# Frequency Dependent Response of Materials

Preamble: General treatment of response functions, or "The generalized susceptibility"
(Taken from Landau & Lifshitz, Stat. Phys. 1, Sec 123).

Let $s(t)$ describe the state of a system, on which a "force" $f(t)$ acts through a "susceptibility" $\chi(t)$. In our applications we have cases where this terminology is very appropriate, e.g., for $s(t)$ could be $\vec{J}(t)$, and $f(t)$ the electric field $\vec{E}(t)$ (literally a force).

We will use Fourier transforms and their inverses for all quantities:

eg $$s(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{s}(\omega), \quad \tilde{s}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} s(t)$$

Now $$s(t) = \int_{-\infty}^{t} dt' \chi(t-t') f(t')$$

Note that the integral goes up to $t'=t$ and no further because causality dictates that the force $f(t')$ does not affect $s(t)$ for times $t'>t$.

Alternatively, $$s(t) = \int_{-\infty}^{\infty} dt' \chi(t-t') f(t')$$

with $\chi(t-t') = 0$ for $t-t'<0$, ie, $\chi(t) = 0$ for $t<0$.

Now $\int_{-\infty}^{\infty} dt' f(t') \chi(t-t') = \int_{-\infty}^{\infty} dt' \int \frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\, e^{i\omega_1 t'} e^{i\omega_2 (t-t')} \tilde{f}(\omega_1)\tilde{\chi}(\omega_2)$

$$= \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \tilde{f}(\omega_1)\tilde{\chi}(\omega_2) e^{i\omega_2 t} \underbrace{\int dt'\, e^{i(\omega_1-\omega_2)t'}}_{=2\pi\,\delta(\omega_1-\omega_2)}$$

$$= \int \frac{d\omega_1}{2\pi} e^{i\omega_1 t} \tilde{f}(\omega_1)\tilde{\chi}(\omega_1)$$

So that $\tilde{s}(\omega) = \tilde{\chi}(\omega)\tilde{f}(\omega)$

Examples:

For conductors $\vec{\tilde{j}}(\omega) = \tilde{\sigma}(\omega)\vec{\tilde{E}}(\omega)$, for dielectrics $\vec{\tilde{D}}(\omega) = \tilde{\epsilon}(\omega)\vec{\tilde{E}}(\omega)$

We want to study properties of $\tilde{\chi}(\omega)$. Let $\tilde{\chi}(\omega) = \tilde{\chi}_1(\omega) + i\,\tilde{\chi}_2(\omega)$ that is $\tilde{\chi}_1 = \mathrm{Re}\,\tilde{\chi}$ and $\tilde{\chi}_2 = \mathrm{Im}\,\tilde{\chi}$. Since $\chi(t)=0$ for $t<0$ we have

$$\tilde{\chi}(\omega) = \int_0^{\infty} dt\, e^{i\omega t}\chi(t)$$

Moreover, $\chi(t)$ is real. Therefore

1. $\tilde{\chi}^*(\omega) = \tilde{\chi}(-\omega)$

That is $\chi_1(-\omega) = \chi_1(\omega)$ and $\chi_2(-\omega) = -\chi_2(\omega)$ (even & odd functions).

For $\chi(t)$ having support over some interval of size $T$ we expect $\tilde{\chi}(\omega)$ to have support over $\Delta\omega \sim \frac{1}{T}$, so $\tilde{\chi}(\omega)\to 0$ as $\omega\to\infty$. Some care is required for $T\to\infty$ (as in $\chi(t)=1$) and for $T\to 0$ (as is $\chi(t) = \delta(t-t_1)$) but we'll assume $\lim_{\omega\to\infty}\tilde{\chi}(\omega) = 0$.

2. $\omega \chi_2(\omega) > 0$

That is $\chi_2(\omega) > 0$ for $\omega > 0$.

The proof relies on the 2nd Law of Thermodynamics and the interpretation of $f$ as a generalized force and $s$ as a generalized displacement. In the absence of $f(t)$, the evolution of $s$ is determined by a Hamiltonian $H_0$, and the effect of $f$ is described as a perturbation $H' = -s f(t)$. The sign is so that $\dot{p} = -\frac{\partial H}{\partial s} = f$.

Now $f$ acts on body, and changes to the state of the body are accompanied by dissipation (heat lost in the process). Then

$$\frac{dE}{dt} = \frac{\partial H}{\partial t} = -s \frac{df(t)}{dt}$$

Now for any two functions

$$\int_{-\infty}^{\infty} dt\, a(t) b(t) = \int \frac{d\omega}{2\pi} \tilde{a}(\omega) \tilde{b}(-\omega) = \frac{1}{2} \int \frac{d\omega}{2\pi} \left[ \tilde{a}(\omega) \tilde{b}(-\omega) + \tilde{a}(-\omega) \tilde{b}(\omega) \right]$$

So $$\Delta E = \int \frac{dE}{dt} dt = -\frac{1}{2} \int \frac{d\omega}{2\pi} \left[ \tilde{s}(\omega) \left[ -i(-\omega) \tilde{f}(-\omega) \right] + \tilde{s}(-\omega) \left( -i\omega \tilde{f}(\omega) \right) \right]$$

now use $\tilde{s} = \tilde{\chi} \tilde{f}$ $\rightarrow$

$$= -\frac{i}{2} \int \frac{d\omega}{2\pi} \left[ \left( \tilde{\chi}(\omega) - \tilde{\chi}(-\omega) \right) \omega \tilde{f}(-\omega) \tilde{f}(\omega) \right]$$

$$= -\frac{i}{2} \int \frac{d\omega}{2\pi} \left( 2i \chi_2(\omega) \right) \omega \left| \tilde{f}(\omega) \right|^2$$

Now, $\tilde{f}(\omega)$ is arbitrary and $\Delta E > 0 \Rightarrow \omega \chi_2(\omega) > 0$.

Analytic continuation: extend definition of $\tilde{\chi}(\omega)$ to complex argument, $\omega = \omega_1 + i\omega_2$.

3. $\tilde{\chi}(\omega)$ is analytic for $\mathrm{Im}(\omega) > 0$.

Because

$$\tilde{\chi}(\omega) = \int_0^\infty dt\, e^{i\omega_1 t}\, e^{-\omega_2 t}\, \chi(t)$$

and the integral converges provided $\omega_2 > 0$ (since $\tilde{\chi}(\omega)$ for real $\omega$ is assumed to exist for some range of $\omega$, we need not worry about the integral not converging because $\chi(t) \sim \exp(ct)$). Moreover

$$\frac{d^n \tilde{\chi}(\omega)}{d\omega^n} = i^n \int_0^\infty dt\, e^{i\omega_1 t}\, e^{-\omega_2 t}\, t^n \chi(t)$$

also converges ( $e^{-\omega_2 t} t^n \to 0$ as $t \to \infty$ for any $n$).

Note that this is a consequence of <u>causality</u> (we used $\chi(t) = 0$ for $t < 0$).

1'. $\tilde{\chi}(-\omega^*) = \tilde{\chi}^*(\omega)$

Is the generalization of (1) to complex argument.

Then $\tilde{\chi}_1(-\omega_1 + i\omega_2) = \chi_1(\omega_1 + i\omega_2)$ and $\tilde{\chi}_2(-\omega_1 + i\omega_2) = -\chi_2(\omega_1 + i\omega_2)$

In particular, on the imaginary axis $\chi_2(i\omega_2) = 0 \Rightarrow \chi(i\omega_2)$ is real.

5. For $\omega_2 > 0$ (upper half plane), $\tilde{\chi} \neq 0$, except on $\omega_1 = 0$ (imaginary axis). For $\omega_1 = 0$, $\tilde{\chi}_1(i\omega_2)$ is monotonically decreasing from $\chi_0 = \tilde{\chi}(i0)$ to $\tilde{\chi}(i\infty) = 0$.

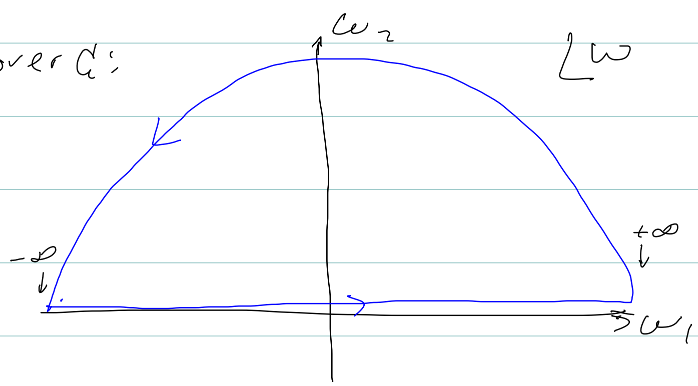
Therefore $\tilde{\chi}(\omega)$ has no zeroes in upper half plane.

Proof: From complex analysy $\frac{1}{2\pi i}\oint_c dz \frac{f'(z)}{f(z)}$.

$N_{Z(P)}$ = number of zeroes (poles) of $f(z)$ in region interior to C.

