* Drude model

→ ideal gas of charged particles driven by external field

→ instantaneous momentum of a particle has the form

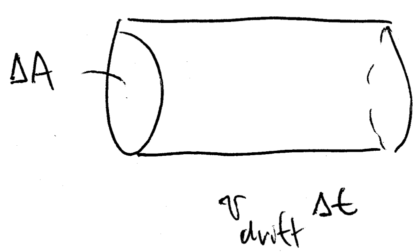
$$\vec{p} = m(\vec{v}_{MB} + \vec{v}_{drift})$$

net motion

drawn from the maxwell-boltzmann distribution

→ heuristic scattering model: complete randomization and no memory between scattering events (separated in time by $\sim\tau$)

* Current is the rate of charge passing through a unit area per unit time



number density of charge carriers

$$j = -\frac{n e\, v_{drift}\, \Delta t \cdot A}{\Delta t \cdot A} = -n e v_{drift}$$

* Between scattering events

$$\Delta\vec{p} = m\vec{v}_{drift} = \int_0^{\tau} \vec{F}\,dt = -e\vec{E}\tau$$

→ drift velocity $\vec{v}_{drift} = -\dfrac{e\vec{E}\tau}{m}$ (directed opposite to $\vec{E}$)

and $\vec{j} = \dfrac{ne^2\tau}{m}\vec{E}$ (directed along $\vec{E}$)

* For an alternating field $\vec{E}(t) = \mathrm{Re}[\vec{E}_0 e^{-i\omega t}]$

complex field strength encodes amplitude and phase

→ substitute $\vec{p}(t) = \mathrm{Re}[\vec{p}_0 e^{-i\omega t}]$
into the force equation $\frac{d\vec{p}}{dt} = -\frac{\vec{p}}{\tau} - e\vec{E}$

→ yields $-i\omega \vec{p}_0 = -\frac{\vec{p}_0}{\tau} - e\vec{E}_0$ or $\vec{p}_0(\omega) = \frac{e\vec{E}_0}{i\omega - \frac{1}{\tau}}$

→ net current is $\vec{j}(t) = \mathrm{Re}[\vec{j}_0(\omega) e^{i\omega t}]$ with

$$\vec{j}_0(\omega) = -\frac{ne\vec{p}_0(\omega)}{m} = -\frac{ne^2}{m}\frac{\vec{E}_0}{i\omega - \frac{1}{\tau}}$$

$$\underbrace{= \frac{ne^2}{m}\frac{1}{\frac{1}{\tau} - i\omega}\vec{E}_0 = \underbrace{\frac{ne^2\tau}{m}}_{= \sigma_0}\frac{1}{1-i\omega\tau}}_{}\vec{E}_0$$

$$\equiv \sigma(\omega) = \frac{\sigma_0}{1-i\omega\tau}$$

complex conductivity

* loose argument for the existence of Ohm's law ($\vec{j} = \sigma \vec{E}$)
  - → rigourously justified by Boltzmann equation approach
  - → weak perturbation out of local equilibrium
  - → quantum treatment of scattering (transport time τ_t) using Fermi's golden rule.

* If this picture is correct
  - → leads to an effective frequency-dependent dielectric constant
  - → implies the existence of <u>plasma oscillations</u>

Start from Maxwell's eqns...

$$\nabla \cdot \vec{E} = 0 \quad \text{(source free)} \qquad \nabla \times \vec{E} = -\frac{1}{c}\frac{\partial \vec{H}}{\partial t}$$

$$\nabla \cdot \vec{H} = 0 \qquad \nabla \times \vec{H} = \frac{4\pi}{c}\vec{j} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t}$$

then

$$\nabla \times (\nabla \times \vec{E}) = -\frac{1}{c}\frac{\partial}{\partial t}(\nabla \times \vec{H})$$

$$= -\frac{1}{c}\frac{\partial}{\partial t}\left(\frac{4\pi}{c}\vec{j} + \frac{1}{c}\frac{\partial \vec{E}}{\partial t}\right)$$

$$= \frac{1}{c}(i\omega)\left(\frac{4\pi\sigma\vec{E}}{c} - \frac{i\omega}{c}\vec{E}\right)$$

or $$-\nabla^2 \vec{E} = \underbrace{\frac{\omega^2}{c^2}\left(1 + \frac{4\pi i \sigma}{\omega}\right)}\vec{E}$$

effective dielectric constant $\varepsilon(\omega)$
controls the propagation speed
in the medium: $\omega_k = \sqrt{\varepsilon}\, ck$

