

# Quantum Condensed-Matter Physics: synopsis (1)

## 1. Classical and semiclassical models for electrons in solids (3L)

Lorentz dipole oscillator, optical properties of insulators. Drude model and optical properties of metals, plasma oscillations. Semiclassical approach to electron transport in electric and magnetic fields, the Hall effect. Sommerfeld model, density of states, specific heat of; electrons in metals, liquid  $^3\text{He}/^4\text{He}$  mixtures. Screening and the Thomas-Fermi approximation.

## 2. Electrons and phonons in periodic solids (6L)

Types of bonding; van der Waals, ionic, covalent. Crystal structures. Reciprocal space, X-ray diffraction and Brillouin zones. Lattice dynamics and phonons; 1D monoatomic and diatomic chains, 3D crystals. Heat capacity due to lattice vibrations; Einstein and Debye models. Thermal conductivity of insulators. Electrons in a periodic potential; Bloch's theorem. Nearly-free-electron approximation; plane waves and bandgaps. Tight-binding approximation; linear combination of atomic orbitals, linear chain and three dimensions, two bands. Pseudopotentials. Band structure of real materials; properties of metals (aluminium and copper) and semiconductors.

Semiclassical model of electron dynamics in bands; Bloch oscillations, effective mass, density of states, electrons and holes in semiconductors

## 3. Experimental probes of band structure (4L)

Photon absorption; transition rates, experimental arrangement for absorption spectroscopy, direct and indirect semiconductors, excitons. Quantum oscillations; de Haas-van Alphen effect in copper and strontium ruthenate. Photoemission; angle-resolved photoemission spectroscopy (ARPES) in GaAs and strontium ruthenate. Tunnelling; scanning tunnelling microscopy. Cyclotron resonance.

Scattering in metals; Wiedemann-Franz law, theory of electrical and thermal transport, Matthiessen's rule, emission and absorption of phonons. Experiments demonstrating electron-phonon and electron-electron scattering at low temperatures.

# Quantum Condensed-Matter Physics: synopsis (2)

## 4. Semiconductors and semiconductor devices (5L)

Intrinsic semiconductors, law of mass action, doping in semiconductors, impurity ionisation, variation of carrier concentration and mobility with temperature - impurity and phonon scattering, Hall effect with two carrier types.

Metal to semiconductor contact. P-n junction; charge redistribution, band bending and equilibrium, balance of currents, voltage bias. Light-emitting diodes; GaN, organic materials.

Photovoltaic solar cell; Shockley-Queisser limit, efficiencies, commercialisation. Field-effect transistor; JFET, MOSFET. Microelectronics and the integrated circuit.

Band-structure engineering; electron-beam lithography, molecular-beam epitaxy. Two-dimensional electron gas, Shubnikov-de-Haas oscillations, quantum Hall effect, conductance quantisation in 1D. Single-electron pumping and current quantisation, single- and entangled-photon emission, quantum cascade laser.

## 5. Electronic instabilities (2L)

The Peierls transition, charge-density waves, magnetism, local magnetic moments, Curie Law. Types of magnetic interactions; direct exchange, Heisenberg Hamiltonian, superexchange and insulating ferromagnets, band magnetism in metals, local-moment magnetism in metals, indirect exchange, magnetic order and the Weiss exchange field.

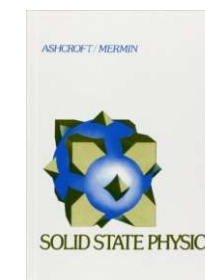
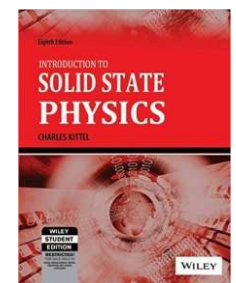
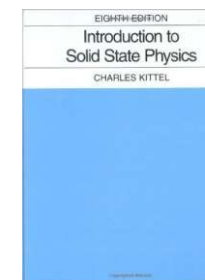
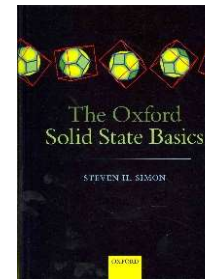
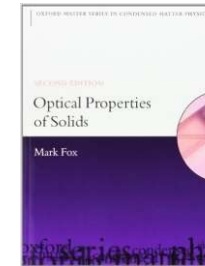
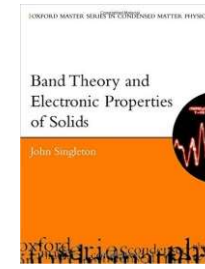
## 6. Fermi Liquids (2L)

Fermi-liquid theory; the problem with the Fermi gas. Liquid helium; specific heat and viscosity. Collective excitations, adiabatic continuity, total-energy expansion for Landau Fermi liquid, energy dependence of quasiparticle scattering rate.

Quasiparticles and holes near the Fermi surface, quasiparticle spectral function, tuning of the quasiparticle interaction, heavy fermions, renormalised band picture for heavy fermions, quasiparticles detected by dHvA, tuning the quasiparticle interaction.  $\text{CePd}_2\text{Si}_2$ ; heavy-fermion magnet to unconventional-superconductor phase transitions.

# Books

1. Band Theory and Electronic Properties of Solids, Singleton J (OUP 2001)
2. Optical properties of Solids, Fox M (2<sup>nd</sup> edn OUP 2010)
3. The Oxford Solid State Basics, Simon S H (OUP 2013)
4. Introduction to Solid State Physics, Kittel C (8th edn Wiley 2004)
5. Solid State Physics, Ashcroft N W and Mermin N D, (Holt, Rinehart and Winston 1976)



- Course material will be useful for several part III courses.
- Printed overheads, reference handout & problem sheets provided.
- All available in pdf on TiS. Extra links at [www.sp.phy.cam.ac.uk/qcmp](http://www.sp.phy.cam.ac.uk/qcmp)











# Quantum Condensed-Matter Physics

## 1. Classical and semiclassical models for electrons in solids (3L)

*Lorentz dipole oscillator, optical properties of insulators. Drude model and optical properties of metals, plasma oscillations. Semiclassical approach to electron transport in electric and magnetic fields, the Hall effect.* Sommerfeld model, density of states, specific heat of: electrons in metals, liquid  $^3\text{He}/^4\text{He}$  mixtures. Screening and the Thomas–Fermi approximation

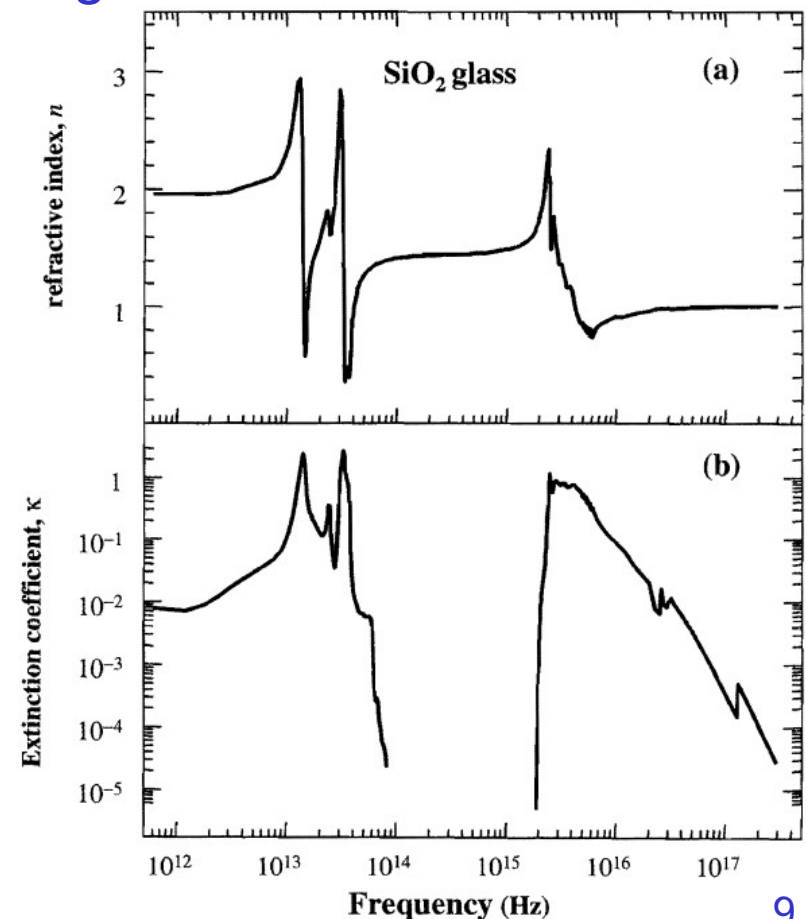
## 2. Electrons and phonons in periodic solids (6L)

## 3. Experimental probes of band structure (4L)

## 4. Semiconductors and semiconductor devices (5L)

## 5. Electronic instabilities (2L)

## 6. Fermi Liquids (2L)

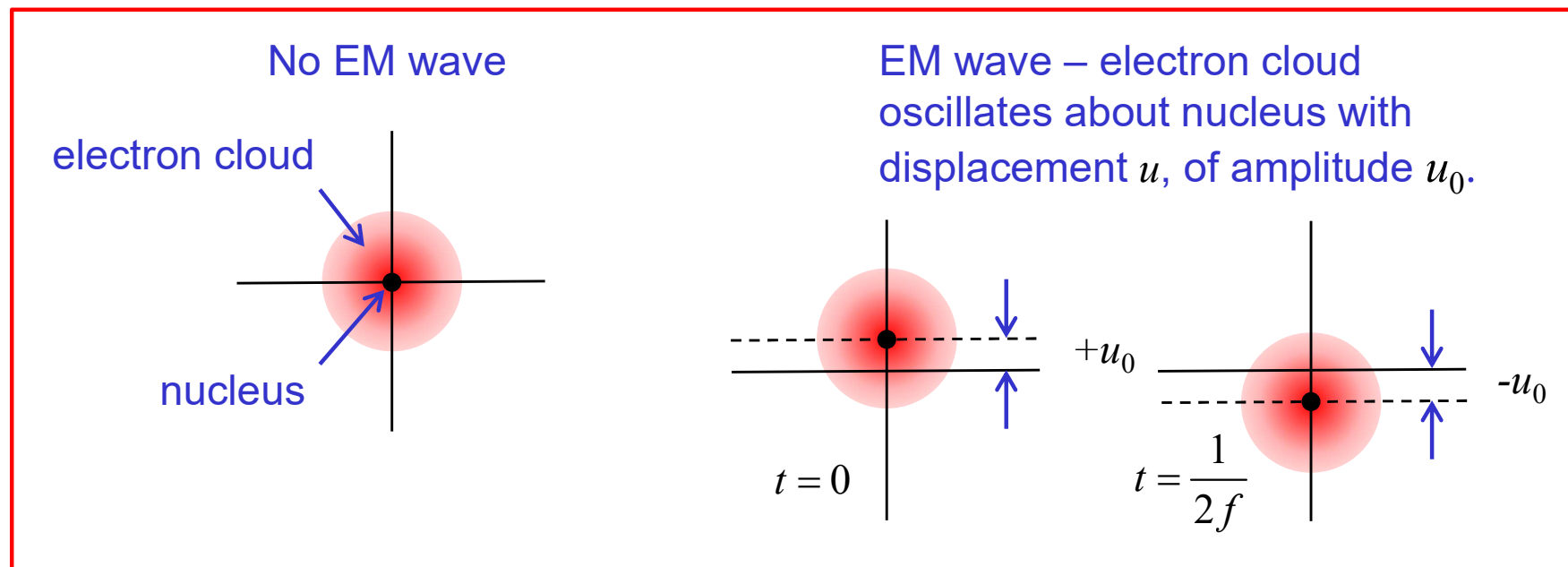


# The course

- Start by considering intuitive, classical models for condensed matter
  - first put forward in the late 19th century
  - Lorentz, or dipole oscillator model
    - oscillation of charges around their average positions is incorporated
  - Drude model
    - electrons are treated similarly to an ideal gas
- Shortcomings of these models will become apparent
- We will progress to more sophisticated models
  - electrons form a degenerate quantum gas
    - states are occupied according to the Pauli exclusion principle
  - Sommerfeld model of the free-electron gas
  - effect of periodic potential produced by the lattice atoms on the electronic states
  - full electronic band structure and the possibility of producing energy gaps
- Finally, in the Easter term, we begin to include the effects of interactions between the electrons
- For now, however, we concentrate on how the electromagnetic response of an insulator is modelled using classical physics...

