

Sec. 7.5 Frequency dispersion

① We can understand much using a simple classical model for $\epsilon(\omega)$

Assumptions

(i) material has low density, with $\mu \approx \mu_0$

(ii) each e^- is bound harmonically, freq. ω_0 , and is subjected to an E-field,

$$\vec{E}(\vec{x}, t) = \vec{E}_0 e^{-i\omega t}$$

This assumes that $e^{i\vec{k} \cdot \vec{x}} \approx \text{constant}$ over the distance scale where the e^- moves.

$$\Rightarrow m \left(\ddot{\vec{x}} + \gamma \dot{\vec{x}} + \omega_0^2 \vec{x} \right) = -e \vec{E}_0 e^{-i\omega t}$$

phenomenological damping term

$\Rightarrow$ Look for a solution at the driving frequency, namely

$$\vec{x}(t) = \vec{x}_0 e^{-i\omega t} \quad \leftarrow \text{plug in}$$

$$\Rightarrow m e^{-i\omega t} \left(-\omega^2 - i\gamma\omega + \omega_0^2 \right) \vec{x}_0 = -e E_0 e^{-i\omega t}$$

$$\text{hence } \vec{x}_0 = \frac{-e}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} \vec{E}_0$$

and the induced electric dipole moment is

$$\vec{p} = -e\vec{x} = \frac{e^2}{m} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} \vec{E}$$

- In this model, imagine each e^- behaving as a classical damped oscillator of frequency ω_0 .

- Suppose there are N molecules
unit volume, each with Z electrons with different frequencies ω_j and damping constants γ_j .

- Call f_j the number of those Z electrons whose frequency is ω_j , i.e. $\sum_j f_j = Z$

$\Rightarrow$ The POLARIZATION is $\vec{P} = N\vec{p}$

or

$$\vec{P} = \frac{Ne^2}{m} \left(\sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i\omega\gamma_j} \right) \vec{E} \equiv \epsilon_0 \chi_e \vec{E}$$

and therefore

$$\frac{\epsilon(\omega)}{\epsilon_0} + 1 = 1 + \chi_e = 1 + \frac{Ne^2}{\epsilon_0 m} \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i\omega\gamma_j}$$

Quantum Derivation

See Fano & Rau,
Atomic collisions & spectra,
p. 29

Let the applied electric field be

$$\vec{E} = \hat{x} E_0 (e^{-i\omega t} + e^{i\omega t})$$

$\Rightarrow$ the potential energy is $V = -exE_0 (e^{-i\omega t} + e^{i\omega t})$

1st-order time-dependent perturbation theory states that

$$\Psi = \Psi^{\text{ground}} + \sum_j \Psi_j e^{-i \overset{\text{energy of } j^{\text{th}} \text{ atomic level}}{\epsilon_j} t / \hbar} c_j(t)$$

$$\text{Where } c_j(t) = \frac{e E_0}{\hbar} \langle \Psi_j | x | \Psi^{\text{ground}} \rangle \times \left[\frac{e^{i(\omega + \omega_j - \frac{1}{2}i\gamma_j)t}}{\omega_j + \omega - \frac{1}{2}i\gamma_j} + \frac{e^{-i(\omega - \omega_j + \frac{i\gamma_j}{2})t}}{\omega_j - \omega - \frac{1}{2}i\gamma_j} \right]$$

where γ_j = decay rate of excited state Ψ_j

$$\text{and } \frac{\epsilon_j - \epsilon_{\text{ground}}}{\hbar} \equiv \omega_j - \frac{1}{2}i\gamma_j$$

simplified notation: call $\Psi^{\text{ground}} \rightarrow |0\rangle$

$$\Psi_j \rightarrow |j\rangle$$

Then the mean dipole moment is:

$$\langle p \rangle = e \langle x \rangle = e \sum_j \left\{ \langle 0 | x | j \rangle c_j(t) e^{-i(\omega_j - i\frac{\gamma_j}{2})t} + c_j^*(t) e^{i(\omega_j + i\frac{\gamma_j}{2})t} \langle j | x | 0 \rangle \right\}$$

$$\Rightarrow \langle p \rangle = \frac{e^2 E_0}{\hbar} \sum_j \langle 0 | x | j \rangle \left(\frac{e^{i\omega t}}{\omega_j^2 - \omega^2 + i\omega\gamma_j} + \frac{e^{-i\omega t}}{\omega_j^2 - \omega^2 - i\omega\gamma_j} \right)$$