Consider $I \equiv \frac{1}{2\pi i}\oint_c d\omega \frac{d\tilde{\chi}(\omega)}{d\omega}\frac{1}{\tilde{\chi}(\omega) - X}$ where $X$ is real and

the integral is over C:



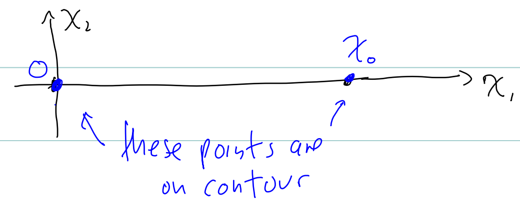

Now, for upper half plane, $\chi$ is analytic $\Rightarrow$ so is $\frac{d\chi}{d\omega}$. So in the statement about complex analysis above, $f = \chi(\omega) - X$ is analytic ($N_p = 0$) and therefore $I$ = number of zeroes of $\chi(\omega) - X$ = number of times $\chi(\omega)$ takes on the real value $X$.

Now compute $I$: change variables:

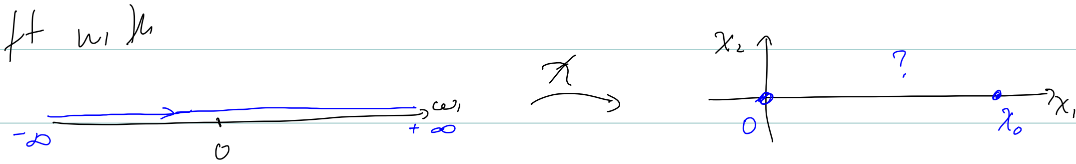
$$I = \frac{1}{2\pi i}\oint_{C'} d\chi \frac{1}{\chi - X}$$

Let's figure out $C'$

Since $C$ goes through $i\omega_2 = 0+$ and $i\omega_2 = +i\infty$, we start with those $\chi(i0+) = \chi_0$ and $\chi(i\infty) = 0$

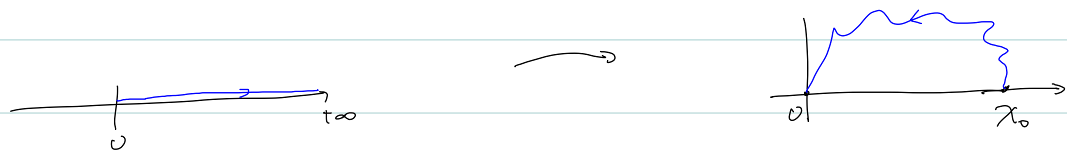



Actually, all of the semi-circle of $C$ maps to $0$, so we are left with

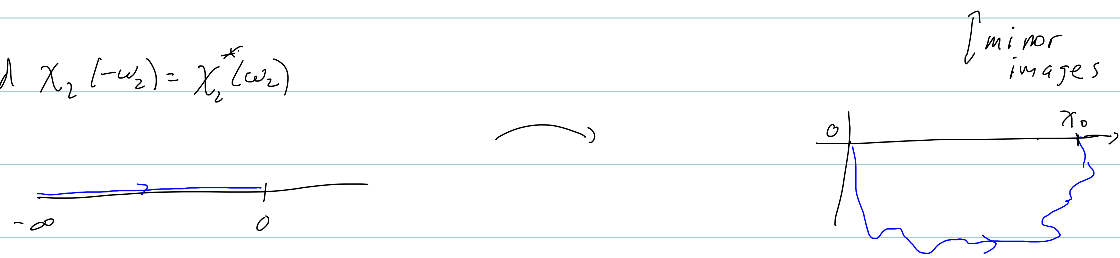



Now $\chi_2 > 0$ for $\omega_1 > 0$ and $\chi_2 < 0$ for $\omega_1 < 0$ by (2).

So




and $\chi_2(-\omega_2) = \chi_2^*(\omega_2)$




The point is $C'$ crosses the real axis only at $0$ and $\chi_0$.

So, $I = 1$ for all values of $\chi$, $0 < \chi < \chi_0$ and $I = 0$ otherwise.

To complete the argument (1) Since $\chi$ is real on the positive imaginary axis, and it is analytic and goes from $\chi_0$ to $0$ on the axis, it must take on every value in the interval $(0, \chi_0)$ along the axis. But it takes on each value only once. It must have $\chi_2 \neq 0$ everywhere else on the upper half plane $\Rightarrow \tilde{\chi}_2 \neq 0$ except at $+i\infty$.

(ii) Since it takes on every value in $(0, \chi_0)$ only once, $\chi(i\omega_2) = \chi_1(i\omega_2)$ cannot have a local minimum or maximum along the line: it is monotonic.

(iii) Since $\tilde{\chi}_2 \neq 0$ everywhere (on upper half plane) except on the imaginary axis, and there $\tilde{\chi}_1(\omega) \neq 0$ except at $\omega = +i\infty$, we have $\tilde{\chi}(\omega) \neq 0$ (except at $+i\infty$).

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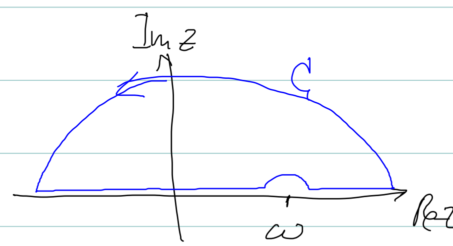
6. Kramers-Kronig relation.

Consider

$$\frac{1}{2\pi i}\oint_C dz\, \frac{\tilde{\chi}(z)}{z-\omega} \quad \text{for } C:$$




Since $\tilde{\chi}(z)$ is analytic for $\mathrm{Im}(z) > 0$ and $\omega$ is outside $C$, there are no poles inside $C$: by Cauchy's theorem the integral vanishes. The integral over the small semicircle is, with $z = \omega + \epsilon e^{i\phi}$

$$\lim_{\epsilon \to 0} \int_{\pi}^{0} \epsilon e^{i\phi}\, i\, d\phi\, \frac{\tilde{\chi}(\omega + \epsilon e^{i\phi})}{\epsilon e^{i\phi}} = -i\pi \tilde{\chi}(\omega)$$

The integral over the real axis is the principal value integral. So

$$0 = -i\pi\tilde{\chi}(\omega) + P\int_{-\infty}^{\infty} d\omega' \, \frac{\chi(\omega')}{\omega'-\omega}$$

or

$$\tilde{\chi}(\omega) = -\frac{i}{\pi} P \int_{-\infty}^{\infty} d\omega' \, \frac{\chi(\omega')}{\omega'-\omega}$$

Taking Im or Re of this equation:

$$\tilde{\chi}_2(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\tilde{\chi}_1(\omega')}{\omega' - \omega}$$

$$\tilde{\chi}_1(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} d\omega' \frac{\tilde{\chi}_2(\omega')}{\omega' - \omega}$$

Kramers–Kronig relations

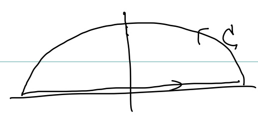
Then, $\tilde{\chi}_1(\omega)$ completely fixes $\tilde{\chi}_2(\omega)$, and viceverza.

Many additional results follow.

Exercises:

(i) Show $\tilde{\chi}_1(\omega) = \frac{2}{\pi} P \int_0^{\infty} d\omega' \frac{\omega' \tilde{\chi}_2(\omega')}{\omega'^2 - \omega^2}$

(ii) By considering $\oint_C dz \frac{z \tilde{\chi}(z)}{z^2 + \omega^2}$ for real $\omega$, along a contour




, show $\int_{-\infty}^{\infty} d\omega' \frac{\omega' \tilde{\chi}(\omega')}{\omega'^2 + \omega^2} = i\pi \tilde{\chi}(i\omega)$

Use this to show $\tilde{\chi}(i\omega) = \frac{2}{\pi} \int_0^{\infty} \frac{\omega' \tilde{\chi}_2(\omega')}{\omega'^2 + \omega_0^2}$

(iii) Use the previous result (integrate over $\omega$) to show

$$\int_0^{\infty} d\omega \, \tilde{\chi}(i\omega) = \int_0^{\infty} \tilde{\chi}_2(\omega) \, d\omega$$

To derive these formulae (including Kramers-Kronig) we only used the fact that $\tilde{\chi}(\omega)$ is regular in the upper half-plane. If in addition we know $\tilde{\chi}^*(\omega) = \tilde{\chi}(-\omega^*)$ so $\tilde{\chi}(i\omega) = \tilde{\chi}_1(i\omega)$ we have $\int_0^{\infty} d\omega \, \tilde{\chi}_1(i\omega) = \int_0^{\infty} \tilde{\chi}_2(\omega) \, d\omega$

## Frequency dependent conductivity

Ohm's Law: $\tilde{\vec{j}}(\omega) = \tilde{\sigma}(\omega)\tilde{\vec{E}}(\omega)$

$\tilde{\sigma}(\omega)$ : frequency dependent conductivity.