# Optical properties of insulators

- Response to high-frequency electric field in electromagnetic (EM) waves
- Wavelength long compared to interatomic spacing
- Classical picture – **Lorentz dipole-oscillator model**
- Model atoms as nucleus + electron cloud
- Applied electric field from EM wave causes displacement of electron cloud:



- Assume restoring force is proportional to displacement

# Optical properties of insulators

- Electron cloud behaves as a damped harmonic oscillator (charge  $q = -e$ )
$$m\ddot{u} + m\gamma\dot{u} + m\omega_T^2 u = qE$$
- $\omega_T$  natural frequency, determined by force constant and mass;  $\gamma$  damping rate (no model for this yet...)
- Consider oscillating electric field  $E(t) = E_\omega e^{-i\omega t}$ , which induces oscillating displacement  $u(t) = u_\omega e^{-i\omega t}$
- Resulting dipole moment per atom at angular frequency  $\omega_T$ :  $p_\omega = qu_\omega$
- Polarisation = dipole moment per unit volume  $P_\omega = p_\omega N/V = n_v p_\omega$   
(with number density  $n_v = N/V$ , use  $n$  for refractive index)
- From  $P_\omega = \epsilon_0 \chi_\omega E_\omega$  and the equation of motion, we obtain for the susceptibility (polarisability/ $\epsilon_0$ ):

$$\chi_\omega = n_v \frac{q^2}{m\epsilon_0(\omega_T^2 - \omega^2 - i\omega\gamma)}$$

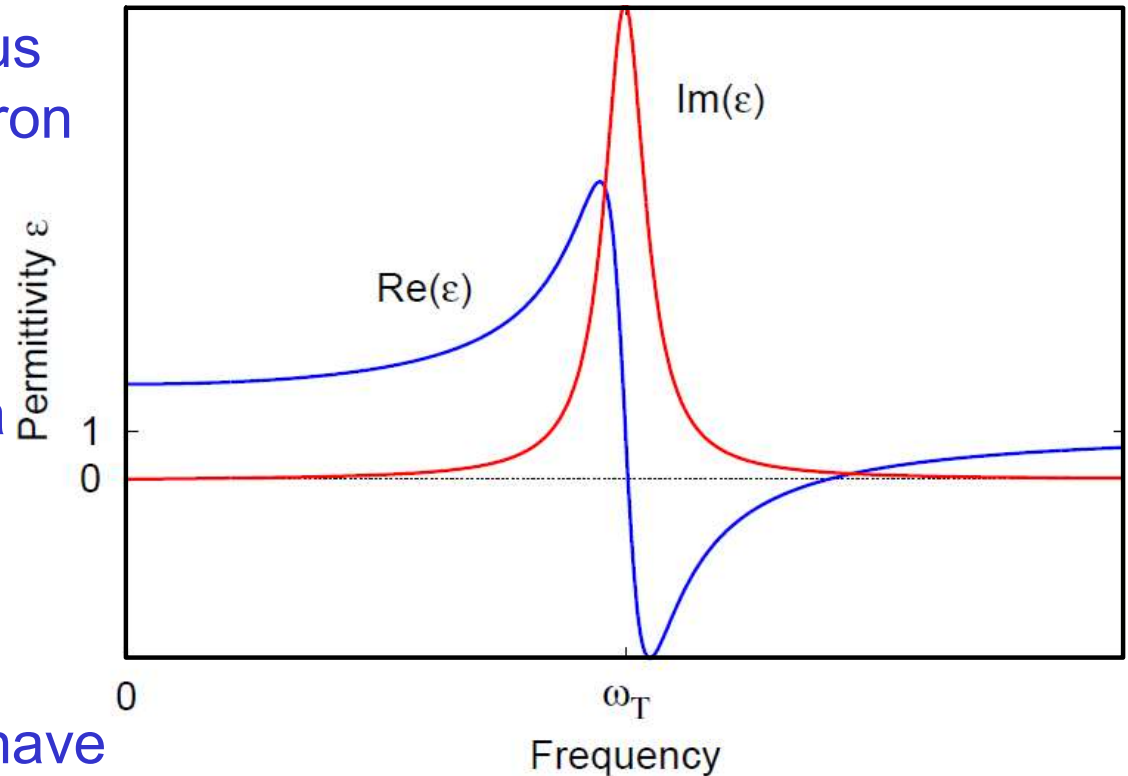
- Frequency dependence of  $\chi_\omega$  is typical of a harmonic oscillator

# Optical properties of insulators

- (Relative) permittivity from model:  $\epsilon_\omega = 1 + \chi_\omega = 1 + n_v \frac{q^2}{m\epsilon_0(\omega_T^2 - \omega^2 - i\omega\gamma)}$
- Figure shows typical frequency dependence
- Analogy with damped SHO tells us that the power absorbed by electron cloud is determined by  $\text{Im}(\epsilon_\omega)$ :  

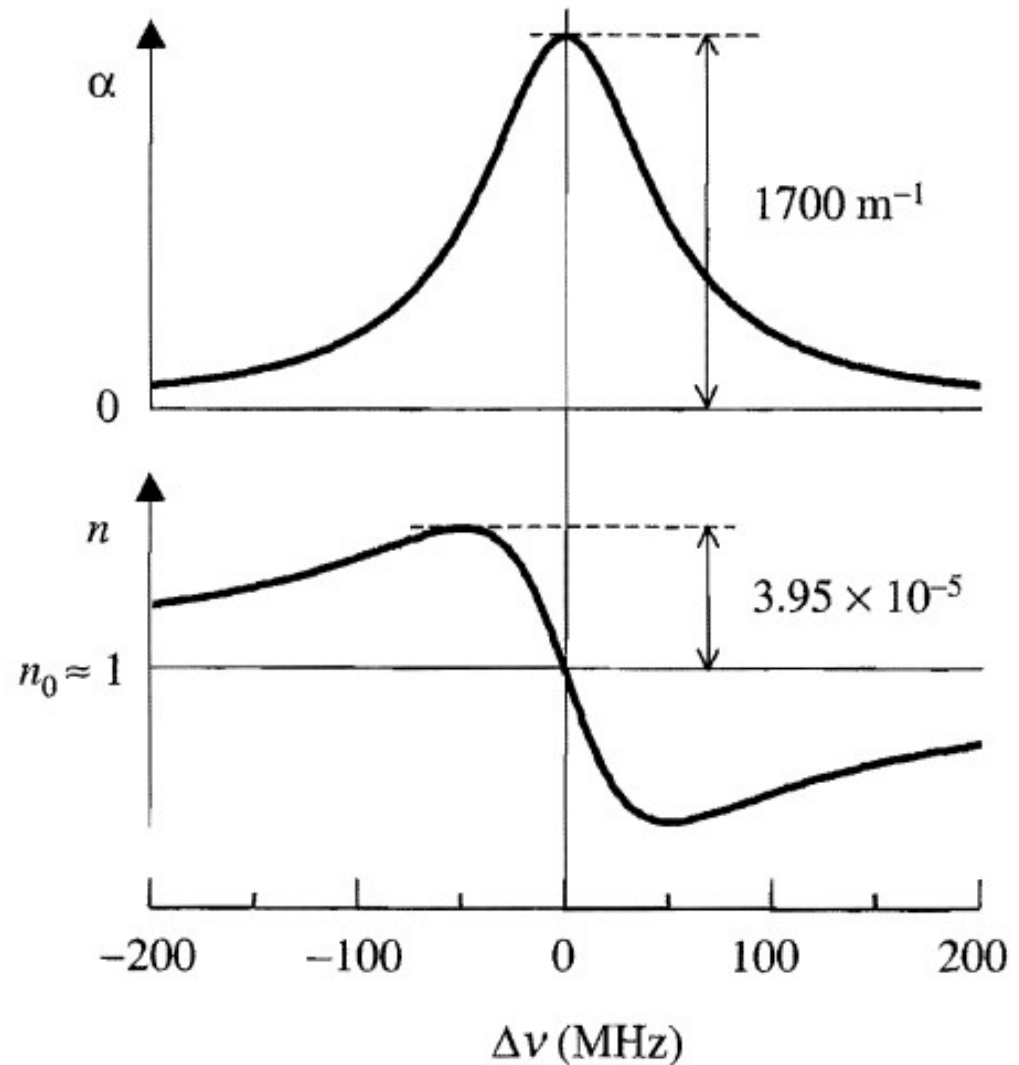
$$P = \frac{1}{2} \omega \epsilon_0 |E_\omega|^2 \text{Im}(\epsilon_\omega)$$
- This is a simple way to think of absorption lines in optical spectra
- At low frequencies:  

$$\epsilon(\omega \rightarrow 0) = 1 + n_v \frac{q^2}{m\epsilon_0 \omega_T^2}$$
- Explains why different materials have very different static permittivities
- Reflectivity between media of different permittivities:  $r = \frac{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}}{\sqrt{\epsilon_1} + \sqrt{\epsilon_2}}$
- Power reflection coefficient given by  $R = |r|^2$
- In a solid, polarisation fields of other atoms can alter resonant frequency



## Example – atomic absorption line (in a gas)

- Absorption coefficient  $\alpha$  and refractive index  $n$  of sodium gas
- Atom density is  $1 \times 10^7 \text{ m}^{-3}$
- $n_0$  is the off-resonance refractive index
- Absorption due to strongest hyperfine component of the D2 line at  $\lambda = 589 \text{ nm}$ 
  - so  $\nu = 5.1 \times 10^{14} \text{ Hz}$
- Linewidth  $\Delta\nu \approx 100 \text{ MHz}$ 
  - hence  $\Delta\nu/\nu = 2 \times 10^{-7}$
  - very narrow.....



Taken from *Optical properties of solids* by M Fox

# Lorentz oscillator model: connection to quantum mechanics

- This classical oscillator model cannot be the whole story – but works as a phenomenological description of the optical response function
- In QM, for two sharp levels, from time-dependent perturbation theory

$$\chi_{\omega} \propto (E_b - E_a - \hbar\omega)^{-1} + i\delta(E_b - E_a - \hbar\omega)$$

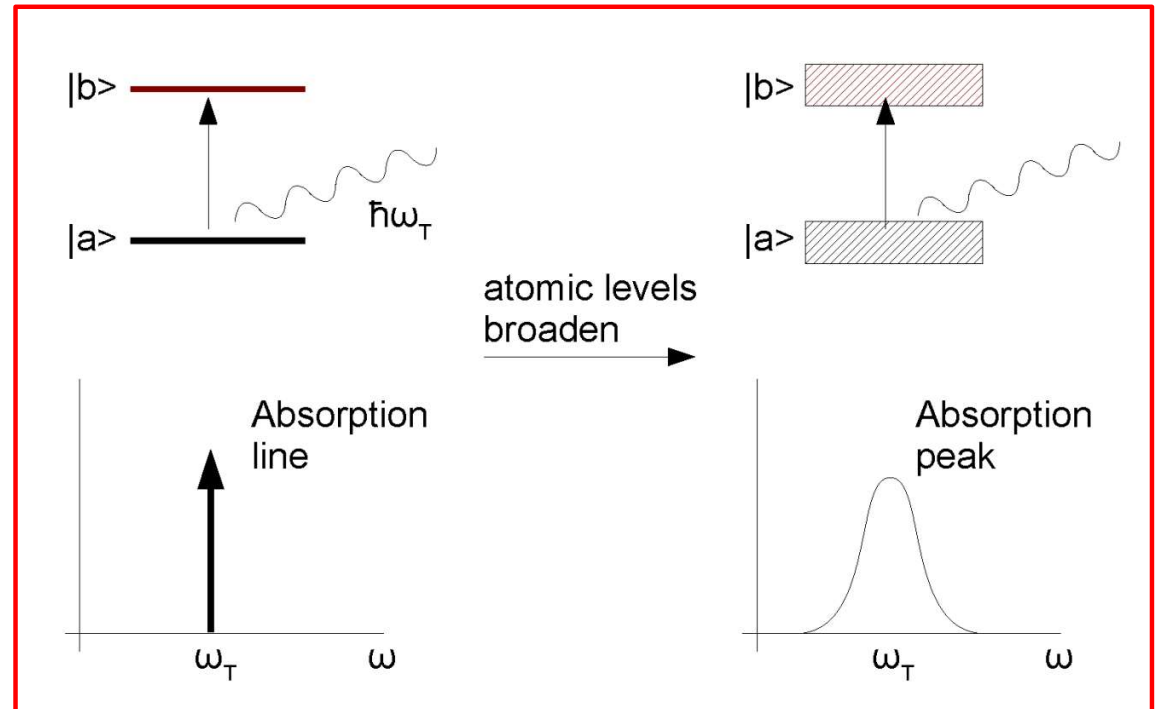
- The imaginary part is the transition rate
- This can also be written

