Handout 1

Drude Model for Metals

In this lecture you will learn:

- Metals, insulators, and semiconductors
- Drude model for electrons in metals
- Linear response functions of materials

Paul Drude (1863-1906)

Inorganic Crystalline Materials

Ionic solids

Mostly insulators
Example: NaCl, KCl

Covalent solids

Semiconductors
Si, C, GaAs, InP, GaN
PbSe, CdTe, ZnO

Insulators
SiO_2, Si_3N_4

Metals
Au, Ag, Al,
Ga, In

Metals

1- Metals are usually very conductive

2- Metals have a large number of "free electrons" that can move in response to an applied electric field and contribute to electrical current

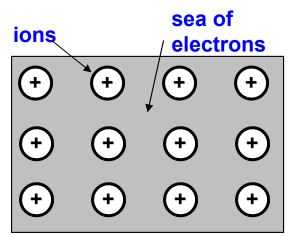
3- Metals have a shiny reflective surface

Properties of Metals: Drude Model

Before ~1900 it was known that most conductive materials obeyed Ohm's law (i.e. *I* =*V/R*).

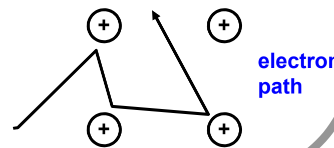
In 1897 J. J. Thompson discovers the electron as the smallest charge carrying constituent of matter with a charge equal to "-*e*"

$$e = 1.6 \times 10^{-19}\ \text{C}$$



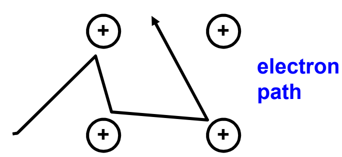
In 1900 P. Drude formulated a theory for conduction in metals using the electron concept. The theory assumed:

1) Metals have a large density of "free electrons" that can move about freely from atom to atom ("sea of electrons")
2) The electrons move according to Newton's laws until they scatter from ions, defects, etc.
3) After a scattering event the momentum of the electron is completely random (i.e. has no relation to its momentum before scattering)



Drude Model - I

Applied Electric Field:



In the presence of an applied external electric field $\vec{E}$ the electron motion, on average, can be described as follows:

Let τ be the scattering time and $1/\tau$ be the scattering rate

This means that the probability of scattering in small time interval time *dt* is: $\dfrac{dt}{\tau}$

The probability of not scattering in time *dt* is then: $\left(1-\dfrac{dt}{\tau}\right)$

Let $\vec{p}(t)$ be the average electron momentum at time *t* , then we have:

$$\vec{p}(t+dt) = \underbrace{\left(1-\frac{dt}{\tau}\right)\left(\vec{p}(t) - e\,\vec{E}(t)\,dt\right)}_{\text{If no scattering happens then Newton's law}} + \underbrace{\left(\frac{dt}{\tau}\right)(0)}_{\text{If scattering happens then average momentum after scattering is zero}}$$

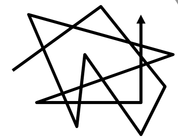
$$\Rightarrow \frac{d\vec{p}(t)}{dt} = -e\,\vec{E}(t) - \frac{\vec{p}(t)}{\tau}$$

Drude Model - II

Case I: No Electric Field

$$\frac{d\vec{p}(t)}{dt} = -\frac{\vec{p}(t)}{\tau}$$

Steady state solution: $\vec{p}(t) = 0$



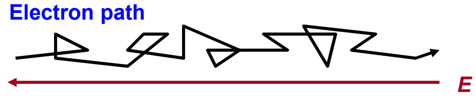
Electron path

Case II: Constant Uniform Electric Field

Steady state solution is:

$$\vec{p}(t) = -e\,\tau\,\vec{E}$$

Electron path



Electron "drift" velocity is defined as:

$$\vec{v} = \frac{\vec{p}(t)}{m} = -\frac{e\,\tau}{m}\vec{E} = -\mu\,\vec{E}$$

$\mu = e\tau/m$ = electron mobility (units: cm^2/V-sec)