where, e.g. $\vec{j}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \tilde{\vec{j}}(\omega)\, e^{-i\omega t}$

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Aside on Fourier Transform of a product.

with $a(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{a}(\omega)$ and $b(t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{b}(\omega)$

where $\tilde{a}(\omega) = \int dt\, e^{i\omega t} a(t)$

Then, the (I)FT of the product is

$$\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} a(\omega) b(\omega) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \int_{-\infty}^{\infty} dt_1\, e^{i\omega t_1} a(t_1) \int_{-\infty}^{\infty} dt_2\, e^{i\omega t_2} b(t_2)$$

$$= \int_{-\infty}^{\infty} dt_1 \int_{-\infty}^{\infty} dt_2\, a(t_1) b(t_2) \underbrace{\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega(t_1+t_2-t)}}_{= \delta(t_1+t_2-t)}$$

$$= \int_{-\infty}^{\infty} dt_1\, a(t_1) b(t-t_1)$$

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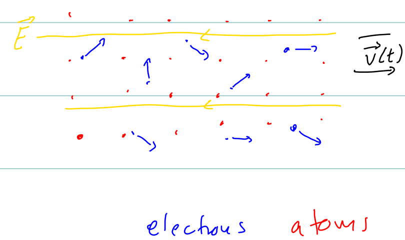
Ohm's law in time domain

$$\vec{j}(t) = \int_{-\infty}^{\infty} dt'\, \sigma(t-t')\, \vec{E}(t')$$

The "response" function $\sigma(t-t')$ must vanish for $t'>t$ since $\vec{E}(t')$ cannot influence the current $\vec{j}(t)$ at prior times (ie for $t<t'$): this follows from causality.

So $\sigma(t) = 0$ for $t<0$.

Drude Model:




- electrons move with average velocity $\vec{v}(t)$
- They accelerate ($\vec{F}=m\vec{a}$) due to electric field $\vec{E}$
- They bounce off fixed atoms.

Simple model: probabilistic

* each electron has probability per unit time $\frac{1}{\tau}$ of colliding
* after collision velocity is randomized

$\Rightarrow$ $\vec{v}(t+\Delta t) - \vec{v}(t) =$ decreased by fraction of electrons $\left(\frac{\Delta t}{\tau}\right)$ that collide, since randomized directions average to zero $+$ (acceleration) $\times \Delta t$

$$= -\frac{\Delta t}{\tau}\vec{v}(t) + \frac{q\vec{E}(t)}{m}\Delta t$$

(textbook uses $q=-e$)

($\tau$ = "relaxation" or "collision" time).

$\Rightarrow$ $\frac{\partial \vec{v}}{\partial t} = -\frac{1}{\tau}\vec{v} + \frac{q\vec{E}}{m}$ ; with $n$ = number density $\vec{j}(t) = nq\vec{v}(t)$ $\Rightarrow$ $\frac{\partial \vec{j}}{\partial t} = -\frac{1}{\tau}\vec{j} + \frac{nq^2}{m}\vec{E}$

or, after Fourier transform $-i\omega\tilde{\vec{j}} = -\frac{1}{\tau}\tilde{\vec{j}} + \frac{nq^2}{m}\tilde{\vec{E}}$

Solving for $\tilde{\vec{j}}$

$$\boxed{\tilde{\sigma}(\omega) = \frac{\frac{nq^2}{m}}{\frac{1}{\tau} - i\omega} = \frac{nq^2\tau}{m}\frac{1}{1-i\omega\tau}}$$

Notes:

- $\tau \sim 10^{-14}$ sec is typical. So for frequencies $\omega \ll \frac{1}{\tau} \sim 10^{14}$ Hz $\tilde{\sigma}(\omega) \approx \sigma_0 = \frac{nq^2\tau}{m}$

Using $n \sim 10^{22}\ \text{cm}^{-3}$ and $q, m$ for electron $\rightarrow \sigma_0 \sim 10^{18}\ \text{sec}^{-1}$ or $\frac{1}{\sigma_0} \sim 10^{-6}$ ohm cm

- Opposite limit : $\omega >> \tau^{-1}$ $\Rightarrow$ $\boxed{\tilde{\sigma}(\omega) = i\,\frac{nq^2}{m\omega}}$ $(\cancel{A})$

is purely imaginary, and $\sim \frac{1}{\omega}$.

This is as if there were no collisions $\rightarrow$ response is inertial (ie from $F=ma$)

and $\tilde{\sigma} \rightarrow 0$ as $\omega \rightarrow \infty$ means

$$\frac{dv}{dt} = \frac{q}{m}\tilde{E}e^{-i\omega t} \rightarrow V = \frac{e^{-i\omega t}}{-i\omega}\frac{q\tilde{E}}{m} \rightarrow 0 \text{ as } \omega\rightarrow\infty$$

, ie electrons can't keep up / respond.

$(\cancel{A})$ is purely from applied $\vec{E}$, so very general (independent of model of collisions of electrons). Will use this!

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ASIDE

- If magnetic field is present, add to force a $\frac{q}{c}\vec{v}(t)\times\vec{B}(t)$ term. Then after multiplying by $nq$, $\frac{q}{c}\vec{j}(t)\times\vec{B}(t)$.

The FT of a product

$$\int dt\;\; a(t)\,b(t)e^{i\omega t} = \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\;\tilde{a}(\omega_1)\,\tilde{a}(\omega_2)\underbrace{\int dt\; e^{it(\omega-\omega_1-\omega_2)}}_{=2\pi\,\delta(\omega-\omega_1-\omega_2)}$$

$$= \int\frac{d\omega'}{2\pi}\; a(\omega')\,b(\omega-\omega')$$

So $$-i\omega\,\vec{j}(\omega) = -\frac{1}{\tau}\vec{j}(\omega) + \frac{nq^2}{m}\vec{E}(\omega) + \frac{q}{c}\int\frac{d\omega'}{2\pi}\;\tilde{\vec{j}}(\omega')\times\tilde{\vec{B}}(\omega-\omega')$$

Yikes! See Exercise 119.1 for static case.

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## General Properties of $\tilde{\sigma}(\omega)$. (Garg sec 121 – we'll go back to 120 later)

Let's write $\tilde{\sigma} = \tilde{\sigma}_1 + i\tilde{\sigma}_2$ ($\tilde{\sigma}_{1,2}$ are real).

Then (much of this follows from the general susceptibility notes above).

1. $\tilde{\sigma}^*(\omega) = \tilde{\sigma}(-\omega)$

This is because $\vec{E}$ and $\vec{J}$ are real. For any real $f(t)$ its FT has $f^*(\omega) = f(-\omega)$ – we have seen this. And $\tilde{\vec{E}} = \tilde{\sigma}\tilde{\vec{J}}$.

2. $\sigma_1(\omega) > 0$. (This is slightly different than for $\chi$ above)!

Power dissipated $= P_{diss} = \vec{J}\cdot\vec{E} > 0$ by 2nd Law of Thermodyn's.

For

$$\int_{-\infty}^{\infty} dt\ \vec{J}(t)\cdot\vec{E}(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\ \tilde{\vec{J}}(-\omega)\cdot\tilde{\vec{E}}(\omega) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\ \frac{1}{2}\left(\tilde{\vec{J}}^*(\omega)\cdot\vec{E}(\omega) + \tilde{\vec{J}}(\omega)\cdot\tilde{\vec{E}}^*(\omega)\right)$$

$$= \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\ \mathrm{Re}\,\sigma(\omega)\ |\tilde{\vec{E}}(\omega)|^2$$

This must be positive for arbitrary $\vec{E} \Rightarrow \sigma_1(\omega) > 0$.

3. $\sigma(\omega)$ is analytic for $\mathrm{Im}(\omega) > 0$

(Note that this depends on our definition of FT as $\int \frac{d\omega}{2\pi} f(t) e^{-i\omega t}$)

We have seen that causality $\Rightarrow \sigma(t) = 0$ for $t < 0$.

So

$$\sigma(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t}\sigma(t) = \int_{0}^{\infty} dt\, e^{i(\mathrm{Re}\,\omega)t}\, e^{-\mathrm{Im}(\omega)t}\ \sigma(t)$$

For $\mathrm{Im}(\omega) > 0$ the integral converges provided $\sigma(t)$ does not grow exponentially.

We may safely assume $\sigma(t)$ does not grow exponentially. recall

$$\vec{j}(t) = \int_{-\infty}^{t} dt' \sigma(t-t') \vec{E}(t')$$

and we do not expect $\vec{j}(t)$ to depend on $\vec{E}(t')$ as $t' \to -\infty$ as $e^{-t'}$ !

