Lecture 2 - Atoms and Photons

Interaction between matter and radiation

"atom" - quantum system, few levels

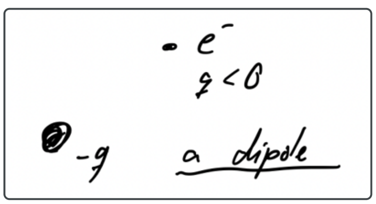
"photon" - non-relativistic, in the visible, IR, microwave, RF

phenomenological coefficients:

- refractive index $n(\omega)$
- absorption coefficient $a(\omega)$

1. Phenomenological approaches

1.1. Lorentz model - elastically bound electron:



$m\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} = -m\omega_0^2\vec{r}$

ω_0 - resonance frequency

Let's add a driving field in the dipole approximation, so no $\vec{r}$-dependence (the atom being much smaller than the wavelength λ):

$\vec{E}(t) = \vec{E}\cos(\omega t)$.

We then have

$$m\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} = -m\omega_0^2\vec{r} + q\vec{E}\cos(\omega t)$$

Introduce the dipole $\vec{d} = q\vec{r}$

$$\frac{\mathrm{d}^2\vec{d}}{\mathrm{d}t^2} + \omega_0^2\vec{d} = \frac{q^2}{m}\vec{E}\cos(\omega t)$$

Notation: We'll often use complex notation:

$$
\begin{aligned}
\vec{E}(\vec{r},t) &= \vec{E}(\vec{r})\cos(\omega t+\phi) \\
&= \vec{E}(\vec{r})\frac{e^{-i\phi}}{2}e^{-i\omega t} + \vec{E}(\vec{r})\frac{e^{i\phi}}{2}e^{i\omega t} \\
&\equiv \vec{E}^{+}(\vec{r})e^{-i\omega t} + \vec{E}^{-}(\vec{r})e^{i\omega t}
\end{aligned}
$$

> Remember: $\vec{E}^{+}$ goes with the *positive* frequency piece $e^{-i\omega t}$, and $\vec{E}^{-}$ goes with the *negative* frequency piece $e^{i\omega t} = e^{-i(-\omega)t}$.
> So then $\vec{E}(t) = \vec{E}^{+}e^{-i\omega t} + \text{c.c} = 2\text{Re}\left\{\vec{E}^{+}e^{-i\omega t}\right\}$
>
> For classical fields this is just for convenience, but for quantum fields the two components will play the role of photon annihilation and creation operators. Note an obvious but awkward factor of two in $\vec{E}^{+} = \frac{\vec{E}}{2}$ between the amplitude of the cosine and the amplitude of the $e^{-i\omega t}$.

So if we know the solution to the following equation:

$$
\frac{\mathrm{d}^2\vec{d}^{+}}{\mathrm{d}t^2} + \omega_0^2\vec{d}^{+} = \frac{q^2}{m}\vec{E}^{+}e^{-i\omega t}
$$

the solution for the (real) dipole is $\vec{d} = 2\text{Re}\left(\vec{d}^{+}\right)$.

Say the $\vec{E}$-field has polarization $\vec{\epsilon}$, so $\vec{E}^{+} = \vec{\epsilon}E_0^{+}$. After a long drive transients will have damped out and the dipole will follow the drive. We thus make the Ansatz:
$\vec{d}^{+} = \vec{\epsilon}\, d_0^{+}e^{-i\omega t}$

We have

$$
\Rightarrow -\omega^2 d_0^{+} + \omega_0^2 d_0^{+} = \frac{q^2E_0^{+}}{m}
$$

and find:

$$
d_0^{+} = \frac{q^2E_0^{+}/m}{\omega_0^2-\omega^2} \approx \frac{q^2E_0^{+}/m}{2\omega(\omega_0-\omega)}
$$

Define polarizability: $\vec{d}_0^{+} = \alpha(\omega)\vec{E}_0^{+}$
with $\alpha(\omega) = \frac{q^2/m}{\omega_0^2-\omega^2}$

(sign check: $\alpha(\omega\to 0) > 0$, as it should be: At DC (so at $\omega = 0$), d is in phase with E).