$$\chi_{\omega} \propto \frac{1}{E_b - E_a - \hbar\omega - i\hbar\gamma/2}$$

where  $\gamma$  is very small

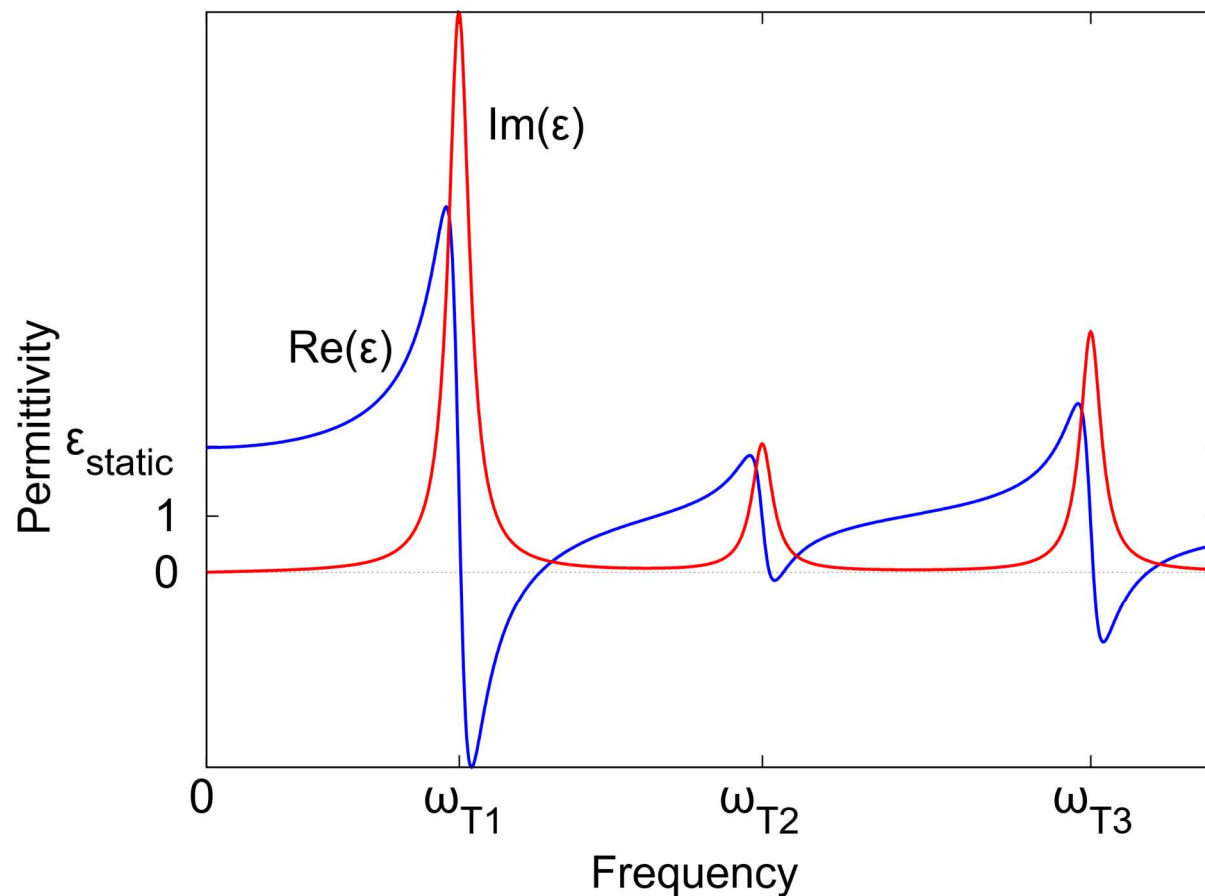
- As energy levels broaden into bands and  $\gamma$  increases, this expression becomes similar to Lorentz model close to resonance where  $\hbar\omega_T = E_b - E_a$
- We multiply by  $\omega_T + \omega$  on top and bottom and approximate  $\omega_T + \omega \approx 2\omega_T$
- Hence

$$\chi_{\omega} \propto \frac{\omega_T + \omega}{\omega_T^2 - \omega^2 - i(\omega_T + \omega)\gamma/2} \simeq \frac{2\omega_T}{\omega_T^2 - \omega^2 - i\omega\gamma}$$



# Optical properties of insulators

- Lorentz oscillator model, superposition of spectra
- May have a number of allowed transitions at energies  $\hbar\omega_{T_1}, \hbar\omega_{T_2}, \dots, \hbar\omega_{T_n}$
- Usually high-frequency – terahertz to ultraviolet
- Resulting frequency-dependent permittivity from adding responses associated with each transition:  $\epsilon(\omega) = 1 + \sum \chi_i(\omega)$





# Optical properties of insulators – comparison with experiments

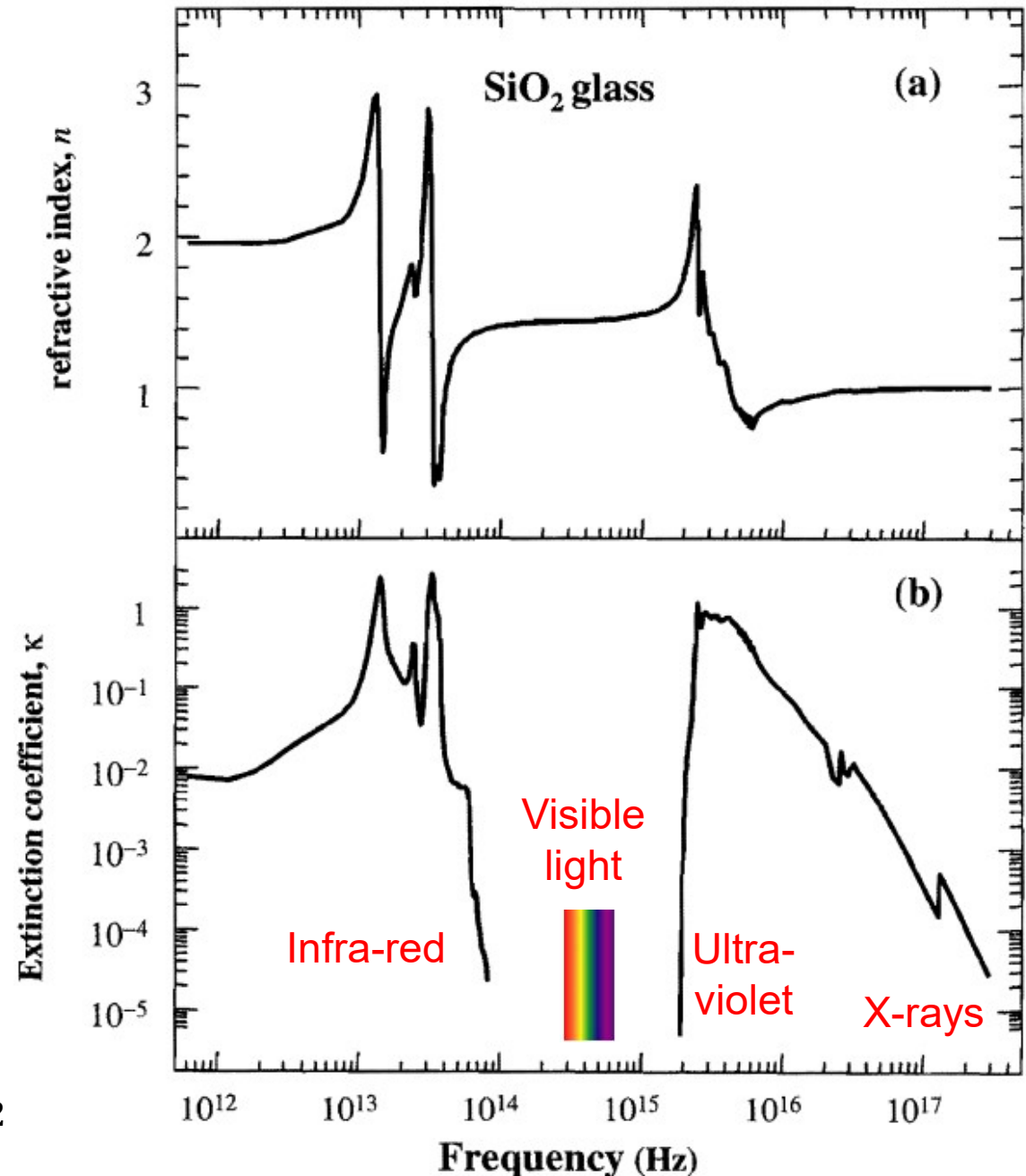
- Fused silica glass  $\text{SiO}_2$
- Expected general characteristics observed
- Transparent in visible light
- Strong absorption peaks in infrared and ultraviolet
- IR peaks due to vibrations of  $\text{SiO}_2$  molecules
- UV absorption background across 10 eV bandgap
- UV absorption peaks caused by inner core-electron transitions in Si and O
- Complex refractive index  $n + ik$

For weakly absorbing medium with  $n \gg \kappa$

$$n \approx \sqrt{\text{Re}(\epsilon)}$$

$$\kappa \approx \frac{\text{Im}(\epsilon)}{2n}$$

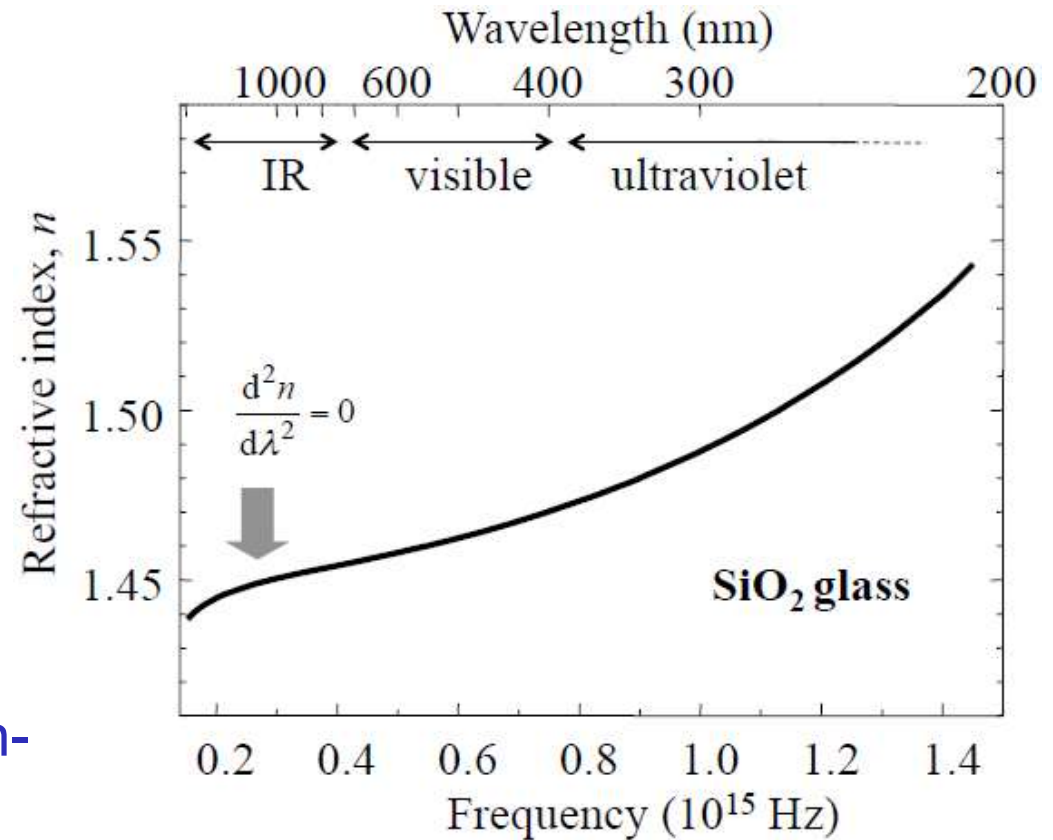
$$\text{since } \epsilon = (n + ik)^2$$



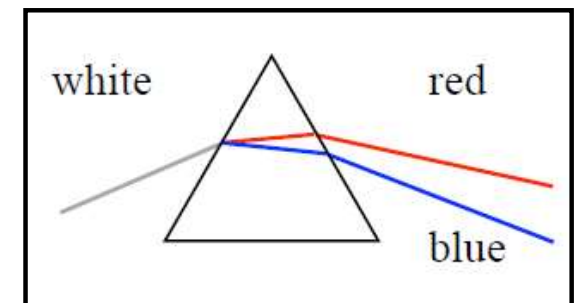
# Dispersion of light

- $\text{SiO}_2$  refractive index in more detail
- $n$  increases with frequency – ‘normal dispersion’ caused by tails of absorption peaks in IR and UV
- Can be used to separate colours of light using a prism
- Short light pulses of duration  $t_p$  have spread of frequencies  $\delta f \approx 1/t_p$
- Different velocities of frequency components causes problems in high-speed optical-fibre communications
- Temporal broadening of pulse  

$$\Delta\tau \propto d^2\omega/dk^2 \propto d^2n/dk^2 \propto d^2n/d\lambda^2$$
- Lorentz model gives  $d^2n/d\lambda^2 < 0$  above one absorption line and  $d^2n/d\lambda^2 > 0$  below next absorption line
- Choosing  $d^2n/d\lambda^2 = 0$  we minimise dispersion
- For  $\text{SiO}_2$  this is at  $\lambda \simeq 1.3 \mu\text{m}$  – a preferred optical-fibre wavelength