Moreover, we can safely take derivatives, as in

$$\frac{d^n \tilde{\sigma}}{d\omega^n} = (-i)^n \int_{-\infty}^{\infty} dt\, t^n e^{i\omega t} \sigma(t)$$

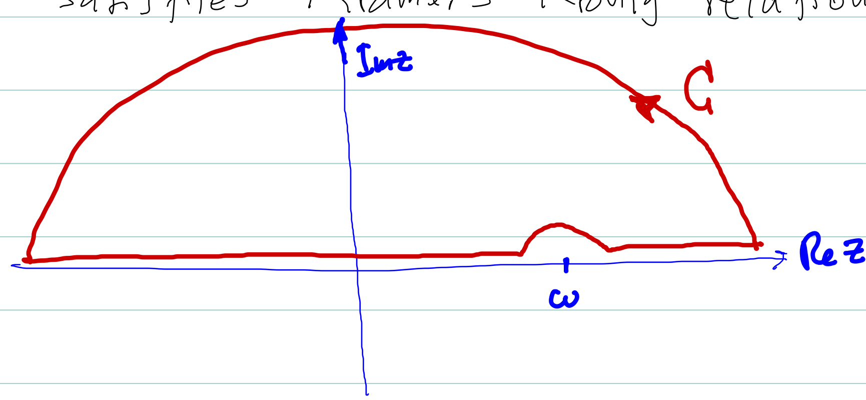
since this is still convergent for $Im(\omega) > 0$.

$\Rightarrow$ $\tilde{\sigma}(\omega)$ is analytic in $Im(\omega) > 0$.

Note also that $\sigma(\omega) \to 0$ as $Im\, \omega \to \infty$.

This (analyticity in upper half plane plus vanishing at $\infty$) means:

4. $\tilde{\sigma}$ satisfies Kramers-Kronig relations




Consider $\oint_C \frac{dz\, \tilde{\sigma}(z)}{z-\omega} = 0$ (Cauchy: $\frac{\tilde{\sigma}(z)}{z-\omega}$ is analytic in region bounded by $C$).

On semicircle $|z| = R \to \infty$ the integral vanishes because $\sigma \to 0$, so $\left|\frac{\sigma}{z-\omega}\right| \to 0$ faster than $\frac{1}{|z|}$.

The small semicircle gives

(use $z = \omega + \epsilon e^{i\phi}$, $\epsilon \to 0$ and $\phi$ goes from $\pi$ to $0$):

$$-\lim_{\epsilon\to 0} \int_0^{\pi} \epsilon e^{i\phi}\, i\, d\phi \; \frac{\sigma(\omega+\epsilon e^{i\phi})}{\epsilon e^{i\phi}} = -i\pi\sigma(\omega)$$

The rest is the principal value of the integral on the real line, so

$$P\int_{-\infty}^{\infty} dx\, \frac{\sigma(x)}{x-\omega} - i\pi\sigma(\omega) = 0$$

Separating into real and imaginary parts, and using $x = \omega'$ so that the dummy variable reminds us it refers to frequency:

$$\sigma_2(\omega) = -\frac{1}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{\sigma_1(\omega')}{\omega-\omega'}$$

Kramers-Kronig relations

$$\sigma_1(\omega) = \frac{1}{\pi} P\int_{-\infty}^{\infty} d\omega' \, \frac{\sigma_2(\omega')}{\omega-\omega'}$$

If you know $\sigma_1$ (or $\sigma_2$) you can compute $\sigma_2$ (or $\sigma_1$)

5. $\tilde{\sigma}(\omega) \neq 0$ in upper half-plane.

This was done for $\tilde{\chi}(\omega)$ above, and won't repeat here.

## 6. f-sum rule

From Kramers-Kronig we have

$$\tilde{\sigma}_2(\omega) = -\frac{2\omega}{\pi} P\int_0^\infty d\omega' \frac{\tilde{\sigma}_1(\omega')}{\omega'^2 - \omega^2}$$

As $\omega \to \infty$ this is

$$\tilde{\sigma}_2(\omega) = \frac{2}{\pi\omega}\int_0^\infty d\omega' \, \tilde{\sigma}_1(\omega')$$

But from Drude's model, $\tilde{\sigma}(\omega) \simeq i\frac{nq^2}{m\omega}$ as $\omega \to \infty$, and we explained this is model independent. Comparing

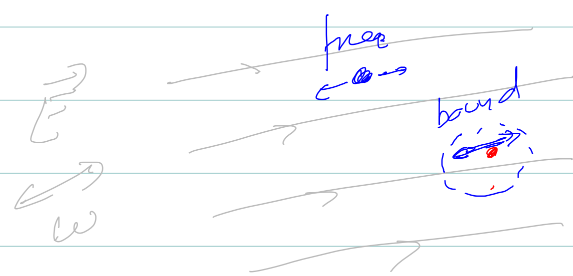
$$\frac{nq^2}{m\omega} = \frac{2}{\pi\omega}\int_0^\infty d\omega' \, \tilde{\sigma}_1(\omega)$$

or

$$\int_0^\infty d\omega' \, \tilde{\sigma}_1(\omega') = \frac{\pi n q^2}{2m} \qquad \text{"f-sum rule"}$$

## Dielectric response function and Garg's "propensity"

The distinction between $\rho_{free}$ and $\rho_{bound}$, and particularly $\vec{J}_{free}$ and $\vec{J}_{pol}$ (and we will see $\vec{J}_{mag}$ too) gets blurred with harmonic fields.




Both free and bound charges exhibit oscillatory motion. At very high frequency they are indistinguishable.

We will later consider a microscopic model of the response of bound electrons. But let's try to 1st capture the ambiguity in free vs bound described above, in a macroscopic description. From Ampere's law

(Here I deviate from Garg slightly: his breaking of $\vec{J} = \vec{J}^{ext} + \vec{J}^{int}$ – external and internal to the material – is non-sense, since these are local quantities, ie, $\vec{J} = \vec{J}(\vec{x},t)$, $\tilde{\vec{J}} = \tilde{\vec{J}}(\vec{x},\omega)$)

$$\vec{\nabla} \times \vec{H} - \frac{1}{c}\frac{\partial \vec{D}}{\partial t} = \frac{4\pi}{c}\vec{J}$$

In $\omega$-domain:

$$\vec{\nabla} \times \tilde{\vec{H}} + \frac{i\omega}{c}\tilde{\vec{D}} = \frac{4\pi}{c}\tilde{\vec{J}} \implies \vec{\nabla} \times \tilde{\vec{H}} + \frac{i\omega}{c}\tilde{\epsilon}\tilde{\vec{E}} = \frac{4\pi}{c}\tilde{\sigma}\tilde{\vec{E}}$$

?

We can rewrite this as

$$\vec{\nabla} \times \vec{H} + \frac{i\omega}{c}\underbrace{\left(\tilde{\epsilon} + i\frac{4\pi\tilde{\sigma}}{\omega}\right)}_{\text{sort of effective permitivity}}\tilde{\vec{E}} = 0 \quad \text{or} \quad \vec{\nabla} \times \tilde{\vec{H}} = \frac{4\pi}{c}\underbrace{\left(\tilde{\sigma} - i\frac{\omega\tilde{\epsilon}}{4\pi}\right)}_{\text{kind of effective conductivity.}}\tilde{\vec{E}}$$

We also have $\vec{\nabla}\cdot\vec{\tilde{D}} = 4\pi\rho$. From continuity $\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{j}$

we have $-i\omega\tilde{\rho} = -\vec{\nabla}\cdot\tilde{\vec{j}}$. Using $\tilde{D} = \epsilon\tilde{E}$ and $\tilde{j} = \tilde{\sigma}\tilde{E}$

$$\vec{\nabla}\cdot\vec{D} = 4\pi\rho \Rightarrow \vec{\nabla}\cdot(\tilde{\epsilon}\tilde{E}) = -\frac{4\pi i}{\omega}\vec{\nabla}\cdot(\sigma\tilde{E})$$

$$\Rightarrow \vec{\nabla}\cdot\left[\left(\tilde{\epsilon} + i\frac{4\pi\tilde{\sigma}}{\omega}\right)\tilde{E}\right] = 0$$

Although you will find some textbooks that state that there is an ambiguity in whether we combine $\tilde{\epsilon}$ & $\tilde{\sigma}$ into permitivity or conductivity, the interpretation of Gauss's law suggests an effective permitivity is a better choice.

Garg invents the term (I have not seen it used elsewhere) "electric propensity" for

$$\zeta(\omega) \equiv \tilde{\epsilon}(\omega) + \frac{4\pi i\,\tilde{\sigma}(\omega)}{\omega}$$

* the squiggle "$\zeta$" is intended as greek-zeta

Much of the literature calls it dielectric constant, or complex dielectric constant, or AC dielectric constant, ... None of these names capture the facts that (i) not a constant, (ii) not purely dielectric and (iii) not the same as $\tilde{\epsilon}(\omega)$ (even though this symbol is often used for $\zeta(\omega)$).

or, to be fair, "full dielectric function"

We'll stick with Garg.