Given N atoms per unit volume, the polarization density is:

$$\begin{aligned}\vec{P}^{+} &= N\vec{d}^{+} = N\alpha(\omega)\vec{E}^{+} \\ &= \vec{\epsilon}\frac{Nq^2/m}{\omega_0^2-\omega^2}\vec{E}_0^{+}e^{-i\omega t}\end{aligned}$$

Susceptibility is defined by: $\vec{P} = \epsilon_0\chi\vec{E}$

with

$$\chi(\omega) = \frac{N}{\epsilon_0}\alpha(\omega) = \frac{Nq^2/m\epsilon_0}{\omega_0^2-\omega^2}$$

the classical susceptibility of the undamped oscillating charge.

Now let's include a damping γ (from radiation reaction - the classical analogue of spontaneous emission - and collisions). Then we have

$$m\frac{\mathrm{d}^2\vec{r}}{\mathrm{d}t^2} + m\omega_0^2\vec{r} + m\gamma\frac{\mathrm{d}\vec{r}}{\mathrm{d}t} = q\vec{E}\cos(\omega t)$$

$$\frac{\mathrm{d}^2\vec{d}^{+}}{\mathrm{d}t^2} + \omega_0^2\vec{d}^{+} + \gamma\frac{\mathrm{d}\vec{d}^{+}}{\mathrm{d}t} = \frac{q^2}{m}\vec{\epsilon}E_0^{+}e^{-i\omega t}$$

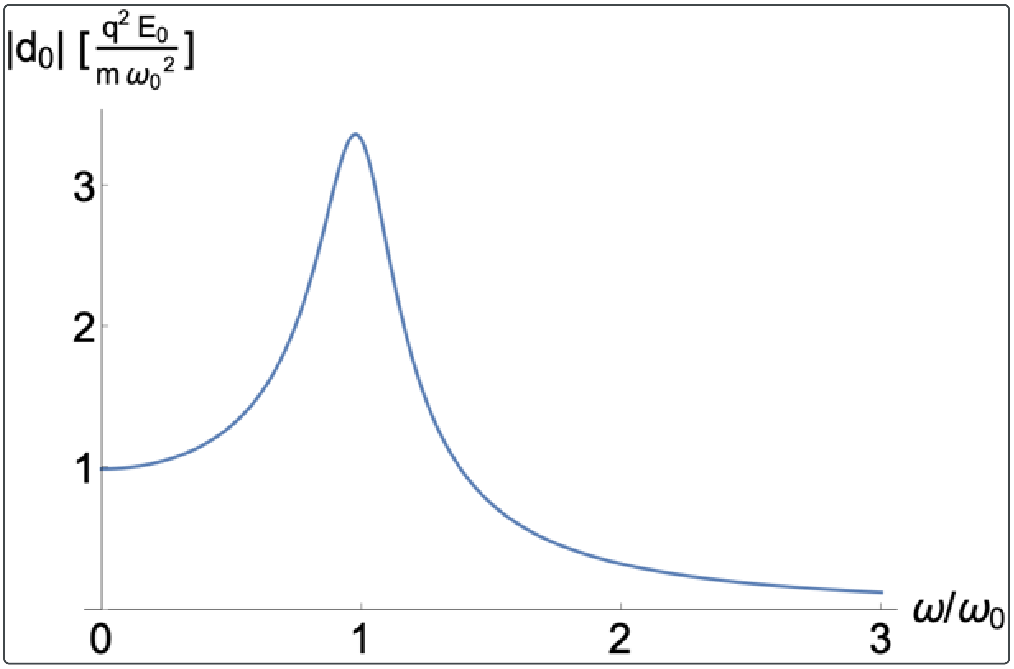
Again making the Ansatz $\vec{d}^{+} = \vec{\epsilon}d_0^{+}e^{-i\omega t}$ gives:

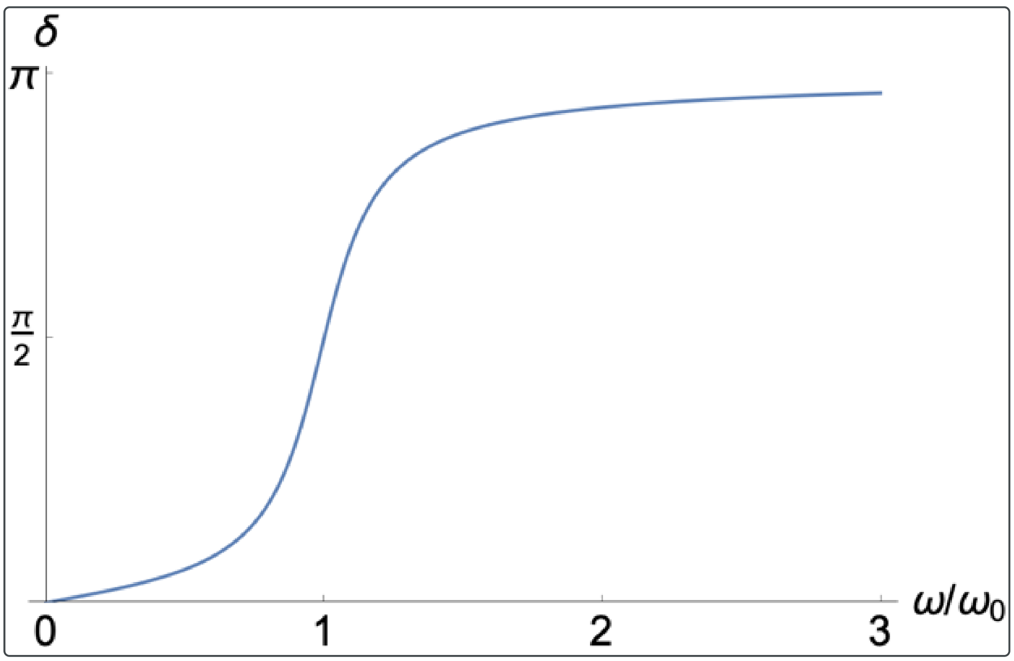
$$-\omega^2 d_0^{+} + \omega_0^2 d_0^{+} - i\gamma\omega d_0^{+} = \frac{q^2E_0^{+}}{m}$$

And we get:

$$d_0^{+} = \frac{q^2E_0^{+}}{m}\frac{1}{\omega_0^2-\omega^2-i\gamma\omega} \equiv |d_0^{+}|e^{i\delta}$$

with magnitude $|d_0^{+}|$ and phase lag δ as shown:





The phase $\delta = \arctan\left(\frac{\gamma\omega}{\omega_0^2-\omega^2}\right)$ is a phase *lag* since $\vec{d}^+ = \vec{\epsilon}|d_0^+|e^{-i\omega t+i\delta} \propto e^{-i(\omega t-\delta)}$, so the (real) dipole goes like $\vec{d} \propto \cos(\omega t - \delta)$. Physically, it is obvious that the driven oscillator lags behind the drive.

Note that the phase $\delta = \pi/2$ when the drive is exactly on resonance with the oscillator, while the magnitude $|d_0^+|$ is not exactly maximal on resonance. Writing

$$\frac{1}{\omega_0^2-\omega^2-i\gamma\omega} = \frac{\omega_0^2-\omega^2+i\gamma\omega}{(\omega_0^2-\omega^2)^2+(\gamma\omega)^2} \equiv \frac{1}{\omega_0^2}(u+iv)$$