Electron current density $\vec{J}$ (units: Amps/cm^2) is:

$$\vec{J} = n\,(-e)\,\vec{v} = n\,e\,\mu\,\vec{E} = \sigma\,\vec{E}$$

Where: n = electron density (units: #/cm^3)

$$\sigma = \text{electron conductivity (units: Siemens/cm)} = ne\mu = \frac{ne^2\tau}{m}$$

Drude Model - III

Case III: Time Dependent Sinusoidal Electric Field

$$\Rightarrow \frac{d\vec{p}(t)}{dt} = -e\,\vec{E}(t) - \frac{\vec{p}(t)}{\tau}$$

There is no steady state solution in this case. Assume the E-field, average momentum, and currents are all sinusoidal with phasors given as follows:

$$\vec{E}(t) = \text{Re}\left[\vec{E}(\omega)\,e^{-i\,\omega\,t}\right] \qquad \vec{p}(t) = \text{Re}\left[\vec{p}(\omega)\,e^{-i\,\omega\,t}\right] \qquad \vec{J}(t) = \text{Re}\left[\vec{J}(\omega)\,e^{-i\,\omega\,t}\right]$$

$$\frac{d\vec{p}(t)}{dt} = -e\,\vec{E}(t) - \frac{\vec{p}(t)}{\tau} \quad \Rightarrow \quad -i\omega\vec{p}(\omega) = -e\vec{E}(\omega) - \frac{\vec{p}(\omega)}{\tau}$$

$$\Rightarrow \quad \vec{p}(\omega) = -\frac{e\,\tau}{1 - i\,\omega\,\tau}\vec{E}(\omega) \quad \Rightarrow \quad \vec{v}(\omega) = \frac{\vec{p}(\omega)}{m} = -\frac{e\,\tau/m}{1 - i\,\omega\,\tau}\vec{E}(\omega)$$

Electron current density:

$$\vec{J}(\omega) = n\,(-e)\,\vec{v}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

Where:

$$\sigma(\omega) = \frac{\dfrac{ne^2\tau}{m}}{1 - i\,\omega\,\tau} = \frac{\sigma(\omega = 0)}{1 - i\,\omega\,\tau}$$

Drude's famous result !!

Linear Response Functions - I

The relationship:

$$\vec{J}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

is an example of a relationship between an applied stimulus (the electric field in this case) and the resulting system/material response (the current density in this case). Other examples include:

$$\vec{P}(\omega) = \varepsilon_o\,\chi_e(\omega)\,\vec{E}(\omega)$$

electric polarization density — **electric susceptibility** — **electric field**

$$\vec{M}(\omega) = \chi_m(\omega)\,\vec{H}(\omega)$$

magnetic polarization density — **magnetic susceptibility** — **magnetic field**

The response function (conductivity or susceptibility) must satisfy some fundamental conditions …. (see next few pages)

Linear Response Functions - II

Case III: Time Dependent Non-Sinusoidal Electric Field

For general time-dependent (not necessarily sinusoidal) e-field one can always use Fourier transforms:

$$\vec{E}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\vec{E}(\omega)\,e^{-i\omega t} \quad \Leftrightarrow \quad \vec{E}(\omega) = \int_{-\infty}^{\infty} dt\;\vec{E}(t)\,e^{i\omega t} \longrightarrow (1)$$

Then employ the already obtained result in frequency domain:

$$\vec{J}(\omega) = \sigma(\omega)\,\vec{E}(\omega)$$

And convert back to time domain:

$$\vec{J}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\vec{J}(\omega)\,e^{-i\omega t} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\sigma(\omega)\,\vec{E}(\omega)\,e^{-i\omega t}$$

Now substitute from (1) into the above equation to get:

$$\vec{J}(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\sigma(\omega)\,\vec{E}(\omega)\,e^{-i\omega t} = \int_{-\infty}^{\infty} dt' \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\,\sigma(\omega)\,e^{-i\omega(t-t')}\right]\vec{E}(t')$$

