Main notebook

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Inhaltsverzeichnis

1 Drude model parameters

The assumptions of the Drude model are simple: we have interaction-free electrons that occasionally undergo some scattering process during a time dt with probability $\frac{dt}{\tau}$, where τ is some phenomenological parameter. This scattering will randomise electron momentum.

Our ultimate goal will be to find the conductivity σ and the dielectric constant ϵ in the Drude model, with Drude relaxation time τ, electron density n and electron mass m. We'll find

$$\sigma_{\mathrm{DC}} = \frac{ne^2\tau}{m} \tag{1}$$

$$\sigma_{\mathrm{AC}} = \frac{ne^2\tau}{m}\frac{1}{1-i\omega\tau} \qquad \text{For SI and Gaussian} \tag{2}$$

$$\epsilon_r = 1 + i\frac{4\pi\sigma}{\omega} \qquad \text{Gaussian} \tag{3a}$$

$$\epsilon_r = 1 + i\frac{\sigma}{\omega\epsilon_0} \qquad \text{SI} \tag{3b}$$

Our dielectric constant can be rewritten to plug in for σ, giving us

$$\begin{aligned}
\epsilon &= 1 + i\frac{4\pi\sigma}{\omega} && (4)\\
&= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1}{1-i\omega\tau} && (5)\\
&= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1}{1-i\omega\tau}\frac{1+i\omega\tau}{1+i\omega\tau} && (6)\\
&= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1+i\omega\tau}{1+\omega^2\tau^2} && (7)\\
&= \left(1 - \frac{4\pi\sigma_{\mathrm{DC}}\omega\tau}{\omega\left(1+\omega^2\tau^2\right)}\right) + i\left(\frac{4\pi\sigma_{\mathrm{DC}}}{\omega\left(1+\omega^2\tau^2\right)}\right) && (8)\\
&= \left(1 - \frac{4\pi\sigma_{\mathrm{DC}}\tau}{1+\omega^2\tau^2}\right) + i\left(\frac{4\pi\sigma_{\mathrm{DC}}}{\omega\left(1+\omega^2\tau^2\right)}\right) && (9)
\end{aligned}$$

This lets us write down the explicit real and imaginary of the Drude dielectric function.

1.1 Limiting forms of the Drude model

We can look at the large and small ω limits for the Drude dielectric function.

1.2 Derivations for Drude model

1.2.1 DC Conductivity

We can start unit-system independently, with the expression

$$\mathbf{j} = \sigma\mathbf{E}. \tag{10}$$

We can also relate our current to our average electron velocity: $\mathbf{j} = ne\mathbf{v}$. Imagine at time $t = 0$ our electron undergoes a Drude collision, and emerges with $\mathbf{v}_{t=0} = \mathbf{v_0}$. After a time t, the electron will accelerate with acceleration $-\frac{e\mathbf{E}}{m}$ (which fortunately remains unit independent). Because it will only accelerate for a time τ on average before a collision, it will end up with velocity

$\mathbf{v} = -\frac{e\mathbf{E}}{m}\tau + \mathbf{v_0}$. The average velocity, and current, will be

$$\begin{aligned} \langle \mathbf{v} \rangle &= -\frac{e\mathbf{E}}{m}\tau + \langle \mathbf{v_0} \rangle && (11) \\ &= -\frac{e\mathbf{E}}{m}\tau && (12) \\ \frac{\mathbf{j}}{ne} &= -\frac{e\mathbf{E}}{m}\tau && (13) \\ \mathbf{j} &= -\frac{ne^2\tau}{m}\mathbf{E}. && (14) \end{aligned}$$

This of course gives us, unit-independently, our DC conductivity $\sigma_{\mathrm{DC}} = \frac{ne^2\tau}{m}$.