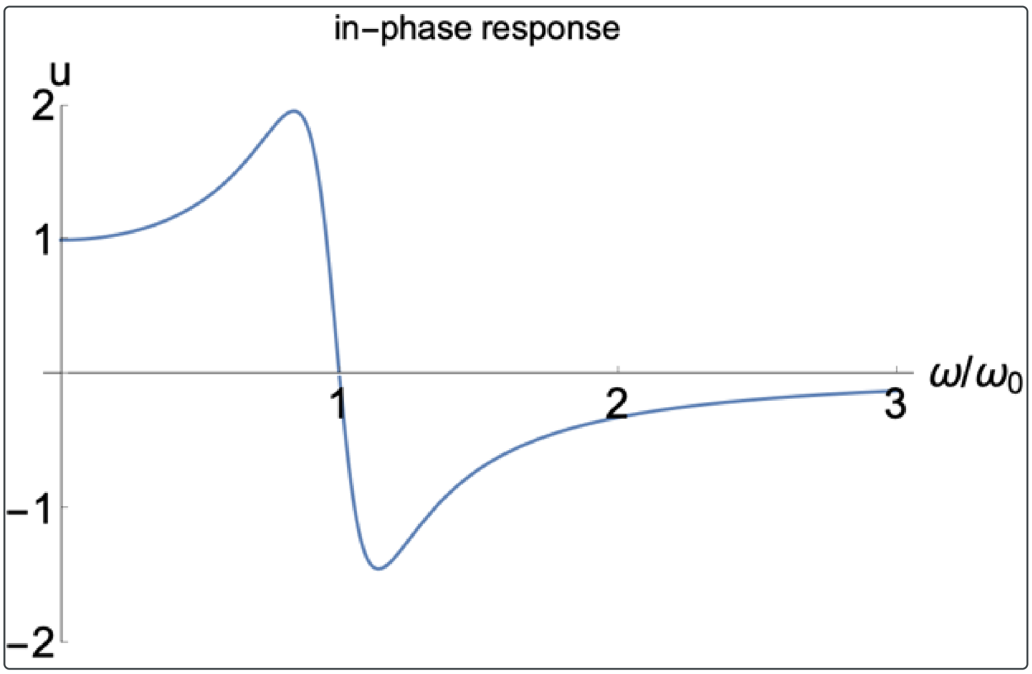
(u, v are thus dimensionless), we have for the (real) dipole:

$$\vec{d} = \mathrm{Re}\left[\frac{q^2 E_0}{m\omega_0^2}(u + iv)e^{-i\omega t}\right] = d_{\mathrm{DC}}(u\cos\omega t + v\sin\omega t)$$

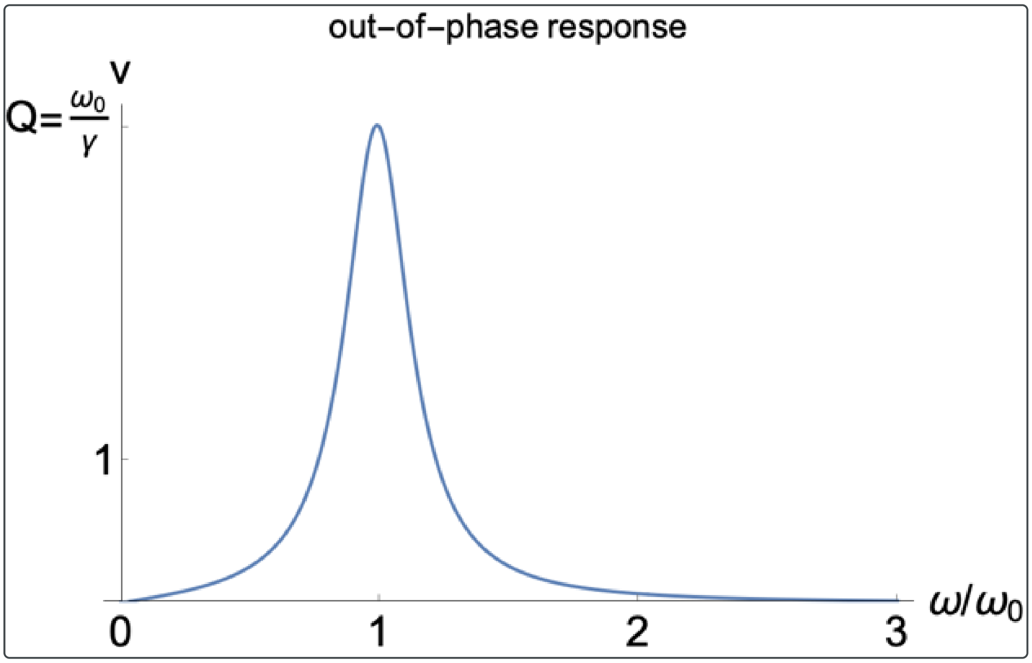
with the DC ($\omega = 0$) reponse $d_{\mathrm{DC}} = \frac{q^2 E_0}{m\omega_0^2}$. So in all glory:

$$\vec{d} = \frac{q^2 E_0}{m}\left\{\frac{\omega_0^2 - \omega^2}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}\cos\omega t + \frac{\gamma\omega}{(\omega_0^2 - \omega^2)^2 + (\gamma\omega)^2}\sin\omega t\right\}$$

We note that the component u that's in phase with the drive (called the elastic amplitude) is a dispersion curve, vanishing on resonance and changing sign from positive at $\omega < \omega_0$ (the dipole faithfully follows a slow drive) to negative above resonance.