* Here, the dielectric is complex-valued and frequency dependent

→ if $\omega\tau \gg 1$ (very high freq.) then

$$\sigma(\omega) = \frac{\sigma_0}{1 - i\omega\tau} \simeq \frac{\sigma_0}{-i\omega\tau} = \frac{ne^2\cancel{\tau}}{-im\omega\cancel{\tau}} = -\frac{ne^2}{im\omega}$$

and $$\varepsilon(\omega) = \left(1 + \frac{4\pi i \sigma}{\omega}\right) \simeq 1 - \frac{4\pi n e^2}{m\omega^2} \equiv 1 - \frac{\omega_p^2}{\omega^2}$$

→ defines a frequency scale $\omega_p = \sqrt{\frac{4\pi n e^2}{m}}$ (plasma freq.)
above which $\varepsilon(\omega) > 0$ and below which $\varepsilon(\omega) < 0$

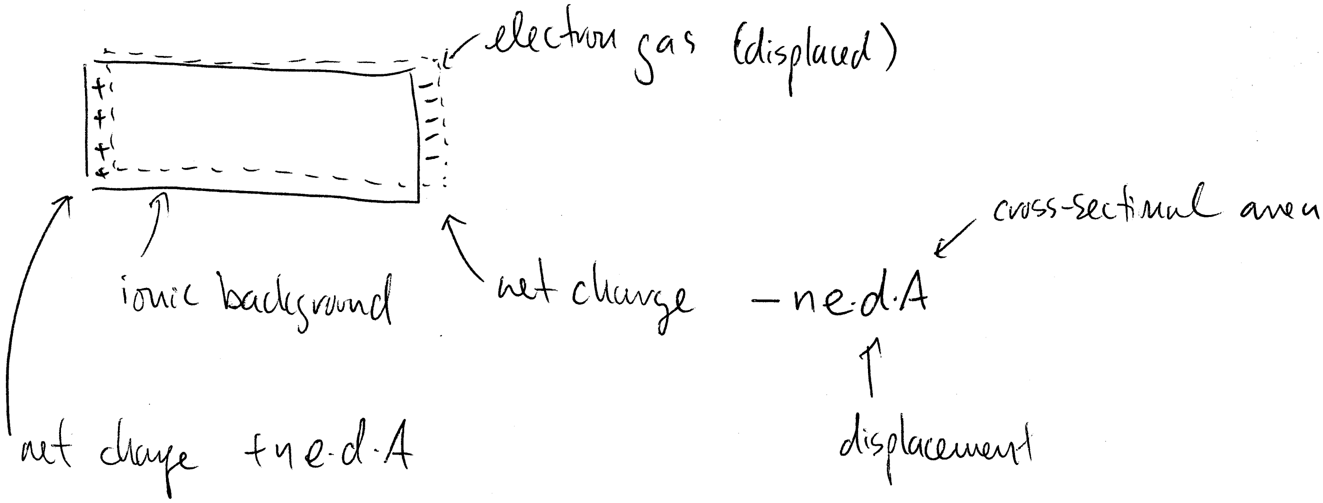
→ crossover from propagating behaviour $\omega = \sqrt{|\varepsilon|}\, ck$
to evanescent behaviour $\omega = \sqrt{-|\varepsilon|}\, ck$
$= i\sqrt{|\varepsilon|}\, ck$

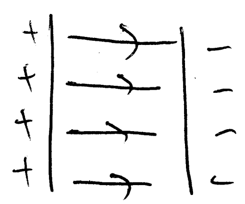
* Expectations for a metallic system

→ transparent to high-frequency EM radiation above ω_p

→ opaque to radiation below that

→ related to global sloshing modes of the electron gas





field $\vec{E} = 4\pi n d e$ between two parallel plates of charge density $+ned$ and $-ned$

equation of motion

$$N m \ddot{d} = -Ne|\vec{E}| = -Ne \cdot 4\pi n d e = -4\pi n e^2 N d$$

plasma oscillations: $\ddot{d} = -\dfrac{4\pi n e^2}{m} d$

harmonic motion with freq $\omega_p = \sqrt{\dfrac{4\pi n e^2}{m}}$

Screening

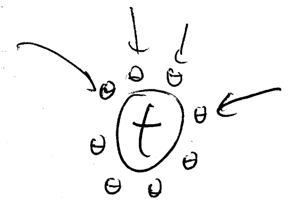
* high frequency modes associated with bulk rearrangements of electrons

  → consistent with our adiabatic picture (Born-Oppenheimer approx; separation of time scales)

* What happens to a positively charged object rigidly fixed in some position?