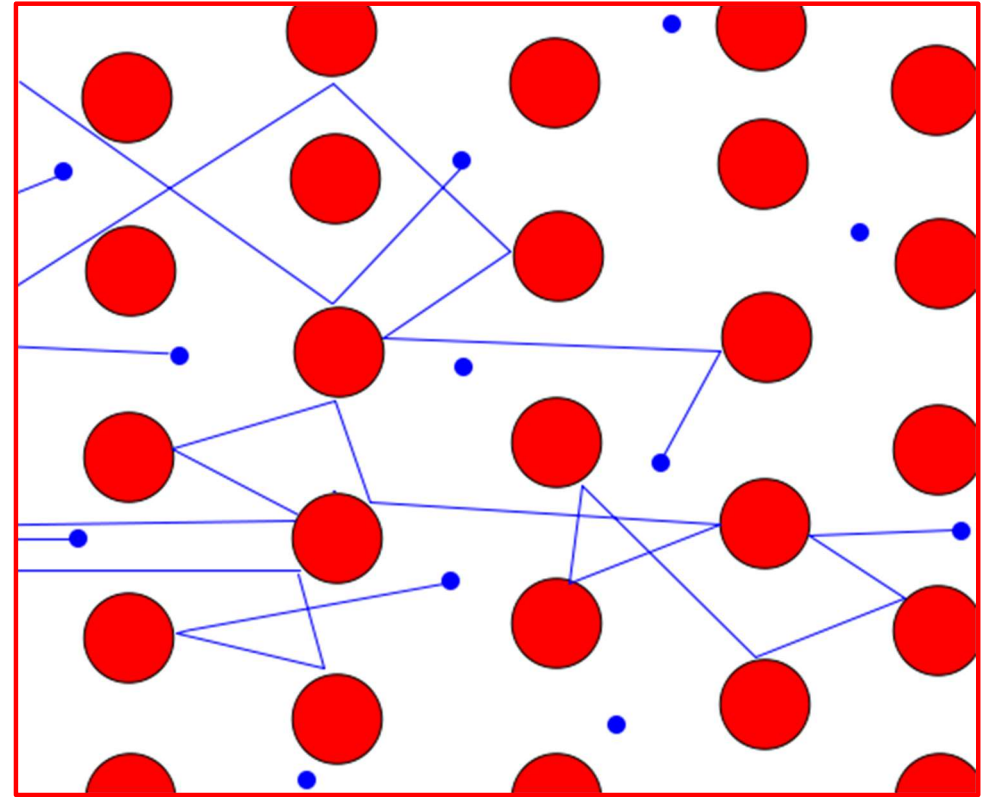


Optical properties of Solids, M Fox



# The Drude model for metals

- Lorentz (dipole) oscillator model extends naturally to metals, if some electrons no longer bound to the ions
- Inner (core) electrons still closely bound and contribute to permittivity according to Lorentz oscillator model
- Outer (conduction) electrons have been cut loose from the ions, now free to roam around entire metal
  - corresponds to spring constant in their linearised force law going to zero, so natural frequency  $\omega_T \rightarrow 0$
  - to model contribution to  $\epsilon(\omega)$ , simply use previous expressions for frequency-dependent permittivity, but drop  $\omega_T$ : resonance now at  $f = 0$
- This picture, in which some electrons are cut loose from the ionic cores, is called the Drude model



Taken from Wikipedia

# Optical properties of metals

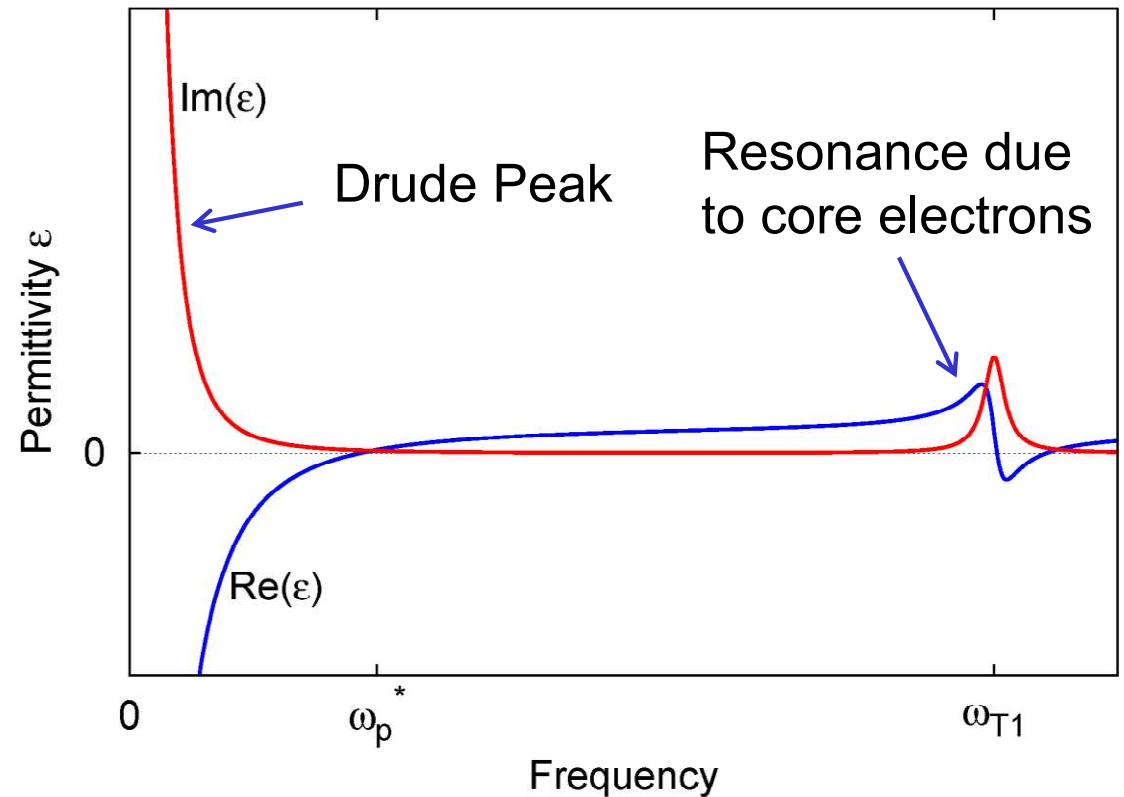
- Use Lorentz oscillator model for bound electrons, giving background  $\epsilon_\infty$
- Use Drude model for conduction electrons, zero restoring force  $\Rightarrow \omega_T = 0$

$$\chi_\omega = \chi_\infty - \frac{nq^2}{m\epsilon_0(\omega_T^2 - \omega^2 - i\omega\gamma)}$$

$$\Rightarrow \epsilon_\omega = \epsilon_\infty - \frac{nq^2}{m\epsilon_0(\omega^2 + i\omega\gamma)}$$

$$= \epsilon_\infty - \frac{\omega_p^2}{(\omega^2 + i\omega\gamma)}$$

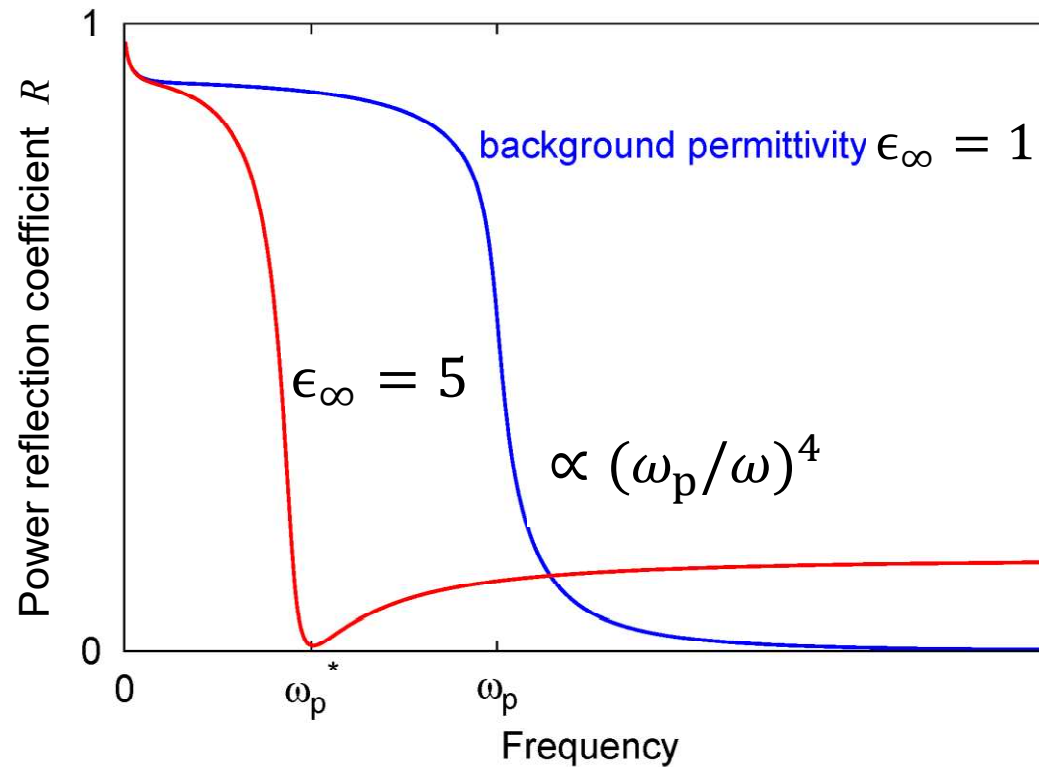
where  $\omega_p^2 = \frac{nq^2}{m\epsilon_0}$



- $|\epsilon(\omega)|$  diverges as  $\omega \rightarrow 0$  so metals are highly reflecting at low frequency
- Peak in  $\text{Im}(\epsilon_\omega)$  at low  $\omega$ , due to enhanced absorption: 'Drude peak'
- $\epsilon(\omega)$  crosses zero at  $\omega_p^*$  and approaches 1 at high frequency so metals become transparent in the ultraviolet

# Optical properties of metals in the Drude model

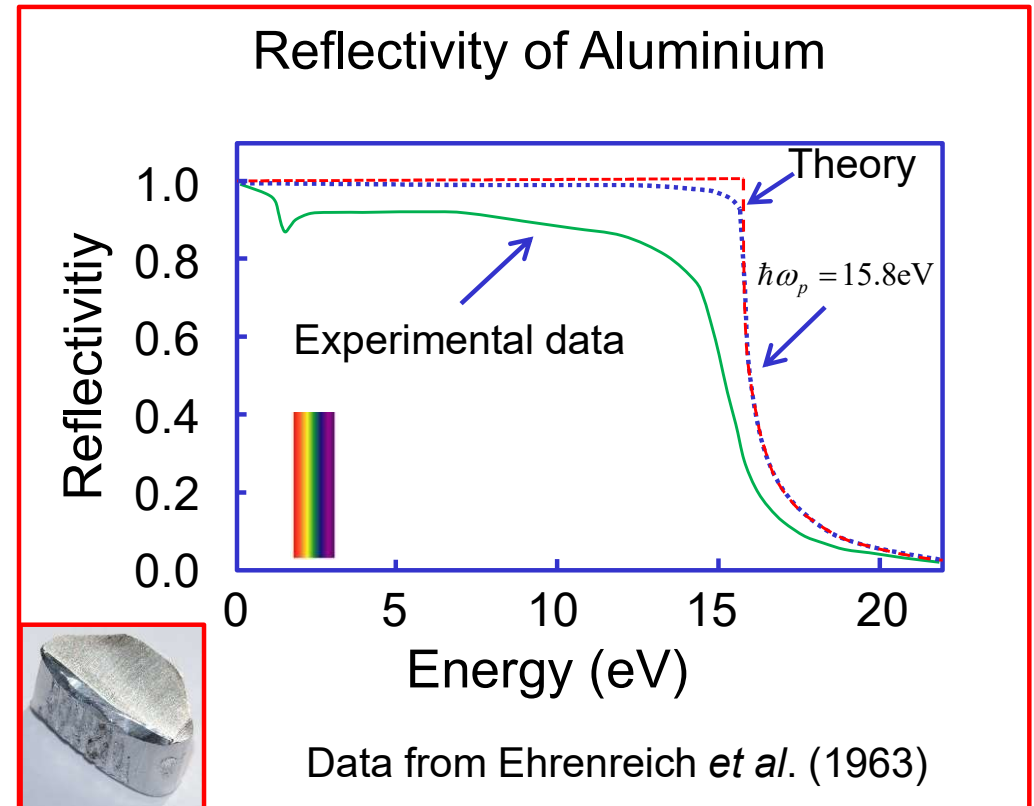
- Reflectivity at the interface between two media using the Drude model
- If permeability is unchanged at interface:  $r = \frac{\sqrt{\epsilon_1} - \sqrt{\epsilon_2}}{\sqrt{\epsilon_1} + \sqrt{\epsilon_2}}$
- Power reflection coefficient  $R = |r|^2$