The component out-of-phase with the drive is an absorptive curve:



Again, although it's almost an academic point, v is not exactly maximal on resonance ($\omega = \omega_0$), but the time-averaged power provided by the drive is. The power (not to be confused with polarizability) is:

$$
\begin{aligned}
P(t) = \vec{F} \cdot \dot{\vec{r}} = \vec{E} \cdot \dot{\vec{d}} &= E_0 \cos(\omega t) d_{\mathrm{DC}} \left[-\omega u \sin(\omega t) + \omega v \cos(\omega t) \right] \\
&= d_{\mathrm{DC}} E_0 \omega \left(-\frac{1}{2} u \sin(2\omega t) + v \cos^2(\omega t) \right)
\end{aligned}
$$

The absorptive (out-of-phase) response always leads to energy put into the atom by the driving field, while the elastic (in-phase) response oscillates between the field putting energy into the oscillator, and the oscillator returning energy to the drive. The elastic portion time-averages to zero. The time-averaged power is purely due to the absorptive (out-of-phase) response

$$
\langle P \rangle = \frac{1}{2} d_{\mathrm{DC}} E_0 \, \omega \, v = \frac{q^2 E_0^2}{2m} \frac{\gamma \omega^2}{(\omega_0^2 - \omega^2)^2 + (\gamma \omega)^2}
$$

As you can check, this is actually maximal on resonance $\omega = \omega_0$, where it's value is $\langle P \rangle = \frac{q^2 E_0^2}{2m\gamma}$.

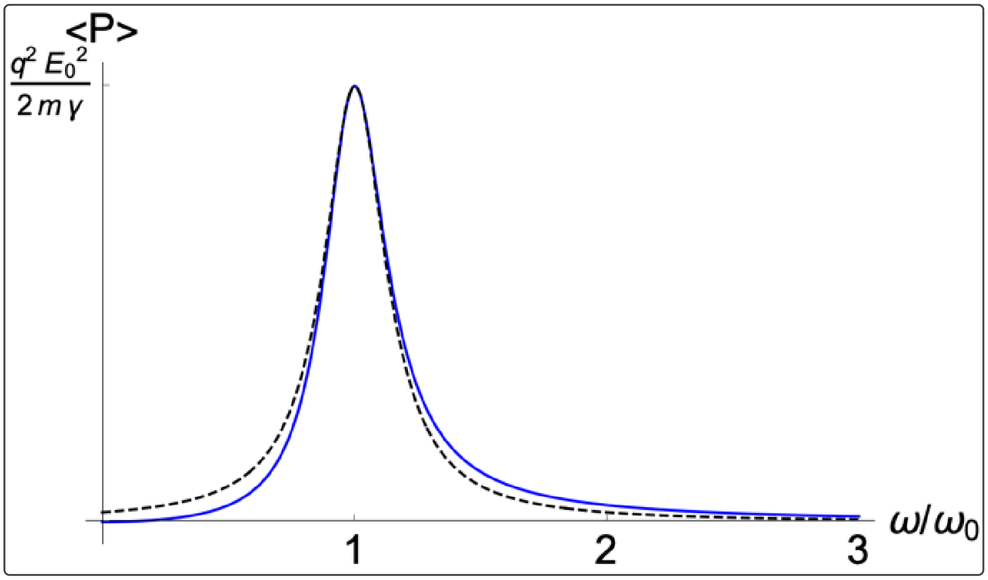
Close to resonance, $\omega \approx \omega_0$, we can use

$$
\omega_0^2 - \omega^2 = (\omega_0 + \omega)(\omega_0 - \omega) \approx 2\omega_0(\omega_0 - \omega)
$$

and the dependence of power with frequency

$$\langle P \rangle \approx \frac{q^2 E_0^2}{8m} \frac{\gamma}{(\omega_0 - \omega)^2 + \frac{\gamma^2}{4}}$$

becomes a Lorentzian of FWHM γ.



