omega_0'}\left(\frac{1}{\omega - \omega_0' + i\gamma} - \frac{1}{\omega + \omega_0' + i\gamma}\right)$$

which is related with index of refraction and absorption coefficient

$$n(\omega) = \sqrt{\frac{1}{2}\left[\epsilon'(\omega) + \sqrt{\epsilon'^2(\omega) + \epsilon''^2(\omega)}\right]} \qquad \alpha(\omega) = \frac{\omega}{n(\omega)c}\epsilon''(\omega)$$

2. Quantum mechanical treatment of an atom in a classical light field

Atom in a light field

- Single electron in an atom described by

$$H_0\psi_n(\mathbf{r}) = \hbar\omega_n\psi_n(\mathbf{r}) \qquad H_0 = -\frac{\hbar^2\nabla^2}{2m_0} - \frac{e^2}{r}$$

- Coupling to optical field $H_1(t) = -exE(t) = -dE(t)$

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t} = [H_0 + H_1(t)]\psi(\mathbf{r},t)$$

- Expand $\psi(\mathbf{r},t) = \sum_m a_m(t)e^{-i\omega_m t}\psi_m(\mathbf{r})$

$$i\hbar\frac{da_n}{dt} = -E(t)\sum_m e^{-i\omega_{mn}t}\langle n|d|m\rangle a_m$$

$$\omega_{mn} = \omega_m - \omega_n$$

$$\langle n|d|m\rangle = \int d^3r\psi_n^*(\mathbf{r})d\psi_m(\mathbf{r}) = d_{nm}$$

Dipole matrix element

Atom in a light field

- Assume $a_n(t \to -\infty) = \delta_{n,l}$

$$i\hbar \frac{da_n}{dt} = -E(t) \sum_m e^{-i\omega_{mn}t} \langle n|d|m\rangle a_m$$

- Expand in small parameter δ: $a_n = a_n^{(0)} + \delta a_n^{(1)} + \ldots$ $\boxed{E(t) \to \delta E(t)}$
- 0th order

$$\frac{da_n^{(0)}}{dt} = 0 \Rightarrow a_n^{(0)} = \delta_{n,l}$$

- 1st order

$$i\hbar \frac{da_n^{(1)}}{dt} = -E(t) d_{nl} e^{-i\omega_{ln}t} \Rightarrow a_n^{(1)}(t) = -\frac{1}{i\hbar} \int_{-\infty}^{t} dt' E(t') d_{nl} e^{-i\omega_{ln}t'}$$

- F.T. of optical field $E(t) = \lim_{\gamma \to 0} \int \frac{d\omega}{2\pi} E(\omega) e^{-i\omega t} e^{\gamma t}$

Adiabatic switch-on of optical field

$$a_n^{(1)}(t) = -\frac{d_{nl}}{\hbar} \int \frac{d\omega}{2\pi} E(\omega) \frac{e^{-i(\omega+\omega_{ln})t}}{\omega + \omega_{ln} + i\gamma}$$

Atom in a light field

- Wavefunction

$$\psi(\mathbf{r},t) = e^{-i\omega_l t}\left[\psi_l(\mathbf{r}) - \sum_{m\neq l}\frac{d_{ml}}{\hbar}\psi_m(\mathbf{r})\int\frac{d\omega}{2\pi}E(\omega)\frac{e^{-i\omega t}}{\omega+\omega_{lm}+i\gamma}\right] + O(E^2)$$

- Polarization

$$P(t) = n_0\int d^3r\,\psi^*(\mathbf{r},t)\,d\,\psi(\mathbf{r},t)$$

$$P(t) = -n_0\sum_m\frac{|d_{lm}|^2}{\hbar}\int\frac{d\omega}{2\pi}\left[E(\omega)\frac{e^{-i\omega t}}{\omega+\omega_{lm}+i\gamma} + E^*(\omega)\frac{e^{i\omega t}}{\omega+\omega_{lm}-i\gamma}\right]$$

$$= \int\frac{d\omega}{2\pi}(-n_0)\sum_m\frac{|d_{lm}|^2}{\hbar}E(\omega)\left[\frac{1}{\omega+\omega_{lm}+i\gamma} - \frac{1}{\omega-\omega_{lm}+i\gamma}\right]e^{-i\omega t}$$

$$\boxed{\chi(\omega) = -n_0\sum_m\frac{|d_{lm}|^2}{\hbar}\left[\frac{1}{\omega+\omega_{lm}+i\gamma} - \frac{1}{\omega-\omega_{lm}+i\gamma}\right]}$$