- Plateau in  $R$  at low frequency, related to conductivity of material
- $R \propto \omega^{-4}$  at high frequency – blue line on figure
- If background permittivity  $\epsilon_\infty$  (due to polarisability of core electrons) is significant,  $R$  can go to zero at finite frequency – red line

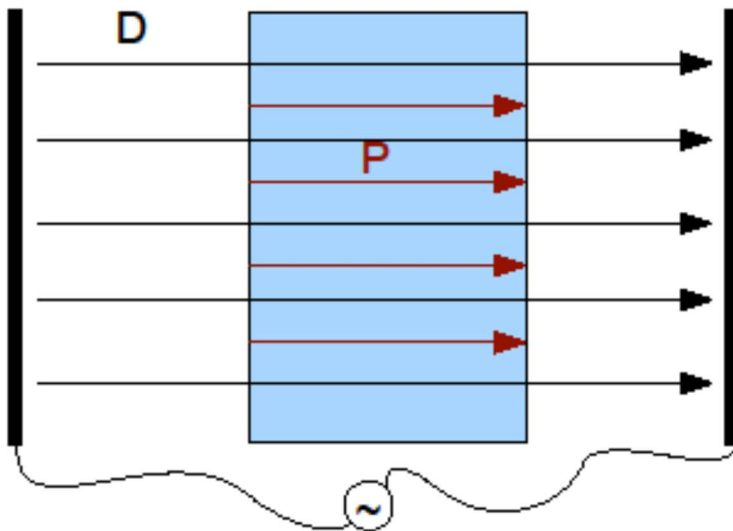
# Experimental reflectivity of aluminium

- Experimental reflectivity of aluminium as a function of photon energy – green curve (solid)
- Reflectivity above 80% for visible region of spectrum - aluminium coating is used for commercial mirrors
- Plasma frequency in ultraviolet
- Both theory curves assume we have  $\hbar\omega_p = 15.8 \text{ eV}$ 
  - red (dashed) no damping
  - blue (dotted) with  $\tau = 8.0 \times 10^{-15} \text{ s}$  – value deduced from DC conductivity – slightly better fit
- Two unexplained features in experimental results: (1) reflectivity is smaller than predicted (2) small dip in reflectivity around 1.5 eV
- Both explained by considering interband absorption rates



# Optical properties of metals: plasma oscillations

- Part IB electromagnetism – “Plasma Oscillations”
- Electrons moving in a positively charged environment – model for metal
- Consider probing a slab of material by applying an oscillating field **D**:



$$\mathbf{D} = \epsilon_0 \epsilon_\omega \mathbf{E} = \epsilon_0 \mathbf{E} + \mathbf{P}$$

$$\Rightarrow \mathbf{P} = \mathbf{D}(1 - \epsilon_\omega^{-1})$$

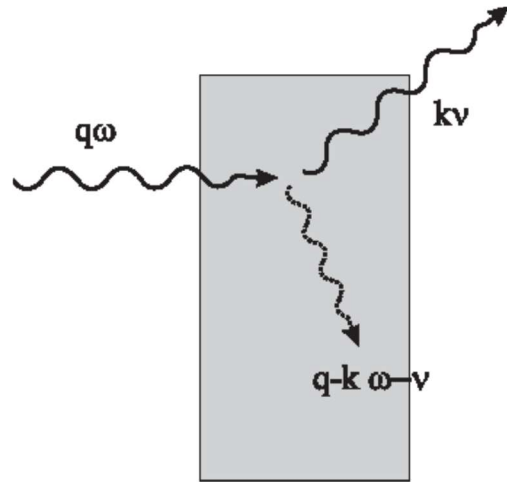
$$\epsilon_\omega = \epsilon_\infty - \frac{\omega_p^2}{(\omega^2 + i\omega\gamma)}$$

$$\epsilon_\infty \approx 1 \Rightarrow \epsilon_\omega^{-1} = \frac{\omega^2 + i\omega\gamma}{\omega^2 - \omega_p^2 + i\omega\gamma}$$

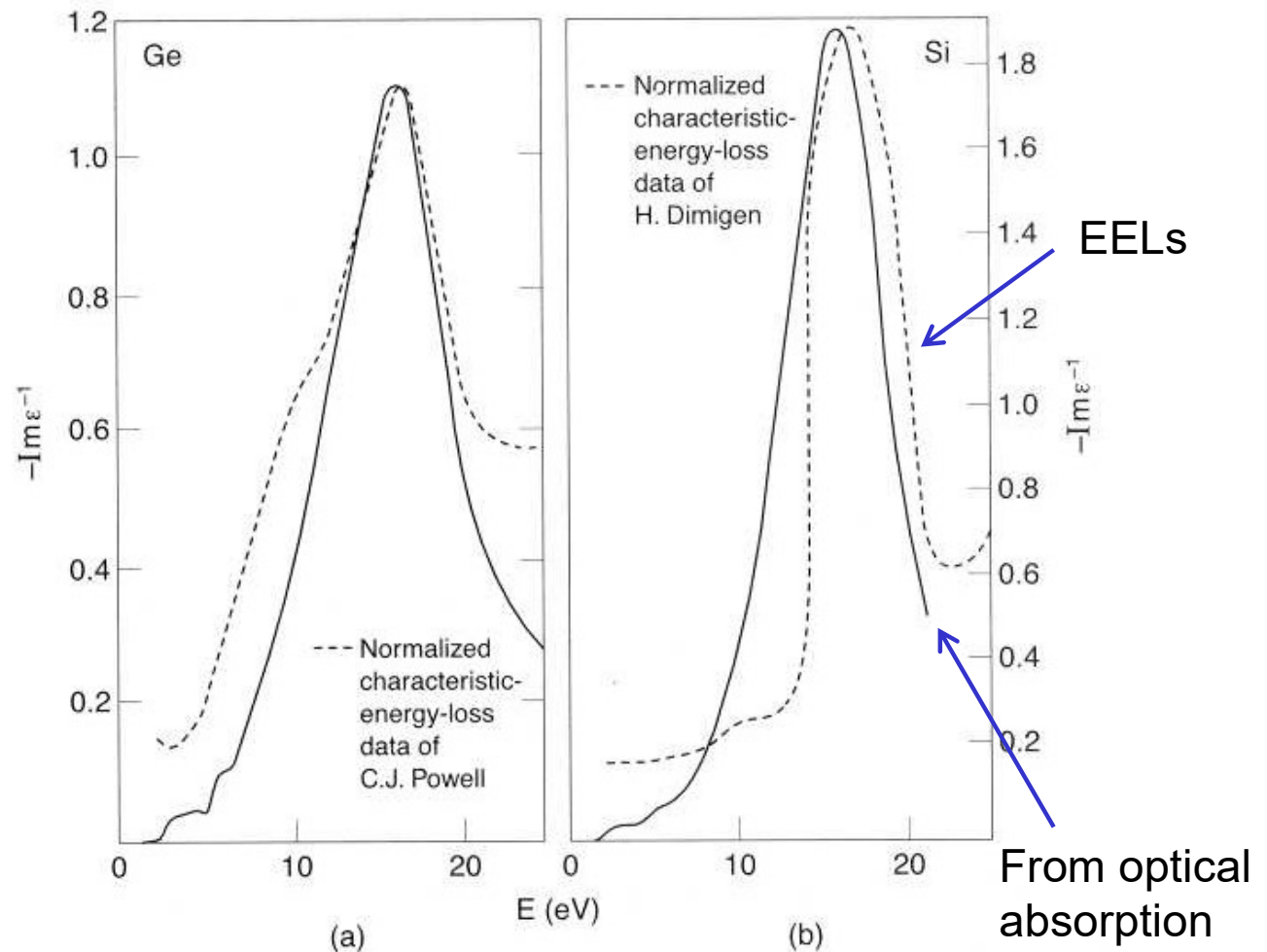
- In metals  $\omega_p \gg \gamma = \tau^{-1}$  and usually  $\epsilon_\infty = 1$  so  $\epsilon_\omega^{-1}$  peaks and  $\epsilon_{\omega_p} \approx 0$
- More generally, as  $\epsilon_\omega \rightarrow 0$  at  $\omega = \omega_p^* \equiv \omega_p \epsilon_\infty^{-1/2}$  we get *plasma oscillations* at  $\omega_p^*$
- Polarisation causes build-up of surface charge, which generates the restoring force driving the oscillations – the electrons slosh back and forth



# Optical properties of metals: plasma oscillations and Electron Energy-Loss Spectroscopy in Ge and Si



- Incoming electron at wavevector  $q$ , energy  $\hbar\omega$
- Outgoing electron at wavevector  $k$ , energy  $\hbar\nu$
- Plasmon generated with energy  $\hbar(\omega - \nu)$

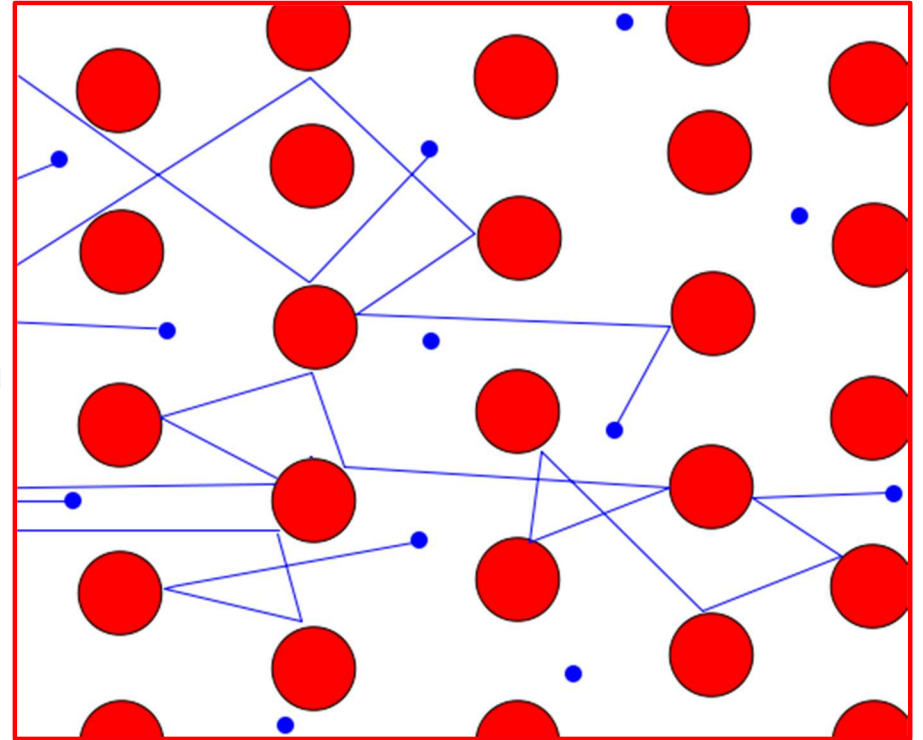


- Response to oscillating applied  $\mathbf{D}$  field given by  $\epsilon_{\omega}^{-1} = \frac{\omega^2 + i\omega\gamma}{\omega^2 - \omega_p^2 + i\omega\gamma}$
- Resonance at plasma frequency  $\omega_p^2 = \frac{ne^2}{m\epsilon_0}$ , width  $\tau^{-1}$



# Metals – the Drude model

- Assumes we have a gas of electrons free to move between positive ion cores
  - electrons only scattered by the ion cores
- Between collisions with the ion cores electrons do not interact with each other
- Collisions are instantaneous, resulting in a change of electron velocity (randomisation of momentum)
- The probability an electron has collision in unit time is  $\tau^{-1}$ , the scattering rate
- Electrons achieve thermal equilibrium with surroundings only through collisions