$$\equiv E_0 \alpha(\omega) e^{-i\omega t} + E_0 \alpha^*(\omega) e^{i\omega t}$$

and the polarizability is

$$\alpha(\omega) = \frac{e^2}{m} \sum_j \frac{f_j}{\omega_j^2 - \omega^2 - i\gamma_j \omega}$$

where the quantal oscillator strength is

$$f_j = \frac{2m\omega_j^2}{\hbar} |\langle j | x | 0 \rangle|^2$$

which is dimensionless

Aside: can prove in nonrelativistic QM that

$$\sum_j f_j = Z,$$

Which is the Thomas - Reiche - Kuhn sum rule.

- see Fano & Cooper, Rev. Mod. Phys. 40, 441 (1968).

⑧ Anomalous Dispersion

Recall, from Chap. 4, $\chi_e = \frac{\alpha N}{1 - \frac{1}{3} \alpha N} \approx \alpha N$

And typically $\gamma_j \ll \omega_j$, so damping is not very important except when ω is near resonance,
 $\omega_j^2 \approx \omega^2$

First look at two limits:

Low ω $\frac{\epsilon(\omega)}{\epsilon_0} \xrightarrow{\omega \rightarrow 0} 1 + \frac{e^2 N}{\epsilon_0 m} \sum_{j>0} \frac{f_j}{\omega_j^2} + \frac{ie^2 N}{\epsilon_0 m} \frac{f_0}{\omega(\gamma_0 - i\omega)}$

this term is present
if an $\omega_0 = 0$
resonant frequency
exists

High ω

$$\frac{\epsilon(\omega)}{\epsilon_0} \xrightarrow[\omega \gg \text{all } \omega_j]{\omega \rightarrow \infty} 1 - \frac{Ne^2 Z}{m \epsilon_0 \omega^2} \equiv 1 - \frac{\omega_p^2}{\omega^2}$$

where $\omega_p^2 \equiv \frac{NZe^2}{\epsilon_0 m}$ is called
the PLASMA FREQUENCY
(squared)

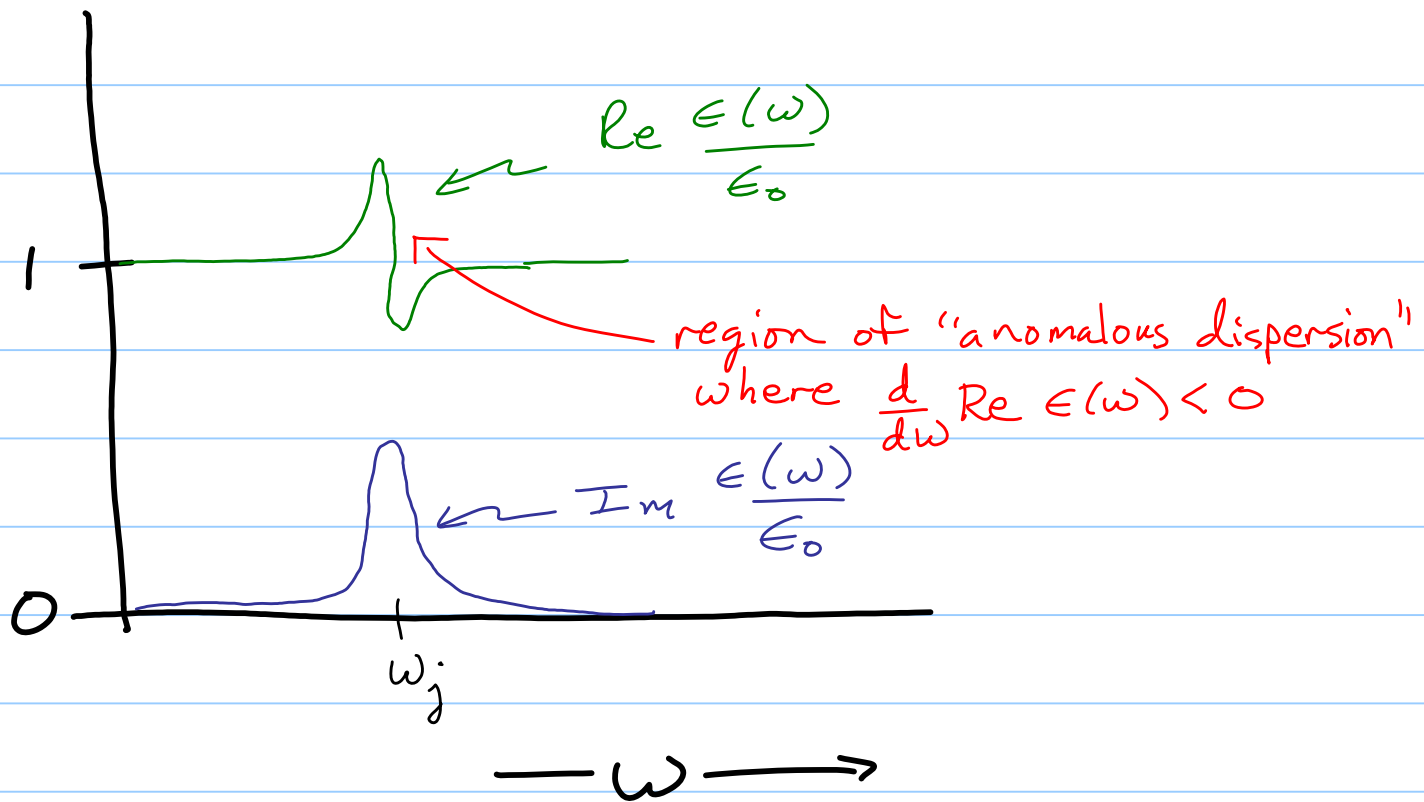
Intermediate ω near resonant ω_j :