Atomic optical susceptibility

Oscillator Strength

- Comparison with oscillator model

$$\chi(\omega) = -\frac{n_0 e^2}{2m_0\omega_0'}\left(\frac{1}{\omega-\omega_0'+i\gamma}-\frac{1}{\omega+\omega_0'+i\gamma}\right)$$

$$\chi(\omega) = -n_0\sum_m \frac{|d_{lm}|^2}{\hbar}\left(\frac{1}{\omega+\omega_{lm}+i\gamma}-\frac{1}{\omega-\omega_{lm}+i\gamma}\right)$$

$$= \frac{n_0 e^2}{2m_0}\sum_n \frac{f_{nl}}{\omega_{nl}}\left(\frac{1}{\omega-\omega_{ln}+i\gamma}-\frac{1}{\omega+\omega_{ln}+i\gamma}\right)$$

- Many oscillators with strength

$$\boxed{f_{nl} = \frac{2m_0}{\hbar}|x_{nl}|^2\omega_{nl}}$$

Oscillator strength

Sum Rule

- Sum over all oscillator strengths

$$\sum_n f_{nl} = \sum_n \frac{2m_0}{\hbar}|x_{nl}|^2\omega_{nl} = \frac{2m_0}{\hbar}\sum_n \langle n|x|l\rangle\langle l|x|n\rangle(\omega_n - \omega_l)$$

- Using $H_0\psi_n(\mathbf{r}) = \hbar\omega_n\psi_n(\mathbf{r})$ $\quad \langle l|x|n\rangle(\omega_n - \omega_l) = -\frac{1}{\hbar}\langle l|[H_0, x]|n\rangle$

$$\sum_n f_{nl} = -\frac{2m_0}{\hbar^2}\langle l|[H_0, x]x|l\rangle$$

- Similarly

$$\langle n|x|l\rangle(\omega_n - \omega_l) = \frac{1}{\hbar}\langle n|[H_0, x]|l\rangle \rightarrow \sum_n f_{nl} = \frac{2m_0}{\hbar^2}\langle l|x[H_0, x]|l\rangle$$

i.e. $\sum_n f_{nl} = \frac{m_0}{\hbar^2}\langle l|[x, [H_0, x]]|l\rangle$ with $[x, [H_0, x]] = [x, \frac{-i\hbar}{m_0}p_x] = \frac{\hbar^2}{m_0}$

$$\boxed{\sum_n f_{nl} = 1}$$

Optical Bloch Equations

- Two level system/atom

$$i\hbar\frac{da_1}{dt} = -E(t)e^{-i\omega_{21}}d_{12}a_2 \qquad i\hbar\frac{da_2}{dt} = -E(t)e^{i\omega_{21}}d_{21}a_1$$

- Optical field $E(t) = \frac{1}{2}E(\omega)(e^{-i\omega t} + c.c.)$

$$i\hbar\frac{da_1}{dt} = -\frac{1}{2}d_{12}E(\omega)\left[e^{-i(\omega+\omega_{21})t} + e^{i(\omega-\omega_{21})t}\right]a_2$$

$$i\hbar\frac{da_2}{dt} = -\frac{1}{2}d_{21}E(\omega)\left[e^{-i(\omega-\omega_{21})t} + e^{i(\omega+\omega_{21})t}\right]a_1$$

Optical Bloch Equations

- Around the resonance $\omega \approx \omega_2 - \omega_1$

$$\lim_{\gamma\to 0}\frac{1}{(\omega \pm \omega_{21}) + i\gamma} = P\frac{1}{\omega \pm \omega_{21}} - i\pi\delta(\omega \pm \omega_{21})$$