Taken from Wikipedia

# Drude model - improvements

- Setting  $\omega_T \rightarrow 0$  is somewhat unsatisfactory:
  - if electrons are cut loose from the ionic cores, their average position, around which they are meant to oscillate, is no longer defined. The displacement  $\mathbf{u}$  for an individual electron acquires an arbitrary offset
  - picture of scattering processes (electrons occasionally hit an obstacle and thereby randomise their momentum) prevents us from ascribing the same velocity to all the electrons—need a statistical description
- Make two modifications:
  - instead of equation of motion for electronic displacement, consider rate of change of the velocity  $\mathbf{v} = \dot{\mathbf{u}}$
  - instead of considering velocity of individual electrons, average over a large number of electrons, look for differential equation for *average* electron velocity
  - even if individual electrons have wildly different velocities, the average, or *drift* velocity will follow a simple equation of motion—drift velocity determines the optical and transport properties of the metal

# Optical properties of *metals*: connection to ac conductivity

- Let  $\mathbf{u}$  be the electron's displacement
- Current density  $\mathbf{j} = nq\dot{\mathbf{u}}$  (number density x charge x velocity)
- Polarisation  $\mathbf{P} = nq\mathbf{u}$ . Hence,  $\dot{\mathbf{P}}_c = \mathbf{j}$  for the conduction electrons
- Adding in the polarisation of the core electrons via  $\chi_\infty$  (due to the background polarisability) we get:  $\dot{\mathbf{P}} = \mathbf{j} + \epsilon_0\chi_\infty\dot{\mathbf{E}}$
- At angular frequency  $\omega$ , substituting:  
 $\mathbf{E} = \mathbf{E}_\omega \exp(-i\omega t)$ ,  $\mathbf{j} = \mathbf{j}_\omega \exp(-i\omega t)$ ,  $\mathbf{P} = \mathbf{P}_\omega \exp(-i\omega t)$ ,  $\mathbf{P}_\omega = \epsilon_0\chi_\omega\mathbf{E}_\omega$
- We get  $\mathbf{j}_\omega = -i\omega\epsilon_0\mathbf{E}_\omega(\chi_\omega - \chi_\infty) = \sigma_\omega\mathbf{E}_\omega$
- Hence  $\sigma_\omega = -i\omega\epsilon_0(\chi_\omega - \chi_\infty) = -i\omega\epsilon_0(\epsilon_\omega - \epsilon_\infty)$   
$$\Rightarrow \epsilon_\omega = \frac{i\sigma_\omega}{\epsilon_0\omega} + \epsilon_\infty$$
- This relates the imaginary part of the permittivity to the real part of the frequency-dependent conductivity
  - can indirectly determine conductivity of a metal at high frequencies by optical measurement
- If atomic (or background) polarisability is zero, then  $\epsilon_\infty = 1$

# Drude model – relaxation-time approximation

- We need an equation of motion for the drift velocity, and to take into account the loss of momentum through collisions
- The current density  $\mathbf{J}$  due to electrons of number density  $n$  [we used  $n_v$  earlier to distinguish from refractive index], mass  $m$ , of average (“drift”) velocity  $\mathbf{v}$  and momentum  $\mathbf{p}$ , is given by:

$$\mathbf{J} = -nev\mathbf{v} = -\frac{ne}{m}\mathbf{p}$$

- Consider the evolution of  $\mathbf{p}$  in time  $\delta t$  under the action of an external force  $\mathbf{f}(t)$
- Probability of a collision during  $\delta t$  is  $\delta t/\tau$ , where  $\tau$  is the average time between collisions – the **relaxation time**
- Probability of no collision during  $\delta t$  is  $1 - \delta t/\tau$
- For electrons that *have not collided*, momentum increases:

$$\delta\mathbf{p} = \mathbf{f}(t)\delta t + O(\delta t)^2$$

- So the contribution to the average momentum during  $\delta t$  for electrons that *have not collided* is:

$$\mathbf{p}(t + \delta t) = (1 - \delta t/\tau)(\mathbf{p}(t) + \mathbf{f}(t)\delta t + O(\delta t)^2)$$

# Drude model – relaxation-time approximation

- Electrons that *have* collided are a fraction  $\delta t/\tau$  of the total
- The momentum they will have acquired since colliding (where their momentum was randomised) is  $\sim \mathbf{f}(t)\delta t$
- So contribution to average momentum for electrons that have collided is of order  $(\delta t)^2$  – small
- Thus, for momentum, from previous slide:

$$\mathbf{p}(t + \delta t) = (1 - \delta t/\tau)(\mathbf{p}(t) + \mathbf{f}(t)\delta t + O(\delta t)^2)$$

- If  $\delta t \rightarrow 0$  we can rearrange this to give

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t)$$

- Hence the collisions produce frictional damping
- Apply to electrical conductivity  $\sigma$  defined by  $\mathbf{J} = \sigma\mathbf{E}$ , assume **steady state** so  $\frac{d\mathbf{p}(t)}{dt} = 0$ , and that the force on an electron is  $\mathbf{f}(t) = -e\mathbf{E}$
- From previous slide,  $\mathbf{J} = -\frac{ne}{m}\mathbf{p}$

- Hence

$$\mathbf{f}(t) = \frac{\mathbf{p}(t)}{\tau} = -\frac{m}{ne\tau}\mathbf{J} = -e\mathbf{E} \Rightarrow \sigma = \frac{ne^2\tau}{m}$$

# Drude model

- From the relaxation-time approximation, for a force  $\mathbf{f}(t)$ :

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + \mathbf{f}(t)$$

- In magnetic and electric fields:  $\mathbf{f} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$  and  $\mathbf{j} = nq\mathbf{v}$
- Hence we can write the same equation in different forms:

$$\frac{d\mathbf{p}(t)}{dt} = -\frac{\mathbf{p}(t)}{\tau} + q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$\frac{d\mathbf{v}(t)}{dt} = -\frac{\mathbf{v}(t)}{\tau} + \frac{q}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$\frac{d\mathbf{j}(t)}{dt} = -\frac{\mathbf{j}(t)}{\tau} + \frac{nq^2}{m}(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

$$\frac{d\mathbf{j}(t)}{dt} = -\frac{\mathbf{j}(t)}{\tau} + \frac{nq^2\mathbf{E}}{m} + \frac{q}{m}(\mathbf{j} \times \mathbf{B})$$

# Drude model: frequency-dependent conductivity

- So, if  $B = 0$ ,  $\frac{d\mathbf{j}(t)}{dt} + \frac{\mathbf{j}(t)}{\tau} = \frac{nq^2}{m} \mathbf{E}$ , and if  $\mathbf{j} = \mathbf{j}_\omega \exp(-i\omega t)$ ,  $\mathbf{E} = \mathbf{E}_\omega \exp(-i\omega t)$ ,

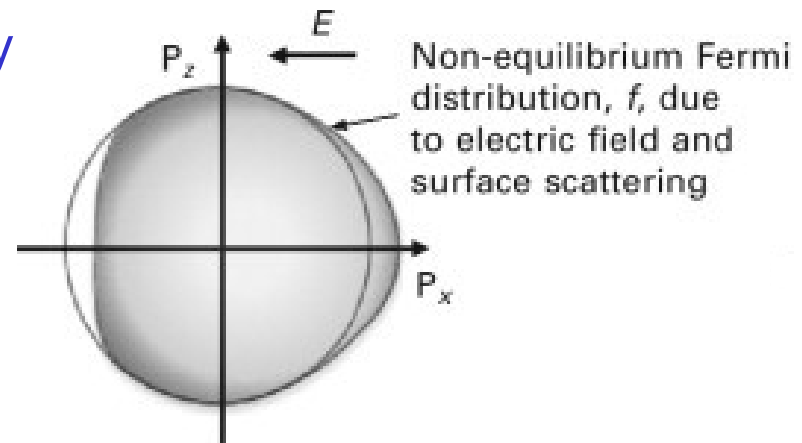
$$(\tau^{-1} - i\omega)\mathbf{j}_\omega = \frac{nq^2}{m} \mathbf{E}_\omega$$

$$\Rightarrow \mathbf{j}_\omega = \frac{nq^2 \mathbf{E}_\omega}{m(\tau^{-1} - i\omega)} = \frac{nq^2 \tau \mathbf{E}_\omega}{m(1 - i\omega\tau)}$$

- And given  $\mathbf{j} = \sigma \mathbf{E}$ , we have  $\sigma_\omega = \frac{nq^2 \tau}{m(1 - i\omega\tau)} = \frac{\epsilon_0 \omega_p^2 \tau}{(1 - i\omega\tau)}$
- Here  $\omega_p^2 \equiv \frac{nq^2}{m\epsilon_0}$  defines the *plasma frequency*
- At low frequencies  $\omega\tau \ll 1$ ,  $\sigma_0 = \frac{ne^2\tau}{m} = ne\mu$ , where  $\mu = \frac{e\tau}{m}$  ( $q = \pm e$ )
- $\mu = \frac{q\tau}{m} = \frac{|\mathbf{v}|}{|\mathbf{E}|}$  called carrier *mobility* (how well carriers respond to  $\mathbf{E}$  field)
- Earlier, we found  $\epsilon_\omega = \frac{i\sigma_\omega}{\epsilon_0 \omega} + \epsilon_\infty$ , so we obtain
 
$$\epsilon_\omega = \epsilon_\infty + \frac{i\omega_p^2 \tau}{\omega(1 - i\omega\tau)} = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega/\tau}$$
- Exactly the expression we obtained right at the start by setting  $\omega_T \rightarrow 0$ , if we identify  $1/\tau$  with  $\gamma$

# Drude model – is it valid?

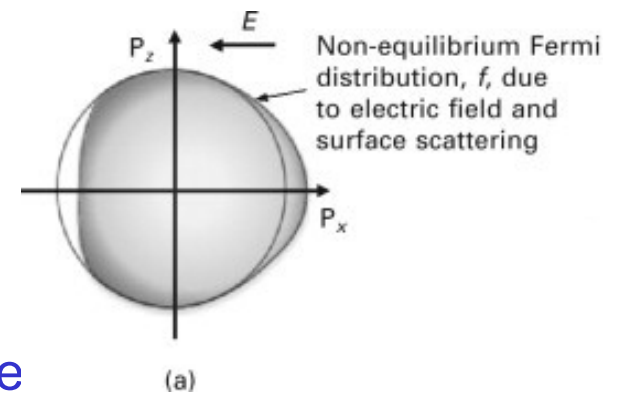
- The Drude model is very crude (devised only 3 years after discovery of electron by J J Thomson in 1897!)
  - assumes electrons have random momentum after a collision (averages to 0)
  - assumes all the positive ions contribute to scattering (but mean free path can be much longer than atomic spacing)
  - no concept of QM, Pauli exclusion principle, fermions, ...
- We should instead consider a Fermi sphere of electrons occupying all the states in  $k$ -space up to the Fermi energy  $E_F$ 
  - only two electrons in each state (two spins)
  - only electrons near Fermi surface can gain energy or scatter
  - Fermi-Dirac function  $f$  gives probability of finding electron in a state
  - distribution function  $f$  is modified by momentum, so there are more electrons moving in one direction than in the opposite one





# Drude model – its replacement

- Describe using Boltzmann transport formalism (Part III major option AQCMP)
  - scattering causes total momentum to decay, same
- Various types of scattering in metals:
  - phonons (dominate at room temperature  $T$ )
  - impurities and lattice defects (important at low  $T$ )
  - other electrons (surprisingly unimportant; total momentum conserved so no effect on current)
  - we will see that the ions themselves have no effect provided that they are in a periodic lattice (band structure)
- Though from the above we now realise its limitations, the Drude model has its uses, so let's see what it can help us calculate



# Transport in electric *and* magnetic fields

- Previously  $\frac{d\mathbf{j}(t)}{dt} = -\frac{\mathbf{j}(t)}{\tau} + \frac{nq^2\mathbf{E}}{m} + \frac{q}{m}(\mathbf{j} \times \mathbf{B})$
- If  $B$  is parallel to  $z$ -axis, taking components

$$\left(\frac{d}{dt} + \tau^{-1}\right)j_y = \frac{q}{m}(nqE_y - Bj_x)$$

$$\left(\frac{d}{dt} + \tau^{-1}\right)j_x = \frac{q}{m}(nqE_x + Bj_y)$$

- Steady state  $\frac{d\mathbf{j}}{dt} = 0$

$$j_y = \frac{q\tau}{m}(nqE_y - Bj_x), \quad j_x = \frac{q\tau}{m}(nqE_x + Bj_y)$$

- Hall effect*: current confined to  $x$ -axis ( $j_y = 0$ ) by transverse field ( $E_y$ ) due to charge build up