  → electrons are attracted to it

  → if there are free carriers, they will rapidly pile up in the vicinity



  → at distances away from charge, it looks much weaker

* Quantitative treatment

  → charged particle with charge density $\rho^{ext}(\vec{r})$

  → an electrostatic potential arises that satisfies Poisson's equation $-\nabla^2 \phi^{ext} = 4\pi \rho^{ext}$

→ the complete physical potential ϕ includes the component arising from the electronic back-reaction

$$-\nabla^2\phi = 4\pi\left(\rho^{ext}(r) + \rho^{ind}(\vec{r})\right)$$

→ ϕ and ϕ^{ext} related by a position-dependent dielectric

$$\phi^{ext}(\vec{r}) = \int dr' \, \varepsilon(\vec{r}-r')\, \phi(\vec{r}')$$

or in fourier space

$$\phi(\vec{q}) = \frac{1}{\varepsilon(\vec{q})}\phi^{ext}(\vec{q})$$

→ In Fourier space, Poisson equations become

$$q^2\phi^{ext} = 4\pi\rho^{ext}$$

$$q^2\phi = 4\pi\rho = 4\pi\left(\underbrace{\rho^{ext}}_{=\frac{q^2\phi^{ext}}{4\pi} = \frac{q^2\phi}{4\pi\varepsilon}} + \rho^{ind}\right)$$

self-consistency: this in term depends on $\phi(\vec{r})$

$$\rho^{ind}(\vec{q}) = \chi(q)\phi(q)$$

$\rightarrow$ leads to $\varepsilon(q) = 1 - \frac{4\pi}{q^2}\chi(q)$

all the difficult work in calculating this factor

* Thomas-Fermi approach assumes that $e\phi(r) = e(\phi^{ext} + \phi^{ind})$ can be treated as a slowly varying change in the local chemical potential

$\rightarrow$ single particle energies shifted $\varepsilon_k = \frac{\hbar^2 k^2}{2m} - e\phi(\vec{r})$

$\rightarrow$ local number density

$$n(\vec{r}) = 2\int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2k^2}{2m} - e\phi(r) - \mu\right)} + 1}$$

$\rightarrow$ induced charge is just the deviation $-en(\vec{r}) + en_0$ from the average

$$n_0(\mu) = 2\int \frac{d^3k}{(2\pi)^3} \frac{1}{e^{\beta\left(\frac{\hbar^2k^2}{2m} - \mu\right)} + 1}$$

$\rightarrow$ hence

$$\rho^{ind}(\vec{r}) = -e\left[n_0(\mu + e\phi(\vec{r})) - n_0(\mu)\right]$$

$$\simeq -e^2 \frac{\partial n_0}{\partial \mu}\phi(\vec{r}) \equiv \int d\vec{r}\,'\, \chi(r - r')\phi(\vec{r}\,')$$

$\rightarrow$ or $\rho^{ind}(\vec{q}) = -e^2 \frac{\partial n_0}{\partial \mu} \phi(q) \equiv \chi(q)\phi(q)$

$\uparrow$ electronic compressibility

related to DOS at the Fermi level

$$\varepsilon(q) = 1 + \frac{4\pi e^2}{q^2}\frac{\partial n_0}{\partial \mu} \equiv 1 + \frac{k_0^2}{q^2}$$

* Consider the case of a point charge

$$\phi^{ext}(r) = \frac{Q}{r} \qquad \phi^{ext}(q) = \frac{4\pi Q}{q^2}$$

$\rightarrow$ combined potential is

$$\phi(q) = \frac{1}{\varepsilon(q)}\phi^{ext} = \frac{1}{1+\frac{k_0^2}{q^2}} \cdot \frac{4\pi Q}{q^2} = \frac{4\pi Q}{k_0^2+q^2}$$

$\uparrow$ long-wavelength cutoff

and in real space $\phi(r) = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}} \frac{4\pi Q}{k_0^2+q^2}$

$$= \int \frac{d^3q}{(2\pi)^3}\, e^{i\vec{q}\cdot\vec{r}}\, \frac{4\pi Q}{(ik_0+q)(-ik_0+q)} \overset{\substack{\text{(contour}\\ \text{integral)}}}{=} \frac{Q}{r}\, e^{-k_0 r}$$