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

ECE 4070 – Spring 2010 – Farhan Rana – Cornell University

Linear Response Functions - III

$$\Rightarrow \vec{J}(t) = \int_{-\infty}^{\infty} dt'\, \sigma(t-t')\, \vec{E}(t') \qquad \text{Where:} \quad \sigma(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \sigma(\omega)\, e^{-i\,\omega(t-t')}$$

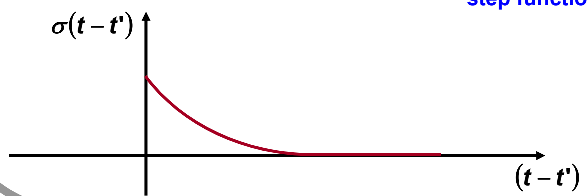
The current at time *t* is a convolution of the conductivity response function and the applied time-dependent E-field

Drude Model: $\sigma(\omega) = \dfrac{\sigma(\omega=0)}{1 - i\,\omega\,\tau}$

$$\sigma(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \sigma(\omega)\, e^{-i\,\omega(t-t')} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \frac{\sigma(\omega=0)}{1 - i\,\omega\,\tau}\, e^{-i\,\omega(t-t')}$$

$$\Rightarrow \sigma(t-t') = \frac{\sigma(\omega=0)}{\tau}\, e^{-\frac{(t-t')}{\tau}}\, \theta(t-t')$$

step function



Linear Response Functions - IV

The linear response functions in time and frequency domain must satisfy the following two conditions:

1) Real inputs must yield real outputs:

Since we had: $\vec{J}(t) = \int_{-\infty}^{\infty} dt' \left[\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, \sigma(\omega)\, e^{-i\,\omega(t-t')} \right] \vec{E}(t')$

This condition can only hold if:

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

2) Output must be causal (i.e. output at any time cannot depend on future input):

Since we had: $\vec{J}(t) = \int_{-\infty}^{\infty} dt'\, \sigma(t-t')\, \vec{E}(t')$

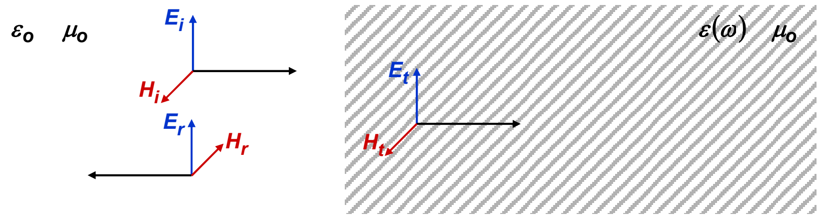
This condition can only hold if:

$$\sigma(t-t') = 0 \quad \text{for} \quad t < t'$$

Both these conditions are satisfied by the Drude model

Drude Model and Metal Reflectivity - I

When E&M waves are incident on a air-metal interface there is a reflected wave:



The reflection coefficient is:

$$\Gamma = \frac{E_r}{E_i} = \frac{\sqrt{\varepsilon_o} - \sqrt{\varepsilon(\omega)}}{\sqrt{\varepsilon_o} + \sqrt{\varepsilon(\omega)}}$$

Question: what is $\varepsilon(\omega)$ for metals?

Drude Model and Metal Reflectivity - II

From Maxwell's equation:

Ampere's law: $\nabla \times \vec{H}(\vec{r},t) = \vec{J}(\vec{r},t) + \varepsilon_o \frac{\partial \vec{E}(\vec{r},t)}{\partial t}$

Phasor form:

$$\begin{aligned} \nabla \times \vec{H}(\vec{r}) &= \vec{J}(\vec{r}) - i\,\omega\,\varepsilon_o\,\vec{E}(\vec{r}) \\ &= \sigma(\omega)\vec{E}(\vec{r}) - i\,\omega\,\varepsilon_o\,\vec{E}(\vec{r}) \\ &= -i\,\omega\,\varepsilon_{eff}(\omega)\,\vec{E}(\vec{r}) \end{aligned}$$

Effective dielectric constant of metals

$$\varepsilon_{eff}(\omega) = \varepsilon_o\left(1 + i\frac{\sigma(\omega)}{\omega\,\varepsilon_o}\right)$$