---

Aside: if there are additional currents $\vec{J}'$ not subject to Ohm's law (eg, superconducting current) then add to right hand side:

$$\vec{\nabla}\times\vec{\tilde{H}} + i\frac{\omega}{c}\tilde{\zeta}\vec{\tilde{E}} = \frac{4\pi}{c}\vec{\tilde{J}}'$$

$$\vec{\nabla}\cdot\tilde{\zeta}\vec{\tilde{E}} = 4\pi\tilde{\rho}'$$

---

Garg also defines $\vec{\tilde{Z}} = \tilde{\zeta}\vec{\tilde{E}}$ so that in $t$-domain

$$\vec{\nabla}\times\vec{H} - \frac{1}{c}\frac{\partial\vec{Z}}{\partial t} = \frac{4\pi}{c}\vec{J}' \quad , \quad \vec{\nabla}\cdot\vec{Z} = 4\pi\rho'$$

Beware than in most of the literature $\vec{\tilde{Z}} = \tilde{\zeta}\vec{\tilde{E}}$ is $\vec{\tilde{D}} = \tilde{\epsilon}\vec{\tilde{E}}$

Best is to understand what you are doing: then you don't get confused with symbols.

# Electromagnetic energy in material media

We saw that $\tilde{\sigma} \neq 0$ in the upper half $\omega$-plane, and in particular $\sigma_1 > 0$ on real axis. This was a result that followed from the 2nd law, that energy is dissipated in the material body.

Now, the microscopic theory tells us exactly where the energy goes:

$$-\vec{\nabla}\cdot\vec{S} = \vec{j}\cdot\vec{e} + \frac{\partial u}{\partial t}$$

as was shown in 203A, where $\vec{S} = \frac{c}{4\pi}\vec{e}\times\vec{b}$ is the (microscopic version of) Poynting vector giving the energy flux and $u = \frac{1}{8\pi}(\vec{e}^2+\vec{b}^2)$ the (microscopic energy density). The question is what replaces this that accounts for rate of heat dissipated in the presence of dielectrics.

The answer is

$$-\vec{\nabla}\cdot\overline{\vec{S}} = \overline{\vec{J}_{free}\cdot\vec{E}} + \frac{d\overline{U}}{dt} + \dot{Q}$$

where (i) Fields are assumed quasimonochromatic

(ii) $\overline{X(t)}$ means $X(t)$ is averaged over the period of the (quasi) monochromatic fields

(iii) $\bar{U}$ has the interpretation of internal energy and $\dot{Q}$ is d(heat)/dt, with

$$\bar{U} = \frac{1}{8\pi}\left[\frac{d}{d\omega}(\omega\epsilon_1(\omega))\overline{E^2} + \frac{d}{d\omega}(\omega\mu_1(\omega))\overline{H^2}\right]$$

and

$$\dot{Q} = \frac{1}{4\pi}\left[\omega\epsilon_2(\omega)\overline{E^2} + \omega\mu_2(\omega)\overline{H^2}\right]$$

The rest of this section is just computations deriving this result (plus a definition of terms, eg, "quasimonochromatic").

---

Consider quasimonochromatic field $\vec{E}(t)$. That is $\vec{\tilde{E}}(\omega)$ has frequencies centered on $\omega_0$ with small dispersion.

We want to show that

$$\vec{E}(t) = \vec{a}(t)e^{-i\omega_0 t} + c.c.$$

To show this, consider

$$\vec{E}(t) = \int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\vec{\tilde{E}}(\omega)e^{-i\omega t} = \int_0^{\infty}\frac{d\omega}{2\pi}e^{-i\omega t}\vec{\tilde{E}}(\omega) + \int_0^{\infty}\frac{d\omega}{2\pi}e^{i\omega t}\vec{\tilde{E}}^*(\omega)$$

Now write $\vec{\tilde{E}}(\omega_0+\alpha) = \vec{\tilde{a}}(\alpha)$ so that ($\omega = \omega_0+\alpha$ above)

$$\vec{E}(t) = e^{-i\omega_0 t}\int_{-\omega_0}^{\infty}\frac{d\alpha}{2\pi}\vec{\tilde{a}}(\alpha)e^{-i\alpha t} + c.c.$$

Now, assume that $\vec{\tilde{a}}(\alpha)$ is localized about some frequencies well above zero. Then we can approximately replace the lower limit by $-\infty$:

$$\vec{E}(t) = \vec{a}(t)e^{-i\omega_0 t} + c.c.$$

which is the desired result.

$\vec{a}(t)$ varies little over a period $\frac{2\pi}{\omega_0}$. So if we average $\vec{E}^2(t)$ over $t \gg \frac{2\pi}{\omega_0}$ the $e^{\pm 2i\omega_0 t}$ terms do not contribute

$$\overline{\vec{E}^2(t)} = 2\, \vec{a}(t)\cdot\vec{a}^*(t)$$

The average is over $t \gg \frac{2\pi}{\omega_0}$ but small over the typical time over which $\vec{a}(t)$ varies.

Likewise for other fields, like $\vec{H}(t)$.

Now, we have shown

$$\vec{\nabla}\cdot\left[-\frac{c}{4\pi}(\vec{E}\times\vec{H})\right] = \vec{J}\cdot\vec{E} + \frac{1}{4\pi}\left(\vec{E}\cdot\frac{\partial\vec{D}}{\partial t} + \vec{H}\cdot\frac{\partial\vec{B}}{\partial t}\right)$$

Integrate over volume, for some $V$. $\int_V d^3r\, \vec{J}\cdot\vec{E}$ = work/time done by $\vec{E}$ on free charges. $-\int d^3r\, \vec{\nabla}\cdot\left[\frac{c}{4\pi}(\vec{E}\times\vec{H})\right] = -\int_{\partial V} d^2r\, \hat{n}\cdot\left[\frac{c}{4\pi}(\vec{E}\times\vec{H})\right]$ is then energy/time flowing into $V$, so $\vec{S} = \frac{c}{4\pi}\vec{E}\times\vec{H}$ = energy flux/vol.

The last term must be the change in internal energy plus heat produced.

Consider $\vec{E}\cdot\frac{\partial\vec{D}}{\partial t}$. Write $\vec{E}$ and $\vec{D}$ in terms of $\tilde{\vec{E}}(\omega)$ and $\vec{D}(\omega) = \hat{\epsilon}(\omega)\tilde{\vec{E}}(\omega)$.

$$\vec{E}\cdot\frac{\partial\vec{D}}{\partial t} = \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\, \tilde{\vec{E}}(\omega_1)^* e^{i\omega_1 t}\cdot(-i\omega_2)\,\epsilon(\omega_2)\,\tilde{\vec{E}}(\omega_2)e^{-i\omega_2 t}$$

$$= \int\frac{d\omega_1}{2\pi}\int\frac{d\omega_2}{2\pi}\, \tilde{\vec{E}}(\omega_2)e^{-i\omega_2 t}\cdot(i\omega_1)\,\epsilon^*(\omega_1)\,\tilde{\vec{E}}(\omega_1)^* e^{i\omega_1 t}$$

so adding these:

$$2\dot{E}\cdot\dot{D} = \int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\int_{-\infty}^{\infty}\frac{d\omega_2}{2\pi}\, e^{i(\omega_1-\omega_2)t}\, \vec{\tilde{E}}(\omega_1)^*\cdot\vec{\tilde{E}}(\omega_2)\; i\left[\omega_1\epsilon^*(\omega_1) - \omega_2\epsilon(\omega_2)\right]$$

Write $\int_{-\infty}^{\infty}\frac{d\omega_1}{2\pi}\, e^{i\omega_1 t}\, \tilde{E}(\omega_1)^*\, i\omega_1\epsilon^*(\omega_1)$

$$= \int_0^{\infty}\frac{d\omega_1}{2\pi}\left[e^{i\omega_1 t}\tilde{E}^*(\omega_1)\, i\omega_1\epsilon^*(\omega_1) + e^{-i\omega_1 t}\tilde{E}(\omega_1)(-i\omega_1)\,\epsilon(\omega_1)\right]$$

and so on, so that we only integrate over positive frequencies. Since we will want to average over quasimonochromatic fields, drop terms $\vec{\tilde{E}}(\omega_1)\cdot\vec{\tilde{E}}(\omega_2)$ or $\vec{\tilde{E}}(\omega_1)^*\cdot\vec{\tilde{E}}(\omega_2)^*$.