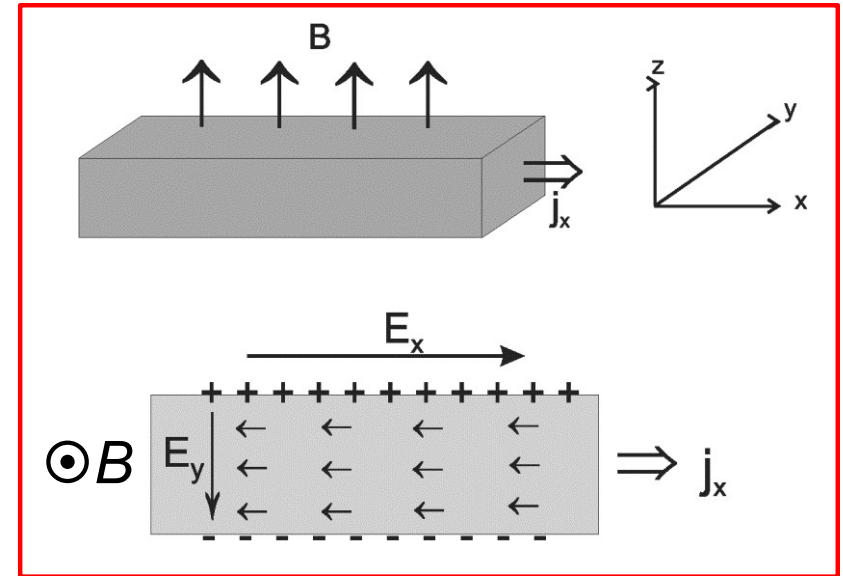
- Hall coefficient  $R_H = \frac{E_y}{j_x B} = \frac{1}{nq}$  gives carrier density and sign of charge

- If  $B = 0$  then  $j_x = \frac{q\tau}{m}nqE_x \Rightarrow \frac{j_x}{nq} = \frac{v_x}{E_x} = \frac{q\tau}{m} = \mu$ , the carrier 'mobility'

– mobility defined as velocity of charge carrier per unit electric field

- $\mathbf{j} = \sigma\mathbf{E} \Rightarrow \sigma = \frac{nq^2\tau}{m} = nq\mu$

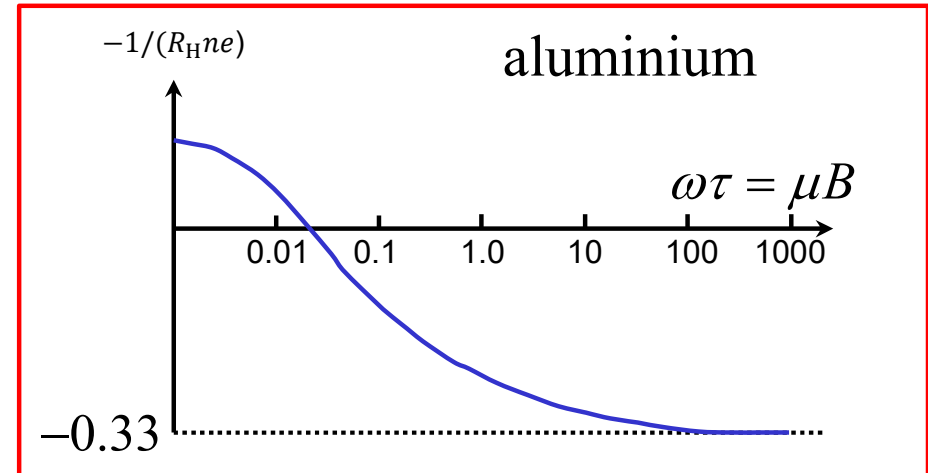
- Cyclotron frequency defined as  $\omega_c = \frac{eB}{m} \Rightarrow \omega_c\tau = \mu B$



# Hall effect in metals

- First measured in 1879 by E H Hall
- From the last slide  $R_H = 1/nq$
- Drude theory predicts  $R_H$  is independent of  $B$  and  $\tau$
- In metals, however, it is found that  $R_H$  does vary with magnetic field as well as temperature and sample purity
- Measuring pure samples at low temperatures and high magnetic fields (1T), limiting values are obtained
- Compare observed and predicted numbers of free electrons per atom for a range of metals
- Theory seems to work quite well for alkali metals & noble metals but not for the others – new theories needed!

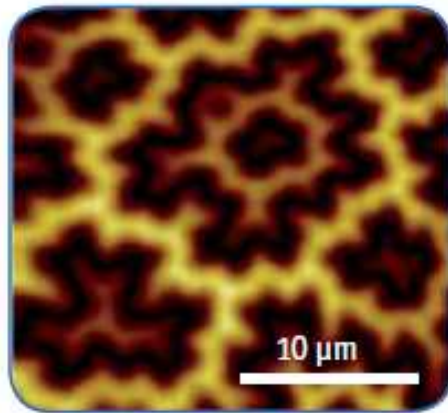
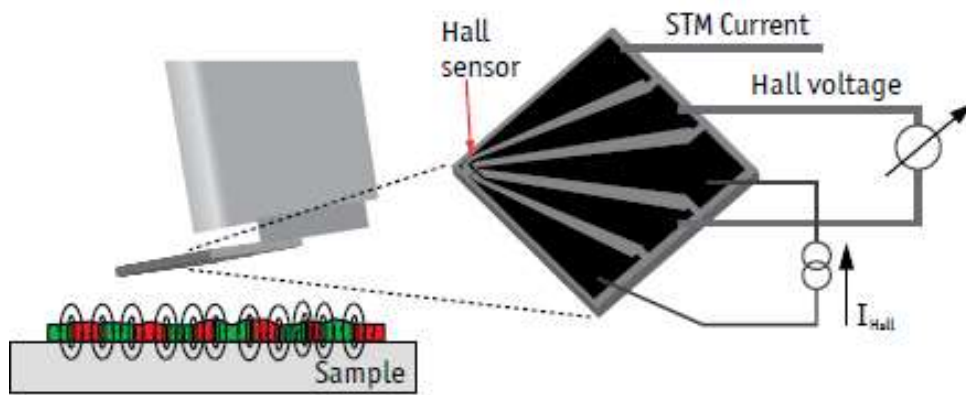
R Lück, *Phys Stat. Sol.* **18**, 49 (1966)



Metal	Valence	$-1/R_H ne$
Li	1	0.8
Na	1	1.2
K	1	1.1
Cu	1	1.5
Ag	1	1.3
Au	1	1.5
Be	2	-0.2
Mg	2	-0.4
In	3	-0.3
Al	3	-0.3

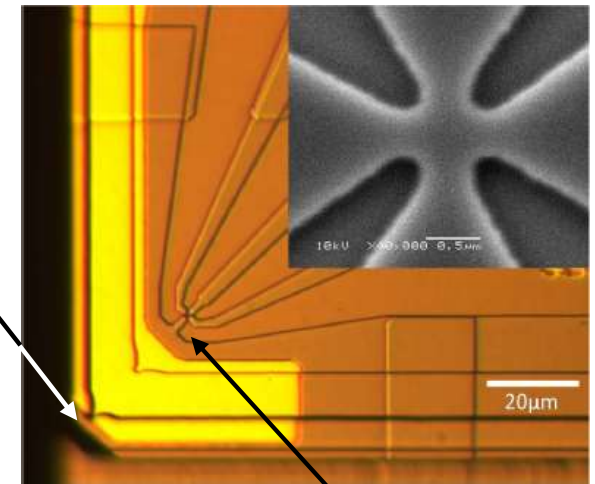
# Scanning Hall-Probe Microscopy

- First report Chang *et al.*, *Appl. Phys. Lett.* **61**, 1974 (1992)
- Hall sensor mounted on scanning system to measure local magnetic field
- Magnetic field sensitivity  $10^{-5}\text{T}$  spatial resolution  $0.35\mu\text{m}$
- Now commercial product from Attocube, Nanomagnetics, Magcam.....

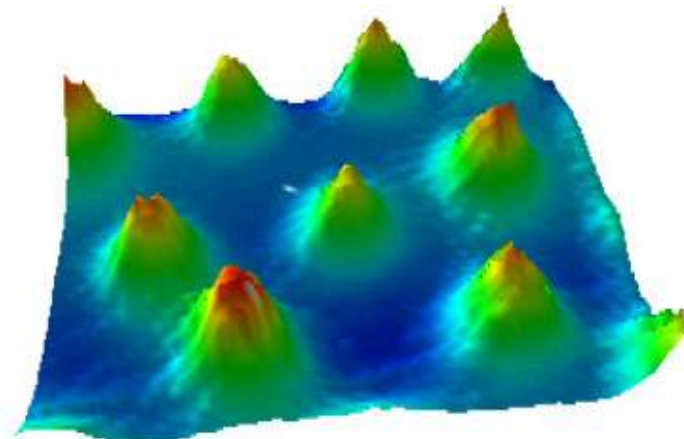


SHPM image of BaFeO, recorded at 4.2 K in constant height mode. The color scale spans 106 mT (black to white), while the S/N ratio of this measurement yields  $2 \times 10^5$ .

Tunnelling probe



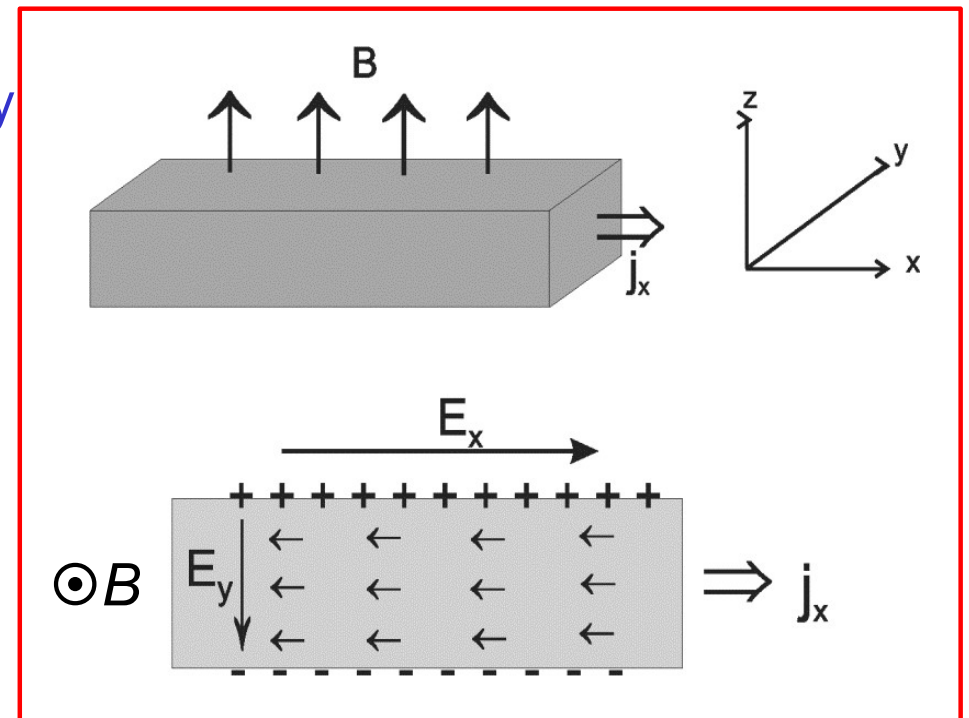
Hall probe



SHPM image of superconducting vortices in a thin Pb film at 4 Kelvin

# Summary

- Introduction to course and recommended text books
- Lorentz oscillator model for optical absorption in solids
  - comparison with atomic absorption
- The Drude model of electron motion in solids
  - relaxation-time approximation, scattering and electrical conductivity
  - frequency-dependent conductivity
  - optical properties of metals
  - experimental reflectivity of aluminium
  - plasma oscillations
  - electron energy-loss spectroscopy
- Hall effect from Drude model
  - scanning Hall-probe microscopy



# Quantum Condensed-Matter Physics

## 1. Classical and semiclassical models for electrons in solids (3L)

Lorentz dipole oscillator, optical properties of insulators. Drude model and optical properties of metals, plasma oscillations. Semiclassical approach to electron transport in electric and magnetic fields, the Hall effect. *Sommerfeld model, density of states, specific heat of; electrons in metals, liquid  $^3\text{He}/^4\text{He}$  mixtures. Screening and the Thomas-Fermi approximation.*