Metal reflection coefficient becomes:

$$\Gamma = \frac{E_r}{E_i} = \frac{\sqrt{\varepsilon_o} - \sqrt{\varepsilon_{eff}(\omega)}}{\sqrt{\varepsilon_o} + \sqrt{\varepsilon_{eff}(\omega)}}$$

Using the Drude expression: $\sigma(\omega) = \frac{\sigma(\omega = 0)}{1 - i\,\omega\,\tau}$

the frequency dependence of the reflection coefficient of metals can be explained adequately all the way from RF frequencies to optical frequencies

Drude Model and Plasma Frequency of Metals

For metals: $\varepsilon_{eff}(\omega)=\varepsilon_o\left(1+i\dfrac{\sigma(\omega)}{\omega\,\varepsilon_o}\right)$ and $\sigma(\omega)=\dfrac{ne^2\tau/m}{1-i\,\omega\,\tau}=\dfrac{\sigma(\omega=0)}{1-i\,\omega\,\tau}$

For small frequencies $(\omega\tau<<1)$:

$$\sigma(\omega)\approx\sigma(\omega=0)=\frac{ne^2\tau}{m}\qquad\Rightarrow\quad\varepsilon_{eff}(\omega)\approx\varepsilon_o\left(1+i\frac{\sigma(\omega=0)}{\omega\,\varepsilon_o}\right)$$

For large frequencies $(\omega\tau>>1)$ (collision-less plasma regime):

$$\sigma(\omega)\approx\frac{\sigma(\omega=0)}{-i\omega\,\tau}=i\frac{ne^2}{m\omega}\qquad\Rightarrow\quad\varepsilon_{eff}(\omega)\approx\varepsilon_o\left(1-\frac{\omega_p^2}{\omega^2}\right)$$

where the plasma frequency is: $\omega_p=\sqrt{\dfrac{ne^2}{\varepsilon_o m}}$

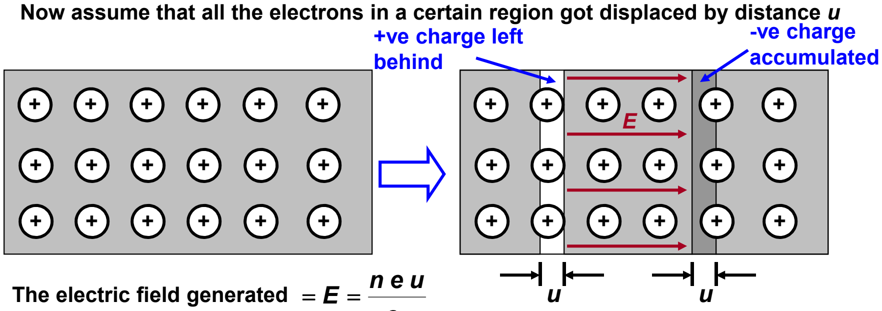
For most good metals this frequency is in the UV to visible range

Electrons behave like a collision-less plasma

Note that for $\omega_p>\omega>>\dfrac{1}{\tau}$ the dielectric constant is real and negative

Plasma Oscillations in Metals

Consider a metal with electron density n
Now assume that all the electrons in a certain region got displaced by distance u



The electric field generated $=E=\dfrac{n\,e\,u}{\varepsilon_o}$

Force on the electrons $=F=-eE=-\dfrac{n\,e^2\,u}{\varepsilon_o}$

As a results of this force electron displacement u will obey Newton's second law:

$$m\frac{d^2u(t)}{dt^2}=F=-eE=-\frac{n\,e^2\,u(t)}{\varepsilon_o}\qquad\Rightarrow\quad\frac{d^2u(t)}{dt^2}=-\omega_p^2\,u(t)$$

← second order system

Solution is: $u(t)=A\cos(\omega_p t)+B\sin(\omega_p t)$

Plasma oscillations are charge density oscillations

Plasma Oscillations in Metals – with Scattering

From Drude model, we know that in the presence of scattering we have:

$$\frac{d\vec{p}(t)}{dt} = -e\,\vec{E}(t) - \frac{\vec{p}(t)}{\tau} \quad \Rightarrow \quad m\frac{d^2u(t)}{dt^2} = -e\,E(t) - \frac{m}{\tau}\frac{du(t)}{dt} \longrightarrow (1)$$