Next average over period $T=\frac{2\pi}{\omega_0}$. Use $\omega=\omega_0+\alpha$, and amp's $\vec{a}(t)$

$$\overline{2\vec{E}\cdot\dot{\vec{D}}} \approx 2\underbrace{\int_{-\omega_0}^{\infty}}_{\approx -\infty}\frac{d\alpha_1}{2\pi}\underbrace{\int_{-\omega_0}^{\infty}}_{\approx -\infty}\frac{d\alpha_2}{2\pi}\; i\left[\omega_1\epsilon^*(\omega_1) - \omega_2\epsilon(\omega_2)\right]\Big|_{\omega_i=\omega_0+\alpha_i}\tilde{\vec{a}}(\alpha_1)^*\cdot\tilde{\vec{a}}(\alpha_2)\, e^{i(\alpha_1-\alpha_2)t}$$

We separate $\epsilon(\omega)$ into real and imaginary parts since physically we expect $\epsilon_2=\mathrm{Im}\,\epsilon$ to be associated to heat (dissipation) while $\epsilon_1=\mathrm{Re}\,\epsilon$ ought to be related to internal energy. For each of this we expand in $\alpha=\omega-\omega_0$ and retain leading terms:

$$\mathrm{Re}\left[\omega_1\epsilon^*(\omega_1)-\omega_2\epsilon(\omega_2)\right] = (\omega_0+\alpha_1)\,\epsilon_1(\omega_0+\alpha_1) - (\omega_0+\alpha_2)\,\epsilon_1(\omega_0+\alpha_2)$$
$$= (\alpha_1-\alpha_2)\frac{d}{d\omega}\left(\omega\epsilon_1(\omega)\right)\Big|_{\omega_0}$$

$$\mathrm{Im}\left[\;\text{idem}\;\right] = -(\omega_0+\alpha_1)\,\epsilon_2(\omega_0+\alpha_1) - (\omega_0+\alpha_2)\,\epsilon_2(\omega_0+\alpha_2)$$
$$= -2\omega_0\,\epsilon_2(\omega_0)$$

Write this in time domain (and drop "0" in $\omega_0$):

$$\overline{\dot{\vec{E}}\cdot\dot{\vec{D}}} = \underbrace{\frac{1}{2}\frac{d}{d\omega}(\omega\epsilon_1(\omega))\quad\frac{d}{dt}\overline{\vec{E}^2(t)}} + \underbrace{\omega\epsilon_2(\omega)\ \overline{\vec{E}^2(t)}}$$

and this $\times\frac{1}{4\pi}$ is $\frac{d}{dt}\bar{U}$ as advertised; this $\times\frac{1}{4\pi}$ is $\dot{Q}$

What remains is justifying the interpretation of the two terms as above. Note that if you proceed slowly and adiabatically in polarizing the medium, the mechanical work done (which should go fully into internal energy) is, $\frac{1}{8\pi}\epsilon_1\vec{E}^2$. But $\frac{1}{8\pi}\frac{d}{d\omega}(\omega\epsilon_1(\omega))E^2$ gives this in the quasistatic approximation. So we interpret the first term as $\frac{d\bar{U}}{dt}$ and infer the $2^{nd}$ is heat that shows up when the process of polarizing the medium is <u>not</u> adiabatic.

Beware of the limits of applicability: we assumed linearity, quasi monochromatic fields, retained leading terms in Taylor expansion, ...

# Electronic Response Model of Drude, Kramers, Lorentz.

Each atom/molecule a polarizable unit.

Model the 'atom' as a charge (electron) bound by a harmonic force, with dissipation and under and applied $\vec{E}$-field force:

$$m\ddot{\vec{r}} + m\gamma\dot{\vec{r}} + m\omega_0^2\vec{r} = q\vec{E}(t) \qquad \begin{pmatrix} q=-e \\ \text{charge of } e^- \end{pmatrix}.$$

If the "atom" is neutral and has no permanent dipole moment then we need a charge $-q$ (ie, $+e$) at the "center" $\vec{r}=0$. The dipole moment is then $\vec{d}(t) = q\vec{r}(t)$

In Fourier space (we have solved this Eq several times before)

$$-\omega^2\tilde{\vec{r}} - i\omega\gamma\tilde{\vec{r}} + \omega_0^2\tilde{\vec{r}} = \frac{q}{m}\tilde{\vec{E}}$$

or

$$\tilde{\vec{r}} = -\frac{q}{m}\tilde{\vec{E}}\,\frac{1}{\omega^2-\omega_0^2+i\omega\gamma}$$

With $n$ = number density of bound electrons/volume

Polarization vector $\vec{P} = nq\tilde{\vec{r}} = -\frac{nq^2}{m}\tilde{\vec{E}}\,\frac{1}{\omega^2-\omega_0^2+i\omega\gamma}$

$$\Rightarrow \quad \tilde{\chi}_e = -\frac{nq^2}{m}\,\frac{1}{\omega^2-\omega_0^2+i\omega\gamma}$$

and $\tilde{\epsilon}(\omega) = 1 + 4\pi \tilde{\chi}_e(\omega) = 1 - \frac{4\pi n^2 q}{m} \frac{1}{\omega^2 - \omega_0^2 + i\omega\gamma}$

This is for rarefied media. For dense media a Clausius-Mossetti model treatment gives

$$\frac{\tilde{\epsilon}(\omega) - 1}{\tilde{\epsilon}(\omega) + 2} = \frac{4\pi}{3} \tilde{\chi}_e(\omega)$$

or $\tilde{\epsilon}\left(1 - \frac{4\pi}{3}\tilde{\chi}_e\right) = 1 + \frac{8\pi}{3}\tilde{\chi}$, $\tilde{\epsilon} = 1 + \frac{4\pi \tilde{\chi}_e}{1 - \frac{4\pi}{3}\tilde{\chi}_e}$

or $\tilde{\epsilon} = 1 + \frac{4\pi n^2 q}{m} \cdot \frac{(-1)}{\omega^2 - \omega_0^2 + i\omega\gamma} \cdot \frac{1}{1 - \frac{4\pi}{3}\frac{n^2 q}{m}\frac{(-1)}{\omega^2 - \omega_0^2 + i\omega\gamma}}$

$$= 1 - \frac{4\pi n^2 q}{m} \frac{1}{\omega^2 - \left(\omega_0^2 - \frac{4\pi}{3}\frac{n^2 q}{m}\right) + i\omega\gamma}$$

$$= 1 + \frac{4\pi n^2 q}{m} \frac{1}{\omega_1^2 - \omega^2 - i\omega\gamma}$$

where $\omega_1^2 = \omega_0^2 - \frac{4\pi}{3}\frac{n^2 q}{m}$

Improvement: many resonant frequencies of electrons in real atoms, given by

$$\hbar\omega_i = \underbrace{\mathcal{E}_i}_{i\text{th energy level}} - \underbrace{\mathcal{E}_0}_{\text{ground state energy}}$$

and introduce $f_i$ = oscillator strength

= amplitude of dipole moment when oscillating between $j$-th state and ground state, with

$$\sum_i f_i = Z = \text{number of electrons in atom}$$

Then, the improved model is

$$\tilde{\epsilon}(\omega) = 1 + \frac{4\pi n q^2}{mZ} \sum_i \frac{f_i}{\omega_i^2 - \omega^2 - i\omega\gamma_i}$$

($\gamma_i$ = damping of response at frequency $\omega_i$).

Note:

This is a rough model. Do not attach too literal a meaning to constants like $n$ & $Z$.

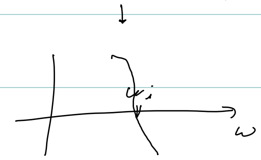
Let's plot $\tilde{\epsilon}_1(\omega)$ and $\hat{\epsilon}_2(\omega)$

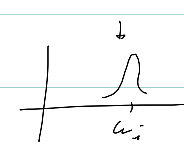
$$\tilde{\epsilon}_1(\omega) = Re(\tilde{\epsilon}(\omega)) = 1 + \frac{4\pi n q^2}{mZ} \sum_i \frac{f_i(\omega_i^2 - \omega^2)}{(\omega_i^2 - \omega^2)^2 + \omega^2\gamma_i^2}$$

$$\tilde{\epsilon}_2(\omega) = Im(\tilde{\epsilon}(\omega)) = \frac{4\pi n q^2}{mZ} \sum_i \frac{f_i \omega \gamma_i}{(\omega_i^2 - \omega^2)^2 + \omega^2\gamma_i^2}$$

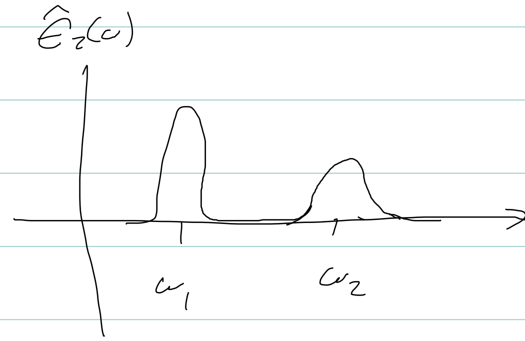
Near resonance $i$,

$$\tilde{\epsilon}_1(\omega) \simeq \frac{4\pi n q^2}{mZ} \frac{f_i(\omega_i^2 - \omega^2)}{\omega_i^2\gamma_i^2} \qquad \tilde{\epsilon}_2(\omega) \simeq \frac{4\pi n q^2}{m} \frac{f_i \omega_i \gamma_i}{(\omega_i^2 - \omega^2)^2 + \omega_i^2\gamma_i^2}$$



So


$\frac{d\tilde{\epsilon}_1}{d\omega} < 0$ "anomalous dispersion" (see later, below)

Notes:

- If $\omega_1 = 0$ the contribution of this resonance to $\tilde{\epsilon} - 1$ is

$$-\frac{4\pi n q^2}{m Z} f_1 \frac{1}{\omega(\omega + i\gamma_1)}$$

which looks like conductivity in Drude's model: and it is! $\omega_1 = 0$ means no restoring force $\Rightarrow$ free electrons.