Yukawa potential with screening length k_0^{-1}

<u>Lindhard screening</u>

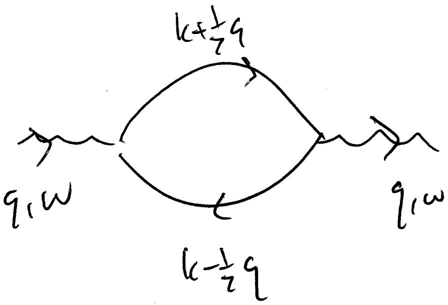
* Leading order in time-dependent perturbation theory

$$\varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q^2}\cdot 2\int \frac{d^3k}{(2\pi)^3}\, \frac{f(\varepsilon_{k+\frac{1}{2}q}-\mu) - f(\varepsilon_{k-\frac{1}{2}q}-\mu)}{\varepsilon_{k-\frac{1}{2}q} - \varepsilon_{k+\frac{1}{2}q} + \hbar\omega}$$

wave vector

freq

where $f(\varepsilon) = (e^{\beta\varepsilon}+1)^{-1}$ is the Fermi-Dirac distribution



particle-hole bubble term (particle and hole with net momentum $\vec{q}$ and energy $\hbar\omega$)

→ subtle order of limits: $q\to 0$ at fixed ω gives the Drude result ; $\omega\to 0$ at fixed q gives the Thomas-Fermi result e.g. $$\frac{f(\varepsilon_{k+\frac{1}{2}q}-\mu)-f(\varepsilon_{k-\frac{1}{2}q}-\mu)}{\varepsilon_{k-\frac{1}{2}q}-\varepsilon_{k+\frac{1}{2}q}+\hbar\omega}$$

$$=\frac{\cancel{f(\varepsilon_k-\mu)}+\frac{1}{2}f'(\varepsilon_k-\mu)\nabla\varepsilon_k\cdot q-\cancel{f(\varepsilon_k-\mu)}+\frac{1}{2}f'(\varepsilon_k-\mu)\nabla\varepsilon_k\cdot q}{\cancel{\varepsilon_k}-\frac{1}{2}\nabla\varepsilon_k\cdot q-\cancel{\varepsilon_k}-\frac{1}{2}\nabla\varepsilon_k\cdot q+\hbar\omega}$$

$$=\frac{+f'(\varepsilon_k-\mu)\nabla\varepsilon_k\cdot q}{-\nabla\varepsilon_k\cdot q+\hbar\omega}$$

if we let $\omega\to 0$ first, then

$$\chi(\vec{q})=2\int\frac{d^3k}{(2\pi)^3}\,\frac{+f'(\varepsilon_k-\mu)\cancel{\nabla\varepsilon_k\cdot q}}{-\cancel{\nabla\varepsilon_k\cdot q}}=2\int\frac{d^3k}{(2\pi)^3}\left(-f'(\varepsilon_k-\mu)\right)$$

$$=2\int d\varepsilon\, D(\varepsilon)\left(-f'(\varepsilon-\mu)\right)$$

$$\simeq 2\int d\varepsilon\, D(\varepsilon)\,\delta(\varepsilon-\mu)$$

$$=2D(\mu)$$

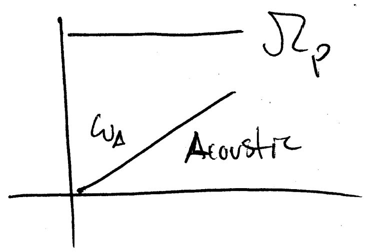
or $$\varepsilon(\vec{q},0)=1+\frac{4\pi e^2}{q^2}\underbrace{2D(\mu)}_{=\frac{\partial n_0}{\partial\mu}}$$

Phonon dispersion

* Long-wavelength acoustic modes are the global sloshing modes of the +vely charged ions

→ why don't they execute plasma oscillations ?

$$\Omega_p^2 = \frac{4\pi n_{ions} (Ze)^2}{M} = \frac{Zm}{M} \omega_p^2$$



→ these oscillations are executed in the presence of the electronic medium;

hence $\omega_A(k) = \dfrac{\Omega_p}{\sqrt{\epsilon(k)}}$ is "dressed"

$$= \frac{\Omega_p}{\sqrt{1 + \frac{k_0^2}{k^2}}} \quad \text{(Thomas-Fermi)}$$

$$= \frac{k\,\Omega_p}{\sqrt{k^2 + k_0^2}} \xrightarrow{k \to 0} \left(\frac{1}{k_0} \sqrt{\frac{4\pi n_{ions} (Ze)^2}{M}} \right) k$$

* Electronic and phonon contributions to the dielectric constant are additive

e.g. $$\varepsilon = 1 + \frac{k_0^2}{q^2} - \frac{\Omega_p^2}{\omega^2}$$

Thomas-Fermi

dressed acoustic mode

$$= \left(1 + \frac{k_0^2}{q^2}\right)\left(1 - \frac{\omega_q^2}{\omega^2}\right)$$