$\Rightarrow$ for $\omega \approx \omega_j$,

$$\alpha(\omega) \approx \frac{e^2}{m} \frac{f_j}{\omega_j^2 - \omega^2 - i\gamma_j \omega}$$

$$\Rightarrow \text{Re } \alpha(\omega) \approx \frac{e^2}{m} f_j \frac{\omega_j^2 - \omega^2}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2 \omega^2}$$

$$\text{Im } \alpha(\omega) = \frac{e^2}{m} f_j \frac{\gamma_j \omega}{(\omega_j^2 - \omega^2)^2 + \gamma_j^2 \omega^2}$$



On your own, read Jackson, Sec. 7.5(E)
pp 314-316, on the importance of the
WATER WINDOW, where water has virtually
no absorption between $\nu \approx 4 \times 10^{14} \text{ Hz} - 8 \times 10^{14} \text{ Hz}$
in the visible region!

Sec. 7.5 Wavepackets, dispersion, group velocity

Recall that the monochromatic plane waves discussed up to now are a mathematical abstraction, a δ -function in $\vec{k}$ -space and in $\omega \Rightarrow$ they extend over all space and exist for all time

Of course, any EM waves occurring in nature will have finite extent & duration

$\Rightarrow$ these require a superposition of frequencies

Moreover, in general $\epsilon(\omega)$ is complex, which has the following implications:

- (1) The phase velocity depends on ω
 $\Rightarrow$ different frequency components in a wavepacket disperse, i.e. drift out of phase
- (2) Energy flows at the group velocity, rather than the phase velocity c/n .
- (3) For $\text{Im } \epsilon(\omega) \neq 0$ there is also dissipation

Sec 7.8 For starters, consider the 1D wave eqn,

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{v^2} \frac{\partial^2}{\partial t^2} \right) u(x, t) = 0$$

This equation has monochromatic plane wave solutions, $u(x, t) = u_0 e^{i(kx - \omega t)}$,

Where $\omega = kv$, or in general $\frac{\omega(k)}{k} = v(k)$
 k = phase velocity

Assume for now that μ, ϵ are real

$\Rightarrow k, \omega(k)$ are real

$\Rightarrow$ DISSIPATION is ignored for now

Next, Form a general wavepacket solution
by superposing monochromatic plane waves,
i.e. $u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx - i\omega(k)t} dk$

In general, to determine $A(k)$, we must specify

BOTH $u(x,0)$ AND $\left. \frac{\partial u(x,t)}{\partial t} \right|_{t=0} \equiv u_t(x,0)$

because this wave equation is 2nd-order in t ;

(This is in contrast to the Schrödinger equation,
first-order in t , which only requires knowledge
of $\psi(x,0)$ to determine $\psi(x,t)$ at all later t .)