As before, the electric field generated $= E(t) = \dfrac{n\,e\,u(t)}{\varepsilon_o} \longrightarrow (2)$

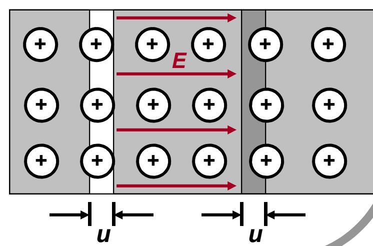
Combining (2) with (1) we get the differential equation:

$$\frac{d^2u(t)}{dt^2} = -\omega_p^2\,u(t) - \frac{1}{\tau}\frac{du(t)}{dt} \longrightarrow \left\{ \omega_p = \sqrt{\frac{ne^2}{\varepsilon_o m}} \right.$$

Or:

$$\frac{d^2u(t)}{dt^2} + \frac{1}{\tau}\frac{du(t)}{dt} + \omega_p^2\,u(t) = 0$$

second order system with damping



Plasma Oscillations in Metals – with Scattering

Case I (underdamped case): $\omega_p > \dfrac{1}{2\tau}$

Solution is:

$$u(t) = e^{-\gamma\,t}\left[A\cos(\Omega_p t) + B\sin(\Omega_p t)\right] \longleftarrow \text{Damped plasma oscillations}$$

Where:

$$\gamma = \frac{1}{2\tau} \qquad \Omega_p = \sqrt{\omega_p^2 - \gamma^2}$$

Case II (overdamped case): $\omega_p < \dfrac{1}{2\tau}$

Solution is:

$$u(t) = A\,e^{-\gamma_1 t} + B\,e^{-\gamma_2 t} \longleftarrow \text{No oscillations}$$

Where:

$$\gamma_1 = \frac{1}{2\tau} + \sqrt{\frac{1}{4\tau^2} - \omega_p^2} \qquad \gamma_1 = \frac{1}{2\tau} - \sqrt{\frac{1}{4\tau^2} - \omega_p^2}$$

Appendix: Fourier Transforms in Time OR Space

Fourier transform in time:

$$f(\omega) = \int_{-\infty}^{\infty} dt \;\; f(t)\, e^{i\,\omega\, t}$$

Inverse Fourier transform:

$$f(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, f(\omega)\, e^{-i\,\omega\, t}$$

Fourier transform in space:

$$g(k) = \int_{-\infty}^{\infty} dx \;\; g(x)\, e^{-i\,k\,x}$$

Inverse Fourier transform:

$$g(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi}\, g(k)\, e^{i\,k\,x}$$

Appendix: Fourier Transforms in Time AND Space

Fourier transform in time and space:

$$h(k,\omega) = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dt \;\; h(x,t)\;\; e^{-i\,k\,x}\; e^{i\,\omega\, t}$$

Inverse Fourier transform:

$$h(x,t) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \;\; h(k,\omega)\;\; e^{i\,k\,x}\; e^{-i\,\omega\, t}$$

Appendix: Fourier Transforms in Multiple Space Dimensions

Fourier transform in space:

$$h(k_x,k_y,k_z)=\int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz \quad h(x,y,z)\; e^{-i k_x x}\, e^{-i k_y y} e^{-i k_z z}$$

Need a better notation!

Let:

$$\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z\, \hat{z}$$

$$\vec{r} = x\, \hat{x} + y\, \hat{y} + z\, \hat{z}$$

$$\int d^3\vec{r} = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dz$$

$$\Rightarrow \qquad h(\vec{k}) = \int d^3\vec{r}\;\; h(\vec{r})\; e^{-i\vec{k}\,.\,\vec{r}}$$

Inverse Fourier transform:

$$h(\vec{r}) = \int \frac{d^3\vec{k}}{(2\pi)^3}\;\; h(\vec{k})\; e^{i\vec{k}\,.\,\vec{r}}$$