Recall the Drude model has

$$\tilde{\sigma}(\omega) = \frac{n_f q^2 \tau}{m} \frac{1}{1 - i\omega\tau} \qquad \text{with } n_f = n \text{ for free } e\text{'s.}$$

and "propensity" is

$$\tilde{\zeta}(\omega) = \tilde{\epsilon}(\omega) + \frac{4\pi i \sigma(\omega)}{\omega}$$

So $\tilde{\zeta}$ in Drude's model has $\tilde{\zeta}(\omega) - \tilde{\epsilon}(\omega) = \frac{4\pi n_f q^2}{m} i\tau \frac{1}{\omega(1 - i\omega\tau)}$

$$= -\frac{4\pi n_f q^2}{m} \frac{1}{\omega(\omega + i\tau^{-1})}$$

which matches the above with

$$n_f = \frac{n f_1}{Z} \quad \text{and} \quad \tau = \gamma_1^{-1}$$

Nice to get a unified treatment in one simple model!

- The static case $\tilde{\epsilon}(0) = 1 + \frac{4\pi n q^2}{mZ} \sum_i \frac{f_i}{\omega_i^2}$

The large frequency limit

$$\tilde{\epsilon}(\omega) = 1 - \frac{4\pi n q^2}{m} \frac{1}{\omega^2}$$

(or $\tilde{\sigma}(\omega)$ = this), where $\frac{1}{Z}\sum_i f_i = 1$ was used. Again, as in the case of $\tilde{\sigma}$, the $\omega \to \infty$ behavior is model independent (does not depend on $f_i, \gamma_i, \omega_i$), since at high frequency electrons are "paralyzed" (in the words of Garg).

We may write $\tilde{\epsilon}(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$

where $\omega_p^2 \equiv \frac{4\pi n q^2}{m}$ is the "Plasma" frequency of the medium.

Addendum: Wave propagation in dispersive medium.

In PHYS 203A we discussed wave propagation in dispersive media briefly. We took

$$\omega(k) = vk = \frac{c}{\sqrt{\tilde{\epsilon}(\omega)\tilde{\mu}(\omega)}}k$$

and then found that $\frac{\omega}{k} = \frac{c}{\sqrt{\tilde{\epsilon}\tilde{\mu}}}$ is the phase velocity, while $v_g = \frac{d\omega}{dk}$ gives the group velocity.

with $\frac{v_g}{c} = \frac{1}{c}\left(\frac{dk}{d\omega}\right)^{-1} = \left[\frac{d}{d\omega}\sqrt{\tilde{\epsilon}\tilde{\mu}}\,\omega\right]^{-1}$

and taking $\tilde{\mu}=1$, we have $\frac{c}{v_g} = \sqrt{\tilde{\epsilon}} + \frac{1}{2}\frac{\omega}{\sqrt{\tilde{\epsilon}}}\frac{d\tilde{\epsilon}}{d\omega}$

Ignoring (for now) the imaginary part of $\tilde{\epsilon}$, we see that in the region of anomalous dispersion $\left(\frac{d\check{\epsilon}}{d\omega} < 0\right)$ $\frac{v_g}{c}$ increases. Worse $\check{\epsilon}_1 < 0$ so even if one neglects $\tilde{\epsilon}_2$, the index of refraction $\tilde{n}(\omega) = \sqrt{\tilde{\epsilon}}$ is purely imaginary so neither $v_p$ nor $v_g$ are well defined.

Sticking to the $\mu = 1$ case, generally

$$\tilde{n} = \tilde{n}_1 + i\tilde{n}_2 = \sqrt{\tilde{\epsilon}_1 + i\tilde{\epsilon}_2} \Rightarrow \tilde{n}_1^2 - \tilde{n}_2^2 = \tilde{\epsilon}_1, \quad 2\tilde{n}_1\tilde{n}_2 = \tilde{\epsilon}_2$$

(Solve: $\tilde{n}_1^2 - \tilde{\epsilon}_1 - \frac{1}{4}\frac{\tilde{\epsilon}_2^2}{\tilde{n}_1^2} = 0 \Rightarrow \tilde{n}_1^2 = \frac{1}{2}\left(\tilde{\epsilon}_1 + \sqrt{\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2}\right) \Rightarrow \tilde{n}_2 = \frac{1}{2}\left(-\tilde{\epsilon}_1 + \sqrt{\tilde{\epsilon}_1^2 + \tilde{\epsilon}_2^2}\right)$

Recall wave equation is $\left(\nabla\times\vec{E} - i\frac{\omega}{c}\vec{B} = 0,\quad \vec{\nabla}\times\vec{B} + i\frac{\omega}{c}\tilde{\epsilon}(\omega)\vec{E} = 0\right)$

$$\left[\vec{\nabla}^2 + \frac{\omega^2}{c^2}\tilde{\epsilon}(\omega)\right]\vec{E} = 0$$

So in $e^{i(kz-\omega t)}$ for plane wave we have

$$k^2 = \frac{\omega^2}{c^2}\tilde{\epsilon}(\omega)$$

$$k = \frac{\omega}{c}\sqrt{\tilde{\epsilon}} = \frac{\omega}{c}(\tilde{n}_1 + i\tilde{n}_2)$$

So the region of anomalous dispersion, which coincides with non-negligible $\tilde{\epsilon}_2$ and therefore $\tilde{n}_2$, one has

$$E_\perp \cdot e^{i\omega(\tilde{n}_1\frac{z}{c} - t)}\, e^{-\tilde{n}_2\frac{\omega}{c}z}$$

and

$$\text{Intensity} \sim |E_\perp|^2 \propto e^{-z/\delta} \qquad \delta^{-1} = 2\frac{\tilde{n}_2\omega}{c}$$

where $\delta$ is the penetration length.

Sec 134: To make sense of velocity of propagation particularly in the region of anomalous dispersion one may define "energy velocity" $\vec{v}_E$:

$$\overline{\vec{S}} = \vec{v}_E \, \overline{U}$$

with Poynting and internal energy defined as previously. Since we are interested in velocity of propagation, but not on atenuation along the wave we ignore absorption (set $\tilde{n}_2 = 0$ so $\vec{k}$ is real). With this $\vec{S}$ is along $\vec{k}$. Moreover $\epsilon |\tilde{E}|^2 = \mu |\tilde{H}|^2$ so

$$\overline{\vec{S}} = \frac{c}{16\pi}\left(\tilde{E} \times \tilde{H}^* + c.c.\right) = \frac{c}{16\pi}\left[\sqrt{\frac{\epsilon}{\mu}}|\tilde{E}|^2 + \sqrt{\frac{\mu}{\epsilon}}|\tilde{H}|^2\right]$$

Now $\overline{U}$ was determined earlier, $\overline{U} = \frac{1}{8\pi}\left\{\frac{d}{d\omega}(\omega \tilde{\epsilon}_1)\overline{|E|^2} + \begin{matrix}\epsilon \to \mu \\ E \to H\end{matrix}\right\}$

so $\overline{S} = \frac{c}{8\pi}\sqrt{\frac{\epsilon}{\mu}}|\tilde{E}|^2$, $\overline{U} = \frac{1}{16\pi}\left[\frac{d(\omega\tilde{\epsilon}_1)}{d\omega} + \frac{\tilde{\epsilon}_1}{\tilde{\mu}_1}\frac{d(\omega\tilde{\mu}_1)}{d\omega}\right]|\tilde{E}|^2$ (the additional $\frac{1}{2}$ from $\overline{E(t)^2} = \frac{1}{2}|\tilde{E}(\omega)|^2$)

$$\Rightarrow \frac{c}{v_E} = \frac{1}{2}\left[\sqrt{\frac{\tilde{\mu}_1}{\tilde{\epsilon}_1}}\frac{d(\omega\tilde{\epsilon}_1)}{d\omega} + \sqrt{\frac{\tilde{\epsilon}_1}{\tilde{\mu}_1}}\frac{d(\omega\tilde{\mu}_1)}{d\omega}\right]$$

$$\text{or} \quad \frac{c}{v_E} = \frac{d}{d\omega}\left(\omega\sqrt{\tilde{\epsilon}_1\tilde{\mu}_1}\right) = \frac{d}{d\omega}(\tilde{n}_1 \omega) = \frac{c}{v_g}$$

the group velocity.

In the region of anomalous dispersion one cannot neglect absorption. The above treatment fails. But for the harmonicly-bound charges model one can compute explicitly.

See details in textbook. It shows $\frac{v_E}{c} \leq 1$.

(End Addendum)

## Note on $\tilde{\mu}(\omega)$

For frequencies $\omega \geq \omega_0$ where $\omega_0$ is no higher than optical, but possibly lower, it makes no physical sense to distinguish between $\vec{H}$ & $\vec{B}$.

Recall

$$\vec{H} - \vec{B} = 4\pi \vec{M} \quad \text{and} \quad \vec{J}_{bound} = c\,\vec{\nabla} \times \vec{M} + \frac{\partial \vec{P}}{\partial t}$$

Under what condition is the 1st term bigger than 2nd?