Then for any real wavepacket $u(x,t)$ we must have:

$$\Rightarrow u(x,0) = \frac{1}{2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk + \text{c.c.}$$

$$\text{and } u_t(x,0) = \frac{1}{2} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (-i\omega(k)) A(k) e^{ikx} dk + \text{c.c.}$$

Next apply "Fourier's Trick" to find $A(k)$,

$$\Rightarrow \text{Set } C_{k'} \equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,0) e^{-ik'x} dx = \frac{A(k') + A^*(-k')}{2}$$

and

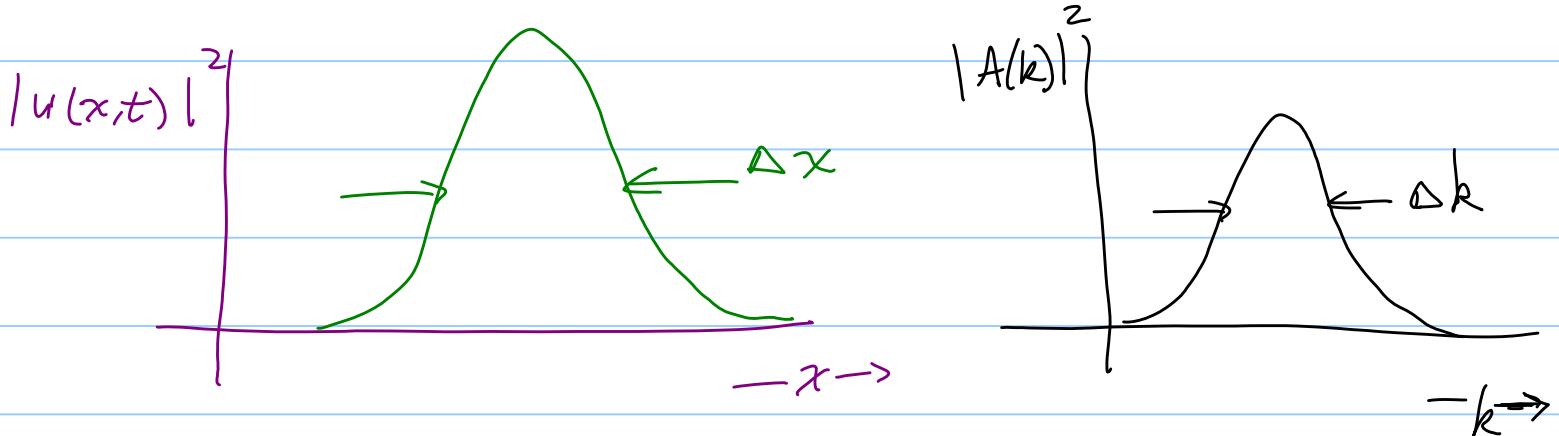
$$\begin{aligned}
 D_{k'} &\equiv \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u_t(x,0) e^{-ik'x} dx \\
 &= -\frac{i}{2} \left(\omega(k') A(k') - \omega^*(-k') A^*(-k') \right) \\
 &= \frac{i}{2} \omega(k') \left(-A(k') + A^*(-k') \right), \\
 &\quad \left(\text{since frequencies here are real} \right. \\
 &\quad \left. \text{and direction-independent} \right)
 \end{aligned}$$

These 2 equations can be solved, giving

$$C_k + \frac{D_k}{i\omega(k)} = A^*(-k) \quad C_k - \frac{D_k}{i\omega(k)} = A(k)$$

$$\Rightarrow A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} \left[u(x,0) + \frac{i}{\omega(k)} u_t(x,0) \right] dx$$

These waves obey an uncertainty relation, both in time and in space, e.g.



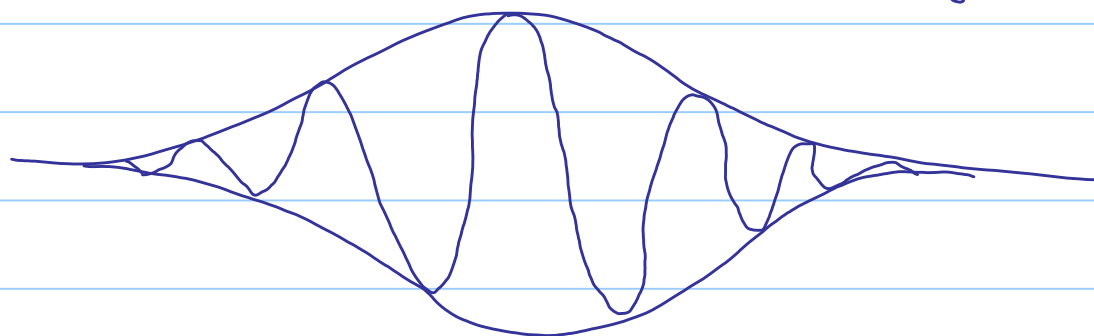
Then from Fourier analysis, $\Delta k \Delta x \geq \frac{1}{2}$
with equality only for a Gaussian pulse

