

1. Complex dielectric constant

Note: ϵ_0 - vacuum permittivity, $\epsilon_0 = \epsilon(0) = \epsilon(\omega = 0)$.

Equation of motion:

$$\ddot{\mathbf{u}} + \gamma\dot{\mathbf{u}} = -\frac{k}{\mu}\mathbf{u} + \frac{q}{\mu}\mathbf{E}_{\text{loc}}, \quad (1)$$

where $\frac{k}{\mu} = \omega_0^2$.

By inserting the ansatz $\mathbf{u} = \mathbf{u}_0 e^{-i\omega t}$ (and implicitly $\mathbf{E}_{\text{loc}} = \mathbf{E}_0 e^{-i\omega t}$) we get

$$-\omega^2 \mathbf{u} - i\omega\gamma \mathbf{u} = -\omega_0^2 \mathbf{u} - \frac{q}{\mu} \mathbf{E}_{\text{loc}} \quad (2)$$

$$\Rightarrow \mathbf{u} = \frac{q}{\mu} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} \mathbf{E}_{\text{loc}}. \quad (3)$$

The polarization can be expressed microscopically as $\mathbf{P} = nq\mathbf{u} + n\alpha\mathbf{E}_{\text{loc}}$ and macroscopically as $\mathbf{P} = (\epsilon - 1)\epsilon_0\mathbf{E}_{\text{mac}}$. Because we are ultimately interested in understanding the behaviour of a single oscillator, we assume a sparse (and isotropic and spherical) sample so that $\mathbf{E}_{\text{loc}} = \mathbf{E}_{\text{mac}} = \mathbf{E}_{\text{ext}} = \mathbf{E}$. Then, we get by setting " $\mathbf{P} = \mathbf{P}$ "

$$nq\mathbf{u} + n\alpha\mathbf{E} = (\epsilon - 1)\epsilon_0\mathbf{E} \quad (4)$$

$$\frac{nq^2}{\mu} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} \mathbf{E} + n\alpha\mathbf{E} = (\epsilon - 1)\epsilon_0\mathbf{E} \quad (5)$$

$$\epsilon = 1 + \frac{nq^2}{\mu\epsilon_0} \frac{1}{\omega_0^2 - \omega^2 - i\omega\gamma} + \frac{n\alpha}{\epsilon_0} \quad (6)$$

Next, let's rewrite this in terms of ϵ_0 and ϵ_∞ . By taking limits $\omega \rightarrow 0$ and $\omega \rightarrow \infty$ we get

$$\epsilon_0 = 1 + \frac{nq^2}{\mu\epsilon_0} \frac{1}{\omega_0^2} + \frac{n\alpha}{\epsilon_0} \quad (7)$$

and

$$\epsilon_\infty = 1 + \frac{n\alpha}{\epsilon_0}, \quad (8)$$

respectively. Note that $\epsilon_0 - \epsilon_\infty = \frac{nq^2}{\mu\epsilon_0} \frac{1}{\omega_0^2}$

Thus, we get

$$\epsilon(\omega) = \epsilon_\infty + \frac{\omega_0^2(\epsilon_0 - \epsilon_\infty)}{\omega_0^2 - \omega^2 - i\gamma\omega}. \quad (9)$$

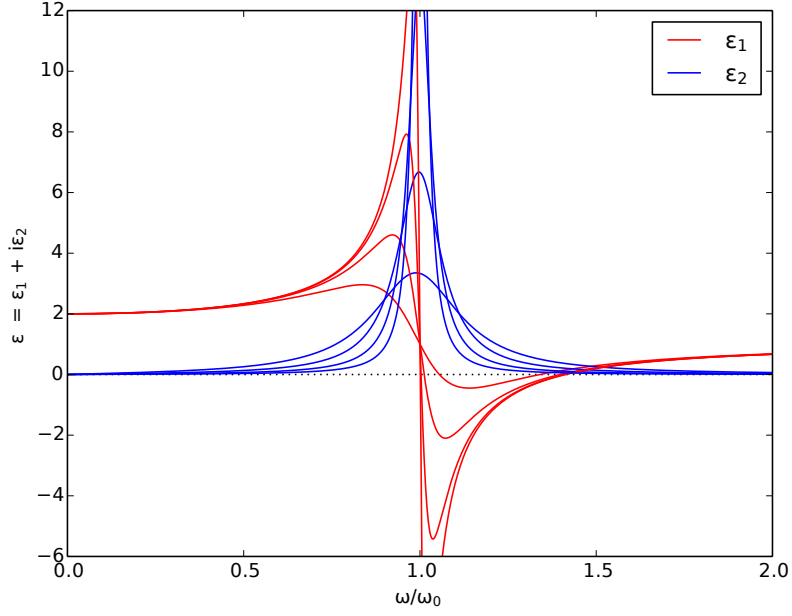
Now, let's separate the real and imaginary parts