The blue curve is the exact expression, the dashed black line the Lorentzian approximation, quite good already for $\gamma = 0.3\omega_0$ used here, so a $Q = \omega_0/\gamma$ of the oscillator of 3.3.

Given the susceptibility χ, we can obtain the index of refraction. Recall from electrodynamics in media that the polarization density causes a displacement field $\vec{D} = \epsilon_0 \vec{E} + \vec{P} \equiv \epsilon \vec{E}$, with the dielectric constant being related to the susceptibility by

$$\epsilon = \epsilon_0 (1 + \chi).$$

Also recall that the index of refraction gives the phase velocity in the medium $v = \frac{1}{\mu\epsilon} = \frac{c}{n}$ and so $n \approx \sqrt{\frac{\epsilon}{\epsilon_0}} = \sqrt{1+\chi} \approx 1 + \frac{\chi}{2}$ in dilute systems where $\chi \ll 1$. Using our result we find

$$\bar{n}(\omega) = 1 + \frac{Nq^2}{2m\epsilon_0\omega_0^2}(u + iv)$$

The complex index of refraction $\bar{n}$ signifies phase shifts and attenuation of a plane wave:

$$E(z) = E_0 e^{ikz} = E_0 e^{ink_0 z} = E_0 e^{i\mathrm{Re}(n)k_0 z} e^{-\mathrm{Im}(n)k_0 z}$$

The phase index is thus

$$n(\omega) = \mathrm{Re}(\bar{n}(\omega)) = 1 + \frac{Nq^2}{2m\epsilon_0\omega_0^2}u = 1 + \frac{1}{2}\chi_{\mathrm{DC}}\, u.$$

The intensity I lost per unit distance from the plane wave is described by the absorption coefficient, as in

$$\frac{\mathrm{d}I}{\mathrm{d}z} = -aI \Rightarrow I(z) = I_0 e^{-az}$$

We thus obtain the absorption coefficient as

$$a(\omega) = 2k_0\mathrm{Im}(\bar{n}(\omega)) = \frac{1}{c}\chi_{\mathrm{DC}}\,\omega v$$

with the DC susceptibility $\chi_{\mathrm{DC}} = \frac{N}{\epsilon}\alpha_{\mathrm{DC}} = \frac{Nq^2}{m\epsilon_0\omega_0^2}$.

As it should be, absorption goes like the dissipated power, and so also has the same absorptive profile versus frequency as we had above, well described by a Lorentzian.

The absorption coefficient directly gives the scattering cross section via $a = \sigma N$, so the classical scattering cross section on resonance is

$$\sigma_{\mathrm{classical}} = \frac{q^2}{m\epsilon_0 c\gamma}$$

The correct quantum mechanical cross section for a two-level atom, averaged over all possible orientations in space, is

$$\sigma_{\mathrm{quantum,isotropic}} = \frac{\lambda_0^2}{2\pi}.$$

The ratio of the quantum to the classical cross section defines the oscillator strength of the transition.

