Main notebook

Deepak Mallubhotla

2017-11-25, Last update 2018-01-21

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

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

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

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

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

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

$$\epsilon = 1 + i\frac{4\pi\sigma}{\omega} \tag{4}$$

$$= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1}{1 - i\omega\tau} \tag{5}$$

$$= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1}{1 - i\omega\tau}\frac{1 + i\omega\tau}{1 + i\omega\tau} \tag{6}$$

$$= 1 + i\frac{4\pi\sigma_{\mathrm{DC}}}{\omega}\frac{1 + i\omega\tau}{1 + \omega^2\tau^2} \tag{7}$$

$$= \left(1 - \frac{4\pi\sigma_{\mathrm{DC}}\omega\tau}{\omega\left(1 + \omega^2\tau^2\right)}\right) + i\left(\frac{4\pi\sigma_{\mathrm{DC}}}{\omega\left(1 + \omega^2\tau^2\right)}\right) \tag{8}$$

$$= \left(1 - \frac{4\pi\sigma_{\mathrm{DC}}\tau}{1 + \omega^2\tau^2}\right) + i\left(\frac{4\pi\sigma_{\mathrm{DC}}}{\omega\left(1 + \omega^2\tau^2\right)}\right) \tag{9}$$

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

1.1 Alternative forms of the Drude model

We can also rewrite the dielectric constant very slightly in terms of the plasma frequency. In Gaussian units:

$$\epsilon = 1 + i\frac{4\pi\sigma}{\omega} \tag{10}$$

$$= 1 + i\frac{4\pi}{\omega}\frac{ne^2\tau}{m}\frac{1}{1 - i\omega\tau} \tag{11}$$

$$= 1 + i\frac{4\pi}{\omega}\frac{ne^2\tau}{m}\frac{1}{1 - i\omega\tau}\frac{i\nu}{i\nu} \tag{12}$$

$$= 1 - \frac{4\pi}{\omega}\frac{ne^2}{m}\frac{1}{i\nu + \omega} \tag{13}$$

With $\omega_p^2 = \frac{4\pi ne^2}{m}$ in Gaussian units, this becomes

$$\epsilon = 1 - \frac{\omega_p^2}{\omega(\omega + i\nu)} \tag{14}$$

We'll see this again later.

1.2 Derivations for Drude model

1.2.1 DC Conductivity

We can start unit-system independently, with the expression

$$\mathbf{j} = \sigma \mathbf{E}. \tag{15}$$

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

$$\langle \mathbf{v} \rangle = -\frac{e\mathbf{E}}{m}\tau + \langle \mathbf{v_0} \rangle \tag{16}$$

$$= -\frac{e\mathbf{E}}{m}\tau \tag{17}$$

$$\frac{\mathbf{j}}{ne} = -\frac{e\mathbf{E}}{m}\tau \tag{18}$$

$$\mathbf{j} = -\frac{ne^2\tau}{m}\mathbf{E}. \tag{19}$$

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 $a\,dt$:

$$\mathbf{v}(dt) = \left(1 - \frac{dt}{\tau}\right)\left(\mathbf{v_0} - \frac{e\mathbf{E}}{m}\,dt\right) \tag{20}$$

$$= \mathbf{v_0} - \frac{dt}{\tau}\mathbf{v_0} - \frac{e\mathbf{E}}{m}\,dt\,, \tag{21}$$

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

$$d\mathbf{v} = \frac{dt}{\tau}\mathbf{v} - \frac{e\mathbf{E}}{m}\,dt \tag{22}$$

$$\frac{d\mathbf{v}}{dt} = \frac{\mathbf{v}}{\tau} - \frac{e\mathbf{E}}{m} \tag{23}$$

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

$$-i\omega v(\omega) = -\frac{v(\omega)}{\tau} - \frac{eE(\omega)}{m} \tag{24}$$

$$v(\omega) = \frac{eE(\omega)}{m\left(\frac{1}{\tau} - i\omega\right)} \tag{25}$$

$$j(\omega) = \frac{ne^2E(\omega)}{m\left(\frac{1}{\tau} - i\omega\right)} \tag{26}$$

$$= \frac{ne^2\tau E(\omega)}{m\left(1 - i\omega\tau\right)}, \tag{27}$$

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 (15).