$$\epsilon(\omega) = \epsilon_\infty + \frac{\omega_0^2(\epsilon_0 - \epsilon_\infty)}{\omega_0^2 - \omega^2 - i\omega\gamma} \cdot \frac{\omega_0^2 - \omega^2 + i\omega\gamma}{\omega_0^2 - \omega^2 + i\omega\gamma} \quad (10)$$

$$= \epsilon_\infty + \frac{(\epsilon_0 - \epsilon_\infty)\omega_0^2(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2} + i \frac{(\epsilon_0 - \epsilon_\infty)\omega_0^2\gamma\omega}{(\omega_0^2 - \omega^2)^2 + \omega^2\gamma^2} \quad (11)$$

$$\equiv \epsilon_1(\omega) + i\epsilon_2(\omega). \quad (12)$$

We note that $\epsilon(\omega)$ has divergence when $\gamma \rightarrow 0$. Thus, when calculating the peak of ϵ_2 and the zeros of ϵ_1 , one needs to first evaluate the condition for peak/zero and only after that take the limit $\gamma \rightarrow 0$. This leads to long but straightforward algebra, which we can avoid by remembering to treat the divergence specially. Figure tells more than thousand words, so see below the plot of $\epsilon(\omega)$ with $\epsilon_0 = 2$, $\epsilon_\infty = 1$, and different damping factors γ (peak gets thinner and the divergence develops as $\gamma \rightarrow 0$).



Peak of ϵ_2 , small damping limit:

When $\gamma \rightarrow 0$,

$$\epsilon_2 \rightarrow \frac{(\epsilon_0 - \epsilon_\infty)\omega_0^2\gamma\omega}{(\omega_0^2 - \omega^2)^2}. \quad (13)$$

The peak corresponds to the divergence at $\omega = \omega_0 \equiv \omega_T$.

Zeros of ϵ_1 , small damping limit:

When $\gamma \rightarrow 0$,

$$\epsilon_1 \rightarrow \epsilon_\infty + \frac{(\epsilon_0 - \epsilon_\infty)\omega_0^2}{\omega_0^2 - \omega^2}. \quad (14)$$

This equals to zero when $\omega^2 = \frac{\epsilon_0}{\epsilon_\infty}\omega_0^2 \equiv \omega_L^2$. Additionally, ϵ_1 diverges at ω_0 and changes sign. Thus, there is a zero at $\omega \approx \omega_0$ when γ is non-zero though small (see the figure above).

2. Plasma frequency in atomic units

In atomic units, the numeric values of the following physical quantities are set to unity:

$$m_e = e = \hbar = \frac{1}{4\pi\epsilon_0} = 1. \quad (15)$$

The units are can be marked, e.g. in the case of mass, as m_e , a.u., or nothing, with the latter two somewhat ambiguous. It can be inferred, that length is in the units of Bohr radius ($a_0 \approx 0.529 \text{ \AA}$) and energy in Hartree ($\text{Ha} \approx 27.211 \text{ eV}$).

The Wigner-Seitz radius r_s is defined by equating the mean volume per particle (here, electron) in a system to a volume of sphere:

$$\frac{4}{3}\pi r_s^3 = \frac{V}{N} = \frac{1}{n}. \quad (16)$$

The plasma frequency is

$$\omega_p = \sqrt{\frac{ne^2}{m_e\epsilon_0}} = \sqrt{\frac{3e^2}{4\pi r_s^3 m_e\epsilon_0}} \quad (17)$$

in SI units [rad/s], or, in atomic units

$$\omega_p = \sqrt{\frac{3}{r_s^3}} \quad (18)$$

In silver $r_s = 3.02$ (a_0), and thus $\omega_p = 0.33$ (Ha/\hbar) or in the units of energy $\hbar\omega_p = 0.33 \text{ Ha} = 8.98 \text{ eV}$.

3. Magnetization

- (a) Let the field be aligned in the z direction, i.e., $\mathbf{B} = (0, 0, B_z)$. For the given $J = 1/2$, we have $J_z = \pm\frac{1}{2}$, i.e., the ion has two possible states. The magnetic moment of the ion is $m_z = -g\mu_B J_z = \mp\mu_B$ and the corresponding energy is $E = -\mathbf{m} \cdot \mathbf{B} = -m_z B_z = \pm\mu_B B_z$.