To proceed farther, consider an $A(k)$ that is peaked around some value, say, k_0 , and Taylor expand $\omega(k)$ about k_0 :

$$\omega(k) \approx \omega_0 + \left. \frac{d\omega}{dk} \right|_{k_0} (k - k_0) + \frac{1}{2} \left. \frac{d^2\omega}{dk^2} \right|_{k_0} (k - k_0)^2 + \dots$$

Then the following model can be solved exactly: Suppose that the $t=0$ solution is

$$u(x, 0) = e^{-x^2/\gamma^2} \cos(k_0 x), \text{ and neglect } u_t(x, 0) \approx 0$$



(This actually corresponds to 2 different pulses moving in the $\pm x$ -directions)

$$\begin{aligned} \text{Then } A(k) &= \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}} e^{-ikx} e^{-x^2/\gamma^2} \cos(k_0 x) \\ &= \frac{1}{2\sqrt{2\pi}} \int dx \left\{ e^{-i(k-k_0)x - x^2/\gamma^2} + e^{-i(k+k_0)x - x^2/\gamma^2} \right\} \end{aligned}$$

To do this integral, complete the square, i.e. set $\frac{x^2}{\gamma^2} + i(k-k_0)x = \frac{1}{\gamma^2} \left[x + \frac{i(k-k_0)\gamma^2}{2} \right]^2 - \frac{(k-k_0)^2\gamma^2}{4}$

and change variables to $x' = x + i(k-k_0)\frac{\gamma^2}{2}$
whereby

$$A(k) = \frac{1}{2\sqrt{2\pi}} e^{-\frac{(k-k_0)^2 \gamma^2}{4}} \underbrace{\int_{-\infty}^{\infty} e^{-\frac{x'^2}{\gamma^2}} dx'}_{\gamma\sqrt{\pi}} + (k \rightarrow -k_0)$$

Now plug into the time-dependent wavepacket integral, with $\omega(k) \approx \omega_0 + v_g(k-k_0) + \frac{1}{2}\omega_0 a^2(k-k_0)^2$
with $v_g \equiv \left. \frac{d\omega}{dk} \right|_{k_0}$, $a^2 \equiv \left. \frac{1}{\omega_0} \frac{d^2\omega}{dk^2} \right|_{k_0}$

⇒ the final wavepacket is

$$u(x,t) = e^{\frac{ik_0 x - i\omega_0 t}{4}} \gamma e^{\frac{-(x - v_g t)^2 / (\gamma^2 + 4ia^2\omega_0 t)}{\sqrt{\gamma^2 + 4ia^2\omega_0 t}}}$$

$$\text{and } |u(x,t)|^2 = \frac{\gamma^2}{16} \frac{e^{-(x - v_g t)^2 \left(\frac{2\gamma^2}{\gamma^4 + 16a^4\omega_0^2 t^2} \right)}}{(\gamma^4 + 16a^4 t^2 \omega_0^2)^{1/2}}$$

And based on this expression, we conclude that:

- ① In media where μ, ϵ , and n are constants, independent of ω, k , the phase and group velocities are equal since
- $$\omega = \frac{kc}{n} \Rightarrow v_g = \frac{d\omega}{dk} = \frac{c}{n} = v_{\text{phase}}$$

② In media where $n \rightarrow n(\omega)$, $k = \frac{n(\omega)\omega}{c}$

$$\Rightarrow v_g = \frac{1}{\left. \frac{dk}{d\omega} \right|_{\omega_0}} = \frac{c}{n + \omega \frac{dn}{d\omega}}$$

NORMAL DISPERSION occurs when $n \geq 1$ and $\frac{dn}{d\omega} > 0$
 $\Rightarrow v_g < c$

ANOMALOUS DISPERSION has $\frac{dn}{d\omega} < 0$ so that

$v_g > c$ could arise. This apparent violation of special relativity (causality) is traceable to a failure of our Taylor approximation to $\omega(k)$.

③ The pulse width spreads in general, as time increases.

When the above approximations are valid, under conditions of normal dispersion, the energy propagates at speed $v_g \leq c$.