2 Reducing Lindhard to Drude

2.1 The longitudinal case

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

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2v_F^2}\frac{(\omega + i\nu)\, f_l(\,(\omega + i\nu)/kv_f\,)}{\omega + i\nu f_l(\,(\omega + i\nu)/kv_f\,)}, \tag{28}$$

where

$$f_l(x) = 1 - \frac{x}{2}\ln\frac{x+1}{x-1}. \tag{29}$$

We can reduce things in the $k \to 0$ limit. The first half of (28) has the simple $\frac{1}{k^2}$ dependence, so we can look at how the rest of it behaves to start with.

2.2 f

$$f_l(\,(\omega + i\nu)/kv_F\,) = 1 - \frac{(\omega + i\nu)/kv_F}{2}\ln\frac{(\omega + i\nu)/kv_F\, + 1}{(\omega + i\nu)/kv_F\, - 1} \tag{30}$$

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

$$f_l(\,(\omega + i\nu)/kv_f\,) = 1 - \frac{(\omega + i\nu)/kv_f}{2}\ln\frac{(\omega + i\nu)/kv_f\, + 1}{(\omega + i\nu)/kv_f\, - 1} \tag{31}$$

$$f_l(\eta/kv_F) = 1 - \frac{\eta}{2kv_F}\ln\frac{\eta+kv_F}{\eta-kv_F} \tag{32}$$

$$f_l = 1 - \frac{\eta}{2v_F}\frac{\ln\frac{\eta+kv_F}{\eta-kv_F}}{k} \tag{33}$$

$$\lim_{k\to 0} f_l = 1 - \frac{\eta}{2v_F}\frac{d\ln\frac{\eta+kv_F}{\eta-kv_F}}{dk} \tag{34}$$

$$= 1 - \frac{\eta}{2v_F}\frac{\eta-kv_F}{\eta+kv_F}\frac{v_F\left(\eta-kv_F\right)+v_F\left(\eta+kv_F\right)}{\left(\eta-kv_F\right)^2} \tag{35}$$

$$= 1 - \frac{\eta}{2}\frac{\eta-kv_F}{\eta+kv_F}\frac{\left(\eta-kv_F\right)+\left(\eta+kv_F\right)}{\left(\eta-kv_F\right)^2} \tag{36}$$

$$= 1 - \frac{\eta}{2}\frac{1}{\eta+kv_F}\frac{2\eta}{\eta-kv_F} \tag{37}$$

$$= 1 - \frac{\eta^2}{\eta^2-k^2v_F^2} \tag{38}$$

$$= \frac{-k^2v_F^2}{\eta^2-k^2v_F^2} \tag{39}$$

$$\lim_{k\to 0} f_l = 0 \tag{40}$$

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

2.3 Series expansion of f

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

$$f_l((\omega+i\nu)/kv_f) = 1 - \frac{(\omega+i\nu)/kv_f}{2}\ln\frac{(\omega+i\nu)/kv_f+1}{(\omega+i\nu)/kv_f-1} \tag{41}$$

$$f_l(\eta/kv_F) = 1 - \frac{\eta}{2v_Fk}\ln\frac{\eta+kv_F}{\eta-kv_F} \tag{42}$$

We want to expand up to k^2 overall, to cancel out the k^2 in the denominator of (28). We're looking at the function.