The probability of a state at a given temperature T is given by the Boltzmann factor $P(E) = e^{-E/k_B T}$. Thus, the thermal average is

$$\langle m_z \rangle = \frac{-\mu_B e^{-\mu_B B_z/k_B T} + \mu_B e^{\mu_B B_z/k_B T}}{e^{-\mu_B B_z/k_B T} + e^{\mu_B B_z/k_B T}} \quad (19)$$

where the denominator normalizes the probabilities. The exponential factors can be rewritten as

$$\langle m_z \rangle = \mu_B \tanh\left(\frac{\mu_B B_z}{k_B T}\right) \quad (20)$$

to yield the magnetization

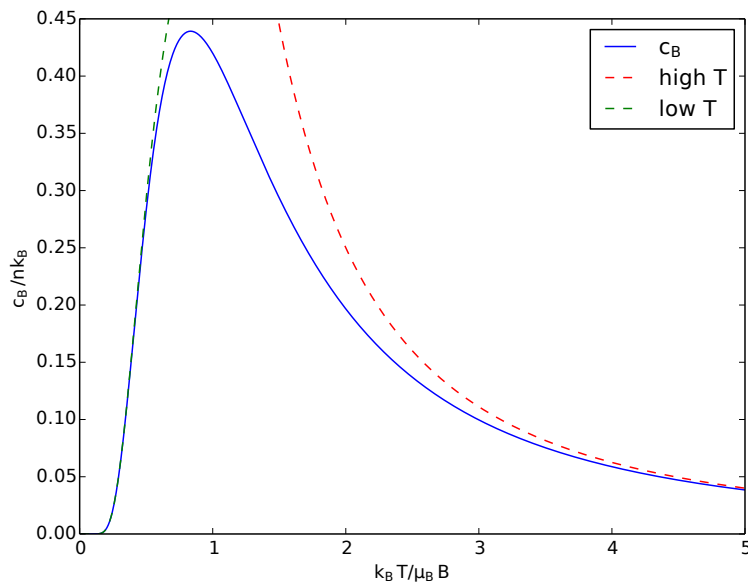
$$M = n\langle m_z \rangle = n\mu_B \tanh\left(\frac{\mu_B B_z}{k_B T}\right), \quad (21)$$

where n is the density of ions.

- (b) The internal energy per unit volume is $u = -\mathbf{M} \cdot \mathbf{B} = -MB_z = -n\mu_B \tanh(\mu_B B_z/k_B T)B_z$. The heat capacity per unit volume in a constant magnetic field B is

$$c_B = \left(\frac{\partial u}{\partial T}\right)_B = nk_B \left(\frac{\mu_B B_z}{k_B T}\right)^2 \frac{1}{\cosh^2\left(\frac{\mu_B B_z}{k_B T}\right)}. \quad (22)$$

See below a plot of c_B and the limiting forms.



By writing $\cosh x$ in terms of exponential functions and using series expansions for them, one gets limiting forms

$$\cosh^2 x = \begin{cases} \left(1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \dots\right)^2 \approx 1, & x \ll 1 \\ \frac{1}{4}(e^x + e^{-x})^2 \approx \frac{1}{4}e^{2x}, & x \gg 1 \end{cases} \quad (23)$$

Thus

$$c_B \approx \begin{cases} nk_B \left(\frac{\mu_B B_z}{k_B T}\right)^2, & T \gg \mu_B B_z/k_B \text{ (high T)} \\ 4nk_B \left(\frac{\mu_B B_z}{k_B T}\right)^2 e^{-2\mu_B B_z/k_B T}, & T \ll \mu_B B_z/k_B \text{ (low T)} \end{cases} \quad (24)$$

Let's calculate the temperature at the peak of $c_B(T)$. The derivative at zero gives ($x \equiv \mu_B B_z / k_B T$)

$$\frac{d}{dx} \left(\frac{x^2}{\cosh^2 x} \right) = \frac{2x \cosh x - 2x^2 \sinh x}{\cosh^3 x} = 0 \quad (25)$$

from which

$$x = 0 \quad \text{or} \quad x \sinh x = \cosh x \quad \Rightarrow \quad x \approx 1.2 \text{ (numerically)}. \quad (26)$$

Thus, c_B has the maximum value at $T \approx \mu_B B_z / 1.2 k_B$, so more accurate conditions for high and low temperature are given by $T \gg \mu_B B_z / 1.2 k_B$ and $T \ll \mu_B B_z / 1.2 k_B$, respectively. Thus, with $B_z = 0.5$ T, we get high temperature regime $T \gg 0.28$ K.