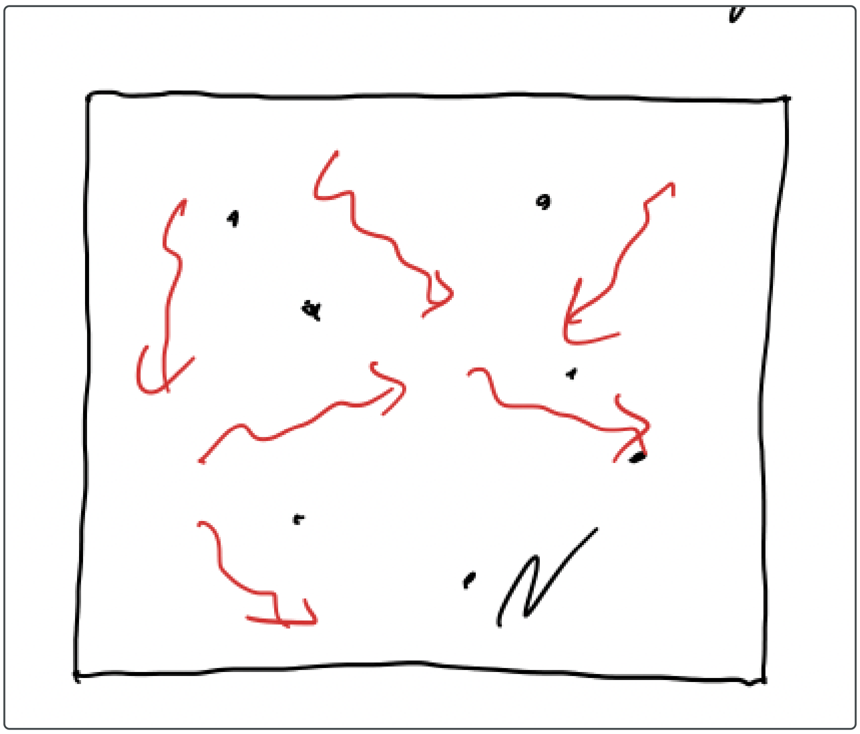
(For atomic dipole moments aligned with the field, the cross section is $\sigma_{\mathrm{quantum}} = \frac{3\lambda_0^2}{2\pi}$.)

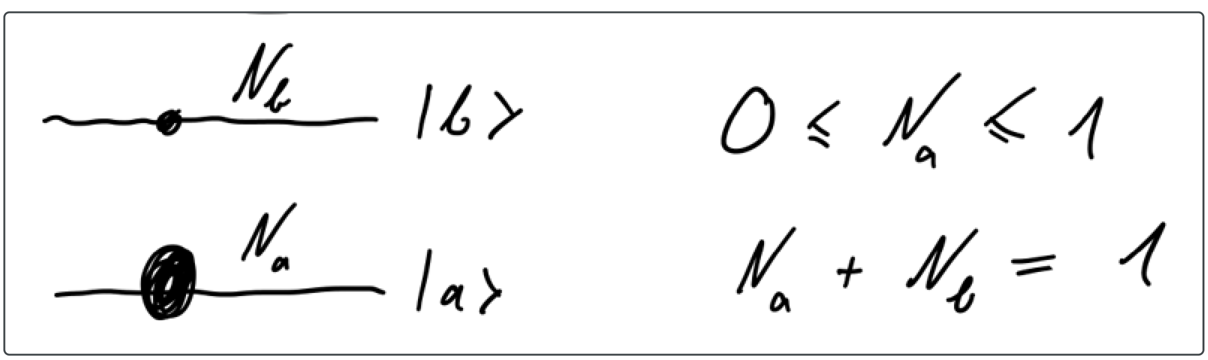
Let's note that the real and the imaginary part of the susceptibility obey the Kramers-Kronig relations

$$\mathrm{Re}\chi(\omega) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Im}\chi(\omega')}{\omega' - \omega}\mathrm{d}\omega'$$

> $$\mathrm{Im}\chi(\omega) = -\frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{\mathrm{Re}\chi(\omega')}{\omega' - \omega}\mathrm{d}\omega'$$
>
> where the $\mathcal{P}$ denotes the "Principal part", i.e. you cut out an infinitesimal region around the pole at $\omega' = \omega$. These relations are a direct consequence of causality, namely that the polarization field can only depend on the elctric field in the present or past. To remember is that there is no dispersion without absorption, and vice versa.