1.2.2 AC Conductivity

The AC conductivity is also simple, but we want to be a bit more formal about it. We can write out the contributions to velocity in terms of probabilities. The velocity at a time dt will have probability dt/τ of being 0, and will otherwise be the original velocity minus $a\,dt$:

$$\begin{aligned} \mathbf{v}(dt) &= \left(1 - \frac{dt}{\tau}\right)\left(\mathbf{v_0} - \frac{e\mathbf{E}}{m}\,dt\right) && (15) \\ &= \mathbf{v_0} - \frac{dt}{\tau}\mathbf{v_0} - \frac{e\mathbf{E}}{m}\,dt\,, && (16) \end{aligned}$$

where we've invoked our inalienable right as physicists to ignore all terms $\mathcal{O}(dt^2)$. This reduces, using the definition of $d\mathbf{v} = \mathbf{v}(dt) - \mathbf{v_0}$, to

$$\begin{aligned} d\mathbf{v} &= \frac{dt}{\tau}\mathbf{v} - \frac{e\mathbf{E}}{m}\,dt && (17) \\ \frac{d\mathbf{v}}{dt} &= \frac{\mathbf{v}}{\tau} - \frac{e\mathbf{E}}{m} && (18) \end{aligned}$$

We can quickly Fourier transform this, using $\frac{d}{dt} \to -i\omega$, and we get (after surreptitiously dropping some vector signs)

$$\begin{aligned} -i\omega v(\omega) &= -\frac{v(\omega)}{\tau} - \frac{eE(\omega)}{m} && (19) \\ v(\omega) &= \frac{eE(\omega)}{m\left(\frac{1}{\tau} - i\omega\right)} && (20) \\ j(\omega) &= \frac{ne^2E(\omega)}{m\left(\frac{1}{\tau} - i\omega\right)} && (21) \\ &= \frac{ne^2\tau E(\omega)}{m\,(1 - i\omega\tau)}, && (22) \end{aligned}$$

which gives us our AC conductivity in equation (2).

Now for our dielectric constant, we have to find some other defining relation on par with (10).

2 Reducing Lindhard to Drude

We want to see how we can reduce the Lindhard dielectric function

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l(\,(\omega + i\nu)/kv_f\,)}{\omega + i\nu f_l(\,(\omega + i\nu)/kv_f\,)}, \tag{23}$$

where

$$f_l(x) = 1 - \frac{x}{2} \ln \frac{x+1}{x-1} \tag{24}$$

We can reduce things in the $k \to 0$ limit. The first half of (23) has the simple $\frac{1}{k^2}$ dependence, so we can look at how the rest of it behaves to start with.

2.1 f

$$f_l(\,(\omega + i\nu)/kv_F\,) = 1 - \frac{(\omega + i\nu)/kv_F}{2} \ln \frac{(\omega + i\nu)/kv_F\, + 1}{(\omega + i\nu)/kv_F\, - 1} \tag{25}$$

Defining $\eta = \omega + i\nu$:

$$\begin{aligned}
f_l(\,(\omega + i\nu)/kv_f\,) &= 1 - \frac{(\omega + i\nu)/kv_f}{2} \ln \frac{(\omega + i\nu)/kv_f\, + 1}{(\omega + i\nu)/kv_f\, - 1} && (26)\\
f_l(\eta/kv_F\,) &= 1 - \frac{\eta}{2kv_F} \ln \frac{\eta + kv_F}{\eta - kv_F} && (27)\\
f_l &= 1 - \frac{\eta}{2v_F} \frac{\ln \frac{\eta + kv_F}{\eta - kv_F}}{k} && (28)\\
\lim_{k \to 0} f_l &= 1 - \frac{\eta}{2v_F} \frac{d \ln \frac{\eta + kv_F}{\eta - kv_F}}{dk} && (29)\\
&= 1 - \frac{\eta}{2v_F} \frac{\eta - kv_F}{\eta + kv_F} \frac{v_F\,(\eta - kv_F) + v_F\,(\eta + kv_F)}{(\eta - kv_F)^2} && (30)\\
&= 1 - \frac{\eta}{2} \frac{\eta - kv_F}{\eta + kv_F} \frac{(\eta - kv_F) + (\eta + kv_F)}{(\eta - kv_F)^2} && (31)\\
&= 1 - \frac{\eta}{2} \frac{1}{\eta + kv_F} \frac{2\eta}{\eta - kv_F} && (32)
\end{aligned}$$

$$= 1 - \frac{\eta^2}{\eta^2 - k^2 v_F^2} \tag{33}$$

$$= \frac{-k^2 v_F^2}{\eta^2 - k^2 v_F^2} \tag{34}$$

$$\lim_{k \to 0} f_l = 0 \tag{35}$$

Note that this goes to 0 for $k \to 0$.