$$\frac{\ln(\eta+kv_F)}{k} - \frac{\ln(\eta-kv_F)}{k} \tag{43}$$

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

$$\left(\frac{g(x)}{x}\right)' = \frac{\pm g'}{x} - \frac{g}{x^2} \tag{44}$$

$$\left(\frac{g(x)}{x}\right)'' = \frac{g''}{x} - \frac{\pm 2g'}{x^2} + \frac{2g}{x^3} \tag{45}$$

$$\left(\frac{g(x)}{x}\right)''' = \frac{\pm g'''}{x} - \frac{3g''}{x^2} + \frac{\pm 6g'}{x^3} - \frac{6g}{x^4} \tag{46}$$

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:

$$\frac{1}{2}\frac{g(a+x)-g(a-x)}{x} = x\frac{g'}{x} - \frac{1}{2}x^2\frac{2g'}{x^2} + \frac{1}{6}x^3\left(\frac{g'''}{x} + \frac{6g'}{x^3}\right) \tag{47}$$

$$= g' - g' + \frac{1}{6}x^2 g''' + g' \tag{48}$$

$$\frac{g(a+x)-g(a-x)}{x} = 2g' + \frac{1}{3}x^2 g''' + \mathcal{O}(x^4) \tag{49}$$

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

$$g'(k=0) = \frac{v_F}{\eta} \tag{50}$$

$$g'''(k=0) = \frac{2v_F^3}{\eta^3} \tag{51}$$

Plugging these into (42) gives us:

$$f_l(\eta/kv_F) = 1 - \frac{\eta}{2v_F k}\ln\frac{\eta+kv_F}{\eta-kv_F} \tag{52}$$

$$= 1 - \frac{\eta}{2v_F}\left(2\frac{v_F}{\eta} + \frac{1}{3}k^2\frac{2v_F^3}{\eta^3}\right) \tag{53}$$

$$= 1 - 1 - \frac{1}{3}k^2\frac{v_F^2}{\eta^2} \tag{54}$$

$$= -\frac{k^2 v_F^2}{3\eta^2} \tag{55}$$

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

2.4 Back to dielectric

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2}\frac{(\omega+i\nu)\, f_l((\omega+i\nu)/kv_f)}{\omega + i\nu f_l((\omega+i\nu)/kv_f)} \tag{56}$$

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

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega} \tag{57}$$

Using (55), we get

$$\begin{aligned}
\epsilon_l &= 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega} &(58)\\
&= 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, \frac{-k^2 v_F^2}{3\eta^2}}{\omega} &(59)\\
&= 1 - 3\omega_p^2 \frac{\eta \frac{1}{3\eta^2}}{\omega} &(60)\\
&= 1 - \frac{\omega_p^2}{\omega\,(\omega + i\nu)} &(61)
\end{aligned}$$

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

2.5 Looking at transverse Lindhard form

It's possible also to show that the transverse Lindhard dielectric function ends up also going to the Drude form in the $k \to 0$ limit.

Writing out ϵ_t:

$$e_t = 1 - \frac{\omega_p^2}{\omega\eta} \left[\frac{3}{2} \frac{\eta^2}{v_F^2 k^2} - \frac{3}{4} \frac{\eta}{v_F k} \left(\frac{\eta^2}{v_F^2 k^2} - 1 \right) \ln \frac{\eta + v_F k}{\eta - v_F k} \right] \tag{62}$$

We can also simplify this slightly, to highlight the similarities between this and the longitudinal forms:

$$\begin{aligned}
e_t &= 1 - \frac{3\omega_p^2}{2\omega\eta} \left[\frac{\eta^2}{v_F^2 k^2} - \frac{1}{2} \frac{\eta}{v_F k} \left(\frac{\eta^2}{v_F^2 k^2} - 1 \right) \ln \frac{\eta + v_F k}{\eta - v_F k} \right] &(63)\\
&= 1 - \frac{3\omega_p^2}{2\omega\eta} \left[\frac{\eta^2}{v_F^2 k^2} - \frac{1}{2} \frac{\eta^2}{v_F^2 k^2} \left(\frac{\eta}{v_F k} - \frac{v_F k}{\eta} \right) \ln \frac{\eta + v_F k}{\eta - v_F k} \right] &(64)\\
&= 1 - \frac{3\omega_p^2}{2\omega\eta} \frac{\eta^2}{v_F^2 k^2} \left[1 - \frac{1}{2} \left(\frac{\eta}{v_F k} - \frac{v_F k}{\eta} \right) \ln \frac{\eta + v_F k}{\eta - v_F k} \right] &(65)\\
&= 1 - \frac{3\omega_p^2 \eta}{2\omega v_F^2 k^2} \left[1 - \frac{1}{2} \left(\frac{\eta}{v_F k} - \frac{v_F k}{\eta} \right) \ln \frac{\eta + v_F k}{\eta - v_F k} \right] &(66)
\end{aligned}$$

There is an extra term within the brackets, as well as an extra factor of $-\frac{1}{2}$ on the outside.

To find the $k \to 0$ limit here, we can do the same series expansion as we did for the longitudinal case. The relevant series to find is for the bracketed portion, which we can break into two parts:

$$1 - \frac{1}{2}\frac{\eta}{v_F k}\ln\frac{\eta + v_F k}{\eta - v_F k} - \frac{1}{2}\frac{v_F k}{\eta}\ln\frac{\eta + v_F k}{\eta - v_F k} \tag{67}$$

We have already done the expansion of the first two terms earlier, and we found that that should equal $-\frac{k^2 v_F^2}{3\eta^2}$. We now need the series expansion of the third term. Like earlier, we can write out the derivatives of $kg(a \pm k)$, keeping in mind that the log will become a difference:

$$(kg)' = g \pm kg' \tag{68}$$
$$(kg)'' = \pm 2g' + kg'' \tag{69}$$

After $k \to 0$ and the subtraction, the only term remaining will be the $2 \pm g'$ term. This will end up giving us

$$\frac{1}{2}\frac{v_F}{\eta}k\ln\frac{\eta + v_F k}{\eta - v_F k} = \frac{1}{2}\frac{v_F}{\eta}\frac{1}{2}k^2 4\frac{v_F}{\eta} \tag{70}$$
$$= \frac{k^2 v_F^2}{\eta^2} \tag{71}$$

Adding this to (67), we end up with

$$1 - \frac{1}{2}\left(\frac{\eta}{v_F k} - \frac{v_F k}{\eta}\right)\ln\frac{\eta + v_F k}{\eta - v_F k} = -\frac{k^2 v_F^2}{3\eta^2} + \frac{k^2 v_F^2}{\eta^2} \tag{72}$$
$$= \frac{2}{3}\frac{k^2 v_F^2}{\eta^2} \tag{73}$$

Plugging this into (66) gives us

$$e_t = 1 - \frac{3\omega_p^2\eta}{2\omega v_F^2 k^2}\left[1 - \frac{1}{2}\left(\frac{\eta}{v_F k} - \frac{v_F k}{\eta}\right)\ln\frac{\eta + v_F k}{\eta - v_F k}\right] \tag{74}$$
$$= 1 - \frac{3\omega_p^2\eta}{2\omega v_F^2 k^2}\frac{2}{3}\frac{k^2 v_F^2}{\eta^2} \tag{75}$$
$$= 1 - \frac{\omega_p^2}{\omega\eta} \tag{76}$$

$$= 1 - \frac{\omega_p^2}{\omega\,(\omega + i\nu)} \tag{77}$$

So to lowest order, both the longitudinal and transverse dielectric functions reduce to the Drude case in the $k \to 0$ limit.

3 Explicit parts of Lindhard function

We want to find the explicit real and imaginary parts of the Lindhard function. To begin with, we can start with the case where $\nu \to 0$, which means long relaxation times.