Optical Stark Shift

- Ignore non-resonant part – rotating wave approximation (RWA)

$$i\hbar\frac{da_1}{dt} = -\frac{1}{2}d_{12}E(\omega)e^{i(\omega-\omega_{21})t}a_2 \qquad i\hbar\frac{da_2}{dt} = -\frac{1}{2}d_{21}E(\omega)e^{-i(\omega-\omega_{21})t}a_1$$

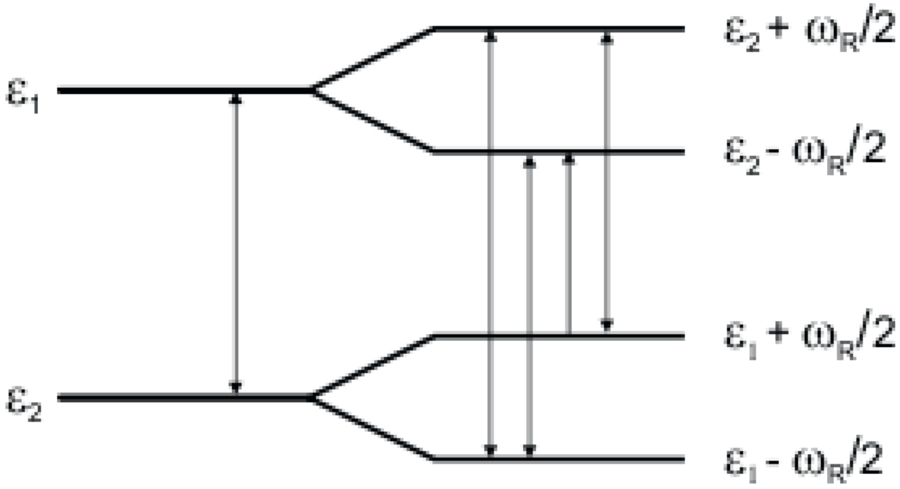
$$\frac{d^2a_2}{dt^2} = i\frac{d_{21}}{2\hbar}E(\omega)\frac{da_1}{dt} = -\left|\frac{d_{12}E(\omega)}{2\hbar}\right|^2 a_2 = -\frac{\omega_R^2}{4}a_2$$

Rabi Frequency $\boxed{\omega_R = \frac{|d_{12}E|}{\hbar}}$

- Solution $a_2(t) = a_2(0)e^{\pm i\omega_R t/2}$

$$\psi(\mathbf{r},t) = a_1(0)e^{-i(\omega_1\pm\omega_R/2)t}\psi_1(\mathbf{r}) + a_2(0)e^{-i(\omega_2\pm\omega_R/2)t}\psi_2(\mathbf{r})$$

Optical Stark Shift



- Similarly in the case of detuning $\nu = \omega_{21} - \omega$

$$\omega_2 \Longrightarrow \Omega_2 = \omega_2 - \frac{\nu}{2} \pm \frac{1}{2}\sqrt{\nu^2 + \omega_R^2}$$

$$\omega_1 \Longrightarrow \Omega_1 = \omega_1 + \frac{\nu}{2} \pm \frac{1}{2}\sqrt{\nu^2 + \omega_R^2}$$

Summary

- Optical response given by atomic susceptibility

$$\chi(\omega) = -n_0 \sum_m \frac{|d_{lm}|^2}{\hbar} \left[\frac{1}{\omega + \omega_{lm} + i\gamma} - \frac{1}{\omega - \omega_{lm} + i\gamma} \right]$$

- Many "oscillators" with strengths

$$f_{nl} = \frac{2m_0}{\hbar} |x_{nl}|^2 \omega_{nl} \qquad \sum_n f_{nl} = 1$$

- Energy levels shift in the presence of a strong light field (optical Stark shift)

Solids

- Energy spectrum consists now of bands and not discrete levels
  - Need to take into account band structure
  - When electrons are excited from filled (valence) bands to empty (conduction) bands, there are effectively 2 types of quasiparticles created: electrons in the CB and holes in the VB
- Confinement: going back to discrete levels but with important differences
- Interaction with environment stronger