Estimate

$$|c\,\vec{\nabla} \times \vec{M}| \sim c \frac{1}{\text{length of variation}} \cdot \chi_m B \sim \frac{\chi_m c B}{l}$$

Also for $\frac{\partial \vec{P}}{\partial t}$, use the induced $\vec{E}$ field (it is magnetic response we care about!) $\vec{\nabla} \times \vec{E} + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} \rightarrow E \sim l\omega B/c$

and $\vec{P} = \chi_e \vec{E} \sim \vec{E}$ $\quad \left|\frac{\partial \vec{P}}{\partial t}\right| \sim l\,\omega^2 B/c$

So for $\left|\frac{\partial \vec{P}}{\partial t}\right| << c|\vec{\nabla} \times \vec{M}|$ we need $l\frac{\omega^2 B}{c} << \chi_m \frac{cB}{l}$

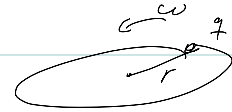
$$\Rightarrow \quad l^2 << \chi_m \frac{c^2}{\omega^2}$$

Moreover,
the dimensions of the body over which variations are considered, $l$, should be much larger than atomic, $l >> a$.

Need to know some rough scaling of $\chi_m$.

For a diamagnetic material (sec. 102)

model atom as bound electron in circular orbit

- $m_M = \frac{1}{2c} q \omega r^2$  ($\vec{m}_M$: magnetic dipole moment).

- $F = ma$: $\underset{\substack{\uparrow \\ \text{mass (not } m_M)}}{m\omega^2 r} = \underset{\substack{\uparrow \\ \text{central}}}{\frac{Zq^2}{r^2}} + \underset{\substack{\uparrow \\ \text{applied } B}}{\frac{q\omega r B}{c}}$ $\left(\vec{F} = \frac{q}{c}\vec{v}\times\vec{B}\right)$

- If $\omega_0$ $F_0$, $B = 0$ then $\omega_0^2 = \frac{Zq^2}{mr^3}$

and $\omega^2 = \omega_0^2 + \omega_0\omega_L$

where $\omega_0\omega_L = \frac{q\omega B}{mc}$

but we work at small B so set $\omega \simeq \omega_0$ on RHS

$\Rightarrow \omega_L = \frac{qB}{mc}$ is the Larmor frequency.

So the change in $m_M$ due to the applied field is

$$\Delta m_M = \frac{q}{2c} r^2 \Delta\omega = \frac{q}{2c} r^2 \left(\frac{\omega_L}{2}\right) = \frac{q^2}{4mc^2} r^2 B$$

Magnetization: $M = n\Delta m_M = \frac{q^2 n}{4mc^2} r^2 B \Rightarrow \chi_m = \frac{q^2 n r^2}{4mc^2}$

Now $\frac{Zq^2}{m} = \omega_0^2 r^3$ and $r^3 n \lesssim 1$ so $\chi_m \lesssim \left(\frac{\omega_0 r}{c}\right)^2$

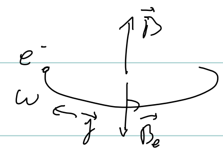
Added comment: there are two problems with the above (correct) argument

(i) we are taking $r$ = constant, but this is not guaranteed.

(ii) $\vec{B}$ does no work but our higher $\omega = \omega_0 + \omega_L$ state has higher energy; $\vec{B}$ as taken ($\perp$ to plane of orbit) does no torque, so $\vec{L} = m\vec{r}\times\vec{v}$ = constant, so $mr^2\omega$ = constant, also not consistent with $r$ = constant

The solution to this is that since $\vec{B}$ increases, $\vec{B} = \vec{B}(t)$ is not constant $\rightarrow$ $\vec{\nabla}\times\vec{E} = -\frac{1}{c}\frac{\partial\vec{B}}{\partial t}$ $\Rightarrow$ $\vec{E}$ is induced, does work and produces torque $\Rightarrow$ $r$ remains constant.

Let's check: increase $\delta\vec{B} = \delta t\,\frac{\partial\vec{B}}{\partial t}$. Assume the current produced by circling electron produces a magnetic field $B_e$ in direction opposite $\vec{B}$




Then $\Delta\vec{B}_e$ is along $\vec{B}_e$ (by Lenz's law): $\int\vec{E}\cdot d\vec{l} = -\frac{1}{c}\int d^2s\,\frac{\partial\vec{B}}{\partial t}$

$\Rightarrow E\,2\pi r = \frac{1}{c}\pi r^2\frac{\Delta B}{\Delta t}$. Note that $E\,2\pi r$ = work done on $e^-$.

and $N = qEr = \frac{q}{2c}r^2\frac{\Delta B}{\Delta t}$ = torque on $e^-$. $\Rightarrow \Delta L = N\,\delta t$.

The initial trajectory has

$$\mathcal{E} = \frac{1}{2}m(\omega_0 r_0)^2 - \frac{Zq^2}{r_0} \quad \text{and} \quad L_0 = m\,\omega_0 r_0^2$$

The final one has

$$\mathcal{E}_f = \frac{1}{2} m (r\omega)^2 - \frac{Zq^2}{r} = \mathcal{E}_0 + \frac{1}{c}\pi r_0^2 \frac{\Delta B}{\Delta t} \qquad L = mr^2\omega$$

Now $L = m(r_0^2 + 2r_0\delta r_0)(\omega_0 + \delta\omega_0) = L_0 + 2mr_0\omega_0\delta r + m r_0^2 \delta\omega$

$$= L_0 + \frac{q}{2c} r^2 \frac{\Delta B}{\Delta t}\delta t \Rightarrow 2mr_0\omega_0\delta r + mr_0^2\delta\omega_0 = \frac{q}{2c} r_0^2 \Delta B$$

The EOM gives $(F = ma)$ $\quad m\omega$

$$m\dot{\omega} r = qE = r\frac{q}{2c}\dot{B} \rightarrow \omega = \omega_0 + \frac{qB}{2mc}$$

note, this already gives

$$\Delta\omega = \frac{1}{2}\omega_L = \frac{qB}{2mc}$$

that we used!

and

$$m\omega^2 r = \frac{Zq^2}{r^2} + \frac{q}{c}\omega r B$$

with $\frac{qB}{c} = m\omega_L$

$$m\omega(\omega - \omega_L) r = \frac{Zq^2}{r}$$

$$\Rightarrow m(\omega_0 - \tfrac{1}{2}\omega_L)(\omega_0 + \tfrac{1}{2}\omega_L) r = \frac{Zq^2}{r} \quad (= m\omega_0^2 r)$$

Something is wrong? Is the statement true only to linear order?

Also $\frac{dL}{dt} = N = qEr = \frac{qr^2}{2c}\frac{dB}{dt}$, $L = mr^2\omega$

$$\frac{dL}{dt} = 2mr\dot{r}\omega + mr^2\dot{\omega} = 2mr\dot{r}\omega + r^2\frac{q\dot{B}}{2c} = \frac{qr^2}{2c}\frac{dB}{dt} \Rightarrow \dot{r} = 0.$$

Clearly $r = r_0 + O(\Delta B^2)$ so good enough for our purpose (linear response); but would be nice to figure it out

END ADDENDUM

Returning to the question of when the frequency response becomes relevant we had

$a^2 \ll l^2 \ll \chi_m \frac{c^2}{\omega^2}$ and now we know $\chi_m \lesssim \left(\frac{\omega_0 a}{c}\right)^2$

($a = r$ = atomic size = atomic separation; the "$\lesssim$" because we used $na^3 = 1$, but for rare media $na^3 \ll 1$).

Hence

$$\boxed{\omega \ll \omega_0 \simeq \text{optical frequencies}}$$

is the condition for $\tilde{\mu}(\omega)$ to make sense physically. For optical frequencies and above (and possibly starting even below that, as the string of "$\gg$" and assumptions above shows) we may as well use $\mu = 1$ and keep track of $c\vec{\nabla}\times\vec{M} + \frac{\partial\vec{P}}{\partial t}$ (dominated by $\frac{\partial\vec{P}}{\partial t}$) through $\tilde{\epsilon}(\omega)$..

[Note added: why keep $r$ fixed when turning $B \neq 0$? $\vec{D}$ does no work and no torque: $E_0 = E_{final}$, $E_0 = \frac{1}{2}m\omega^2 r^2 - \frac{Zq^2}{r} = \frac{1}{2}\frac{L^2}{mr^2} - \frac{Zq^2}{r}$, $L_0 = m\omega_0 r^2 = L_{final}$.

$\Rightarrow m\omega_f r_f^2 = m\omega_0 r_0^2$ and $\frac{L^2}{2mr_0^2} - \frac{Zq^2}{r_0} = \frac{L^2}{2mr^2} - \frac{Zq^2}{r} + \frac{q\omega r B}{2}$

$\Rightarrow$ 2 eqs, 2 unknowns $\Rightarrow$