2.2 Series expansion of f

The previous section gives the limit, but having the actual series expansion is probably more valuable. Again, with $\eta = \omega + i\nu$,

$$f_l((\omega + i\nu)/kv_f) = 1 - \frac{(\omega + i\nu)/kv_f}{2} \ln \frac{(\omega + i\nu)/kv_f + 1}{(\omega + i\nu)/kv_f - 1} \tag{36}$$

$$f_l(\eta/kv_F) = 1 - \frac{\eta}{2v_F k} \ln \frac{\eta + kv_F}{\eta - kv_F} \tag{37}$$

We want to expand up to k^2 overall, to cancel out the k^2 in the denominator of (23). We're looking at the function.

$$\frac{\ln(\eta + kv_F)}{k} - \frac{\ln(\eta - kv_F)}{k} \tag{38}$$

Generally, the derivatives of $\frac{g(a \pm x)}{x}$ are

$$\left(\frac{g(x)}{x}\right)' = \frac{\pm g'}{x} - \frac{g}{x^2} \tag{39}$$

$$\left(\frac{g(x)}{x}\right)'' = \frac{g''}{x} - \frac{\pm 2g'}{x^2} + \frac{2g}{x^3} \tag{40}$$

$$\left(\frac{g(x)}{x}\right)''' = \frac{\pm g'''}{x} - \frac{3g''}{x^2} + \frac{\pm 6g'}{x^3} - \frac{6g}{x^4} \tag{41}$$

When we take the difference, we see that we'll only end up keeping (and doubling) the terms of odd derivatives. Thus, up to this order, the series for $\frac{g(a+x)-g(a-x)}{x}$ will look like:

$$\frac{1}{2}\frac{g(a+x) - g(a-x)}{x} = x\frac{g'}{x} - \frac{1}{2}x^2\frac{2g'}{x^2} + \frac{1}{6}x^3\left(\frac{g'''}{x} + \frac{6g'}{x^3}\right) \tag{42}$$

$$= g' - g' + \frac{1}{6}x^2 g''' + g' \tag{43}$$

$$\frac{g(a+x)-g(a-x)}{x} = 2g' + \frac{1}{3}x^2 g''' + \mathcal{O}(x^4) \tag{44}$$

This type of result is to be expected: we are starting with an even function. For $g = \ln(\eta + kv_F)$, we have

$$g'(k=0) = \frac{v_F}{\eta} \tag{45}$$

$$g'''(k=0) = \frac{2v_F^3}{\eta^3} \tag{46}$$

Plugging these into (37) gives us:

$$f_l(\eta/kv_F) = 1 - \frac{\eta}{2v_F k} \ln \frac{\eta + kv_F}{\eta - kv_F} \tag{47}$$

$$= 1 - \frac{\eta}{2v_F}\left(2\frac{v_F}{\eta} + \frac{1}{3}k^2 \frac{2v_F^3}{\eta^3}\right) \tag{48}$$

$$= 1 - 1 - \frac{1}{3}k^2 \frac{v_F^2}{\eta^2} \tag{49}$$

$$= -\frac{k^2 v_F^2}{3\eta^2} \tag{50}$$

This gives us a simple approximation for f_l in the long wavelength limit.

2.3 Back to dielectric

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega + i\nu f_l((\omega + i\nu)/kv_f)} \tag{51}$$

In the denominator, we can note that ω should dominate $i\nu f$, because f goes to zero, so we can simplify that.

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega} \tag{52}$$

Using (50), we get

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega} \tag{53}$$

$$= 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, \frac{-k^2 v_F^2}{3\eta^2}}{\omega} \tag{54}$$

$$= 1 - 3\omega_p^2 \frac{\eta \frac{1}{3\eta^2}}{\omega} \tag{55}$$

$$= 1 - \frac{\omega_p^2}{\omega\left(\omega + i\nu\right)} \tag{56}$$

This is the Drude limit, keeping in mind that $\omega_p^2 = \frac{4\pi n e^2}{m}$ in Gaussian units.