1.2. Einstein model (1916)

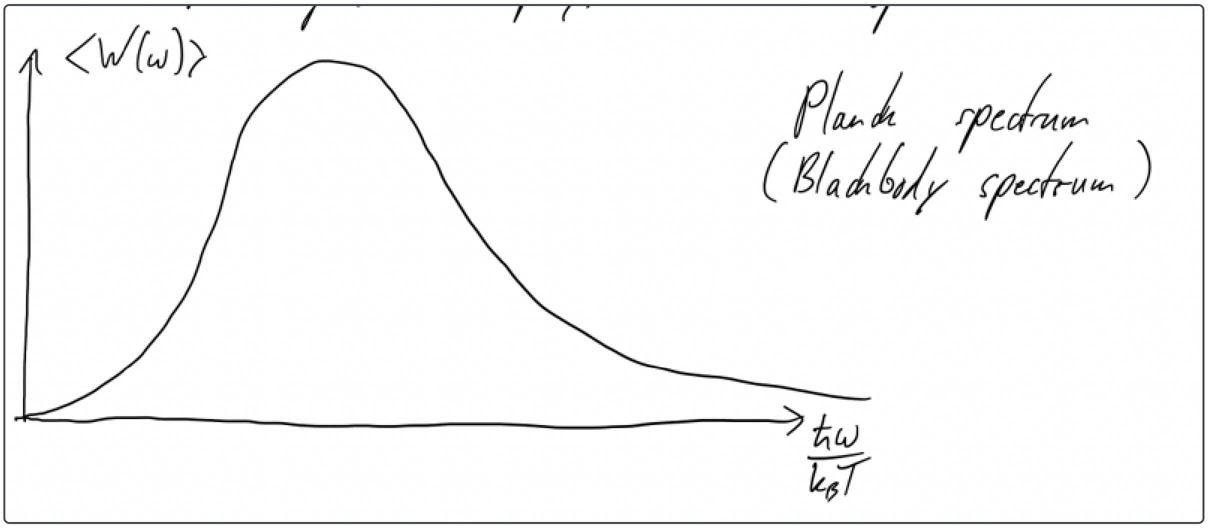




Einstein's idea is that the thermal distribution over energy states in an atom must be reached by interaction with a thermal light field alone, so through absorption and emission processes.

He includes spontaneous emission, as any oscillating charge should radiate energy away. He also includes the possibility that the light field can transfer energy to the atom and vice versa, as as a driving field can perform work on the atom or receive energy back from the atom, depending on the relative phase of the oscillator and the drive. This is stimulated emission and absorption.

The e.m. field is characterized by a spectral energy density $u(\nu) = \frac{\mathrm{d}U}{\mathrm{d}\nu}$. Here, U is the energy density.



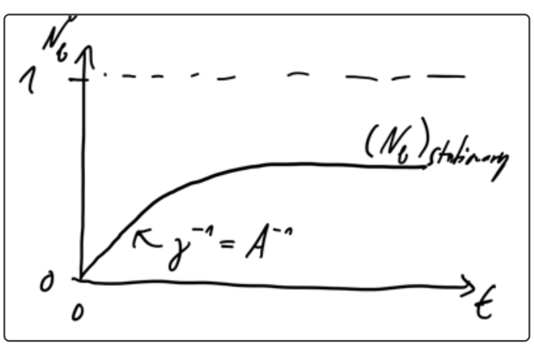
Einstein shows that the rate coefficients of stimulated emission and absorption must be equal. The rate equation is

$$\frac{\mathrm{d}N_b}{\mathrm{d}t} = -\frac{\mathrm{d}N_a}{\mathrm{d}t} = -AN_b + B(N_a - N_b)u\left(\nu = \frac{\omega_0}{2\pi}\right)$$

A describes relaxation, so it will be our γ.

In equilibrium, we should have $AN_b = B(N_a - N_b)u(\nu) = B(1 - 2N_b)u(\nu)$. Thus

$$N_b = \frac{B}{\gamma + 2Bu}u$$



At low $u \ll \gamma/2B$ this is linear in u. However, at large $u \gg \gamma/2B = u_{\text{sat}}$ this gives $N_b \to 1/2$, equilibrium of populations $\Rightarrow$ saturation.

The power exchanged with the field has the sign of $N_b - N_a$. So amplification of light is possible if $N_b > N_a$! $\Rightarrow$ Laser!

In thermal equilibrium, we should find $N_b/N_a = e^{-(E_b-E_a)/k_BT} = e^{-h\nu/k_BT}$.

So then from above: $AN_b = BN_a(1 - N_b/N_a)u(\nu_0)$ or $Ae^{-h\nu/k_BT} = B(1 - e^{-h\nu/k_BT})u(\nu)$ and thus

$$u(\nu) = \frac{A}{B}\frac{1}{e^{h\nu/k_BT} - 1}$$

which is Planck's relation.

Einstein's model works well to describe thermal radiation fields, and populations in laser media.

So far: No photons!