We have our Lindhard form

$$\epsilon_l = 1 + \frac{3\omega_p^2}{k^2 v_F^2} \frac{(\omega + i\nu)\, f_l((\omega + i\nu)/kv_f)}{\omega + i\nu f_l((\omega + i\nu)/kv_f)}, \tag{78}$$

where

$$f_l(x) = 1 - \frac{x}{2} \ln \frac{x+1}{x-1}. \tag{79}$$

3.1 Pines result

From Pines, we have the forms

$$\begin{aligned}\mathrm{Re}[\epsilon_l] = 1 + \frac{k_{TF}^2}{k^2}\Bigg(\frac{1}{2} + \frac{k_F}{4k}\Bigg[\Bigg(1 - \frac{\left(\omega - \frac{\hbar k^2}{2m}\right)^2}{k^2 v_F^2}\Bigg) \ln\left[\frac{\omega - kv_F - \frac{\hbar k^2}{2m}}{\omega + kv_F - \frac{\hbar k^2}{2m}}\right] \\ + \Bigg(1 - \frac{\left(\omega + \frac{\hbar k^2}{2m}\right)^2}{k^2 v_F^2}\Bigg) \ln\left[\frac{\omega + kv_F + \frac{\hbar k^2}{2m}}{\omega - kv_F + \frac{\hbar k^2}{2m}}\right]\Bigg]\Bigg)\end{aligned} \tag{80}$$

$$\mathrm{Im}[\epsilon_l] = \begin{cases} \dfrac{\pi}{2} \dfrac{\omega}{kv_F} \dfrac{k_{TF}^2}{k^2}, & \omega \le kv_F - \frac{\hbar k^2}{2m} \\ \dfrac{\pi}{4} \dfrac{k_F}{k} \left(1 - \dfrac{\left(\omega - \frac{\hbar k^2}{2m}\right)^2}{k^2 v_F^2}\right) \dfrac{k_{TF}^2}{k^2}, & kv_F - \frac{\hbar k^2}{2m} \le \omega \le kv_F + \frac{\hbar k^2}{2m} \\ 0, & \omega \ge kv_F + \frac{\hbar k^2}{2m} \end{cases} \tag{81}$$

3.2 Long relaxation time forms of the logs

In order to analyse the $\nu \to 0$ limit, we can start by looking at what happens to the logarithms in the Lindhard function:

$$\ln \frac{\omega + i\nu + kv_F}{\omega + i\nu - kv_F} \tag{82}$$

The first thing to note is that the numerator will always have a very small, positive argument, while the denominator will have a small argument which may be positive or negative. As Lindhard mentions, these logarithms should all have imaginary parts between $\pm i\pi$. This effectively means we can treat each logarithm as giving the principal value, which give us a result that looks like

$$\ln \frac{\sqrt{(\omega + kv_F)^2 + \nu^2}}{\sqrt{(\omega - kv_F)^2 + \nu^2}} + i\left(\theta_+ - \theta_-\right), \tag{83}$$

where θ_+ and θ_- are the arguments of the numerator and denominator. For small ν, θ_+ is proportional to ν, as it'll be determined by an arcsine. However, the denominator may be negative, which would contribute a factor of $\theta_- = +i\pi$ (with a plus sign because ν would be just above the real line).

$$\ln \frac{\omega + i\nu + kv_F}{\omega + i\nu - kv_F} = \ln \frac{\sqrt{(\omega + kv_F)^2 + \nu^2}}{\sqrt{(\omega - kv_F)^2 + \nu^2}} + i\left(\theta_+ - \theta_-\right) \tag{84}$$

$$= \ln \frac{\sqrt{(\omega + kv_F)^2}}{\sqrt{(\omega - kv_F)^2}} - \sigma i\pi \tag{85}$$

$$= \ln \left| \frac{\omega + kv_F}{\omega - kv_F} \right| - \sigma i\pi, \tag{86}$$

where $\sigma = 1$ if $\omega < kv_F$, and 0 otherwise.