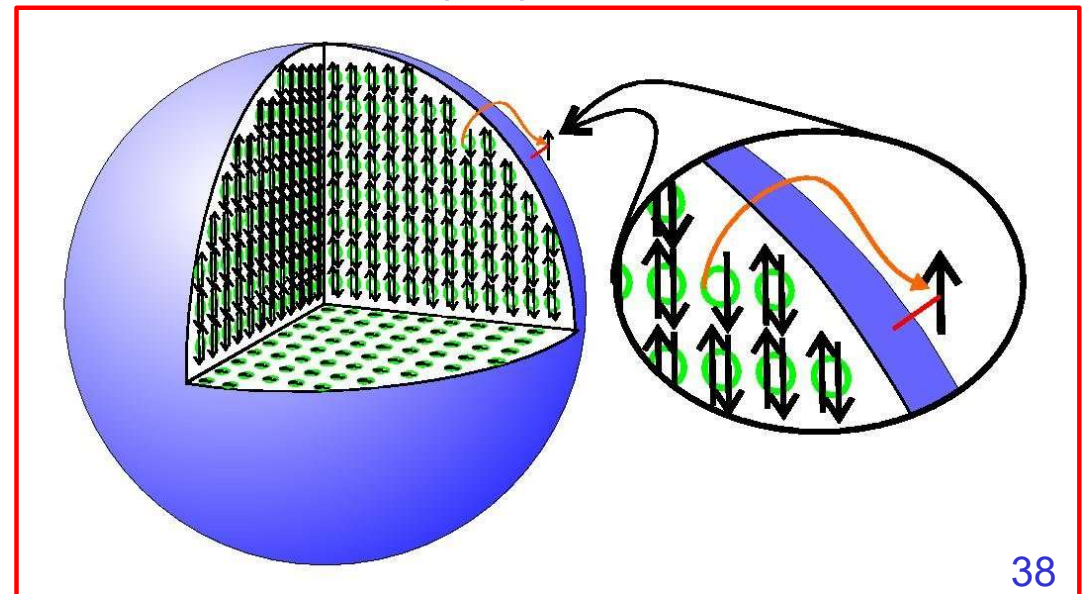
## 2. Electrons and phonons in periodic solids (6L)

## 3. Experimental probes of band structure (4L)

## 4. Semiconductors and semiconductor devices (5L)

## 5. Electronic instabilities (2L)

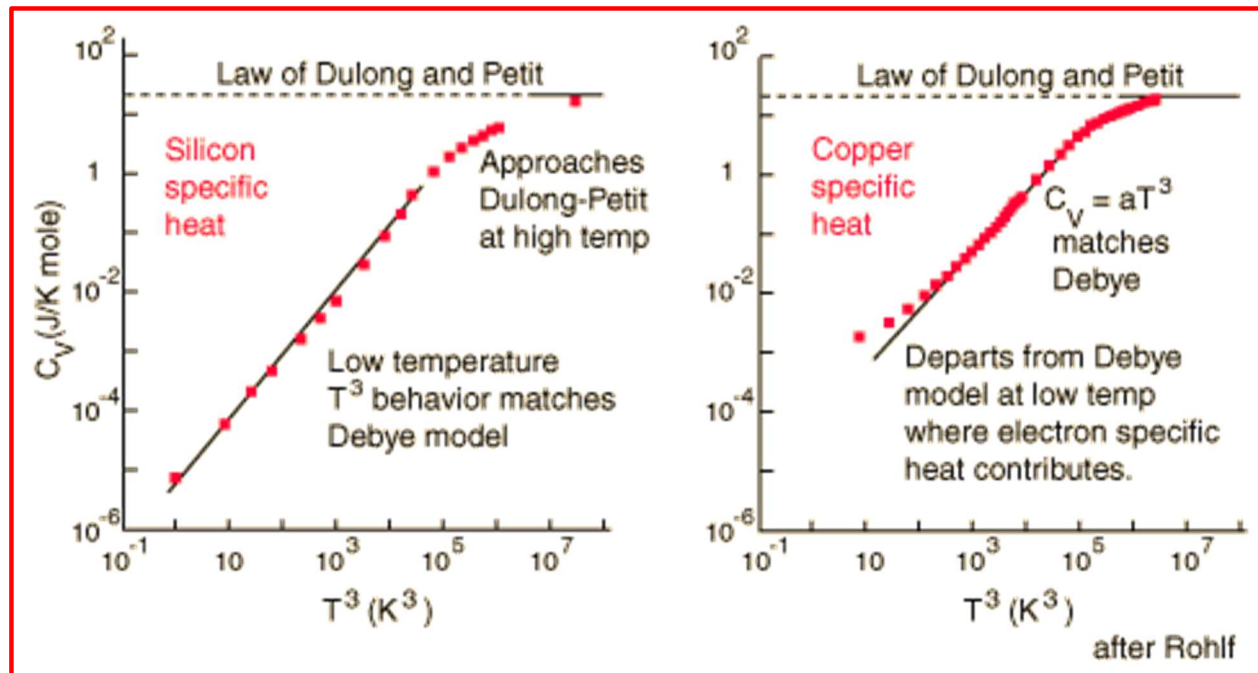
## 6. Fermi Liquids (2L)





# Problems with Drude Theory

- Drude model predicts the electronic heat capacity to be  $C_{el} = \frac{3}{2} n k_B$  from equipartition of energy, independent of  $T$
- Measured heat capacity falls far below that expected from equipartition theorem and is temperature-dependent



- Correct description: degenerate Fermi gas (c.f. Stat. Phys. course)
- Interpret velocity  $u$  in Drude model as *drift velocity*, averaged over many particles
  - individual electrons actually travel at up to 1% of speed of light!

# Failure of Lorentz and Drude models

- Lorentz oscillator model successfully describes optical response of insulators
- Drude theory works surprisingly well modelling optical and transport properties of metals
- Both theories fail dramatically describing thermodynamic properties
  - applying equipartition theorem to the dipole-oscillator model, expect contribution of  $k_B$  to heat capacity of each oscillator
  - similarly, within Drude model (which treats conduction electrons like classical ideal gas), expect contribution to heat capacity of  $\frac{3}{2}k_B$  per conduction electron
- Measured heat capacities for both insulators and metals are far lower
- Reason same as why heat capacity due to lattice vibrations falls below Dulong-Petit limit at low temperature:
  - electronic motion largely frozen out, because in the quantum-mechanical model for electrons, energy required to excite them exceeds thermal energy available

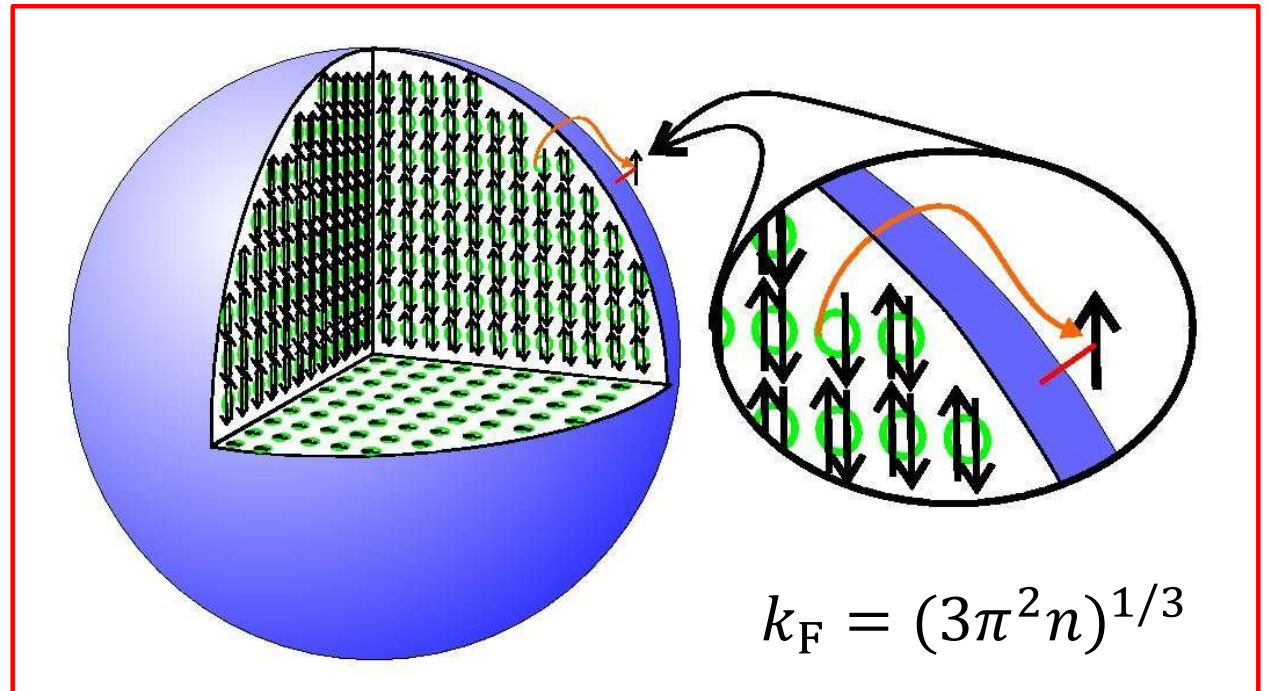


# Introduction to Sommerfeld theory

- More specifically, in insulators, atomic energy levels separated by large energy gaps of order eV ( $\sim k_B \times 11,000$  K)
  - so specific-heat contribution due to electronic excitations in insulators will only become noticeable at temperatures of thousands of K
- In metals, on the other hand, low-energy excitations always possible, but only for a small fraction of electrons
  - we will see (as shown in Thermal and Statistical Physics course) that conduction electrons form a degenerate Fermi gas, in which only a fraction  $\sim k_B T / E_F$  (where Fermi energy  $E_F \sim$  eV) are close enough to chemical potential to contribute to heat capacity, which is therefore proportional to  $T$
- Within Fermi-gas picture, most electrons travel at very high speeds, dictated by the wavevector of the quantum state they occupy
  - these speeds can reach  $10^6$  m/s (c.f. m/s in Drude model)
  - shows again the need to interpret velocity  $v = \dot{u}$  in Drude model as a *drift* velocity, averaged over all particles (a few with huge speeds, most 0!)
- By using quantum statistics, as introduced in Thermal and Statistical Physics course, we can resolve difficulties of Drude model and understand the thermodynamic properties of solids

# Sommerfeld Model – density of states

- Free-electron gas - Schrödinger equation:  $-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) = E\psi(\mathbf{r})$
- Introduce eigenstates
$$\psi_{\mathbf{k}}(\mathbf{r}) = A \exp(i\mathbf{k} \cdot \mathbf{r}), \quad E_{\mathbf{k}} = \hbar^2 |\mathbf{k}|^2 / 2m$$
satisfying periodic boundary conditions  $\psi(x + L, y, z) = \psi(x, y, z)$  etc.
- Allowed values of momentum are discrete:  $\mathbf{k} = 2\pi/L (n_x, n_y, n_z)$ , where  $n_x, n_y, n_z$  are positive or negative integers
- At zero temperature fill up Fermi sphere to the Fermi energy  $E_F$
- Each triplet of quantum numbers corresponds to 2 states – electron spin degeneracy
- Volume in  $k$ -space  $(2\pi/L)^3$



# Sommerfeld Model – density of states

- Number of occupied states in Fermi sphere:  $N = 2 \cdot \frac{\frac{4}{3}\pi k_F^3}{(2\pi/L)^3}$
- Hence if  $n = N/V = N/L^3$  then  $k_F = (3\pi^2 n)^{1/3}$
- Also,  $E_F = \hbar^2 k_F^2 / 2m = \hbar^2 (3\pi^2 n)^{2/3} / 2m \Rightarrow \ln(E_F) = \frac{2}{3} \ln(n) + \text{const}$   

$$\Rightarrow \frac{dE_F}{E_F} = \frac{2}{3} \frac{dn}{n} \Rightarrow g(E_F) \equiv \frac{dn}{dE_F} = \frac{3}{2} \frac{n}{E_F}$$
- **Density of states** (number of states per unit energy)  $g(E)$ :  

$$g(E)dE = 2 \cdot \frac{\text{Volume of shell in } k\text{-space}}{\text{Volume of } k\text{-space per state}} = 2 \cdot \frac{4\pi k^2 dk}{(2\pi)^3 / V}$$
- Hence  $g(E) = 2 \frac{V}{(2\pi)^3} 4\pi k^2 \frac{dk}{dE} = \frac{V}{\pi^2} \frac{m}{\hbar^2} \left( \frac{2mE}{\hbar^2} \right)^{1/2}$ 
  - factor of 2 for spin degeneracy
- Often  $g(E)$  is defined as number of states per unit energy *per unit volume* so  $V$  disappears (as in the first definition above)

# Sommerfeld Model – electronic specific heat

- Occupancy of states in thermal equilibrium – Fermi distribution:

$$f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$$

- At  $T = 0$ , chemical potential  $\mu = E_F$
- Number density of particles  $n = \frac{N}{V} = \frac{1}{V} \sum_i f(E_i) = \int g(E) f(E) dE$
- Internal energy density  $u = \frac{U}{V} = \int E g(E) f(E) dE$
- At room temperature  $k_B T \approx 0.025$  eV
- For metals  $E_F \approx 1 - 10$  eV, hence  $k_B T \ll E_F$
- From above,  $c_V = \partial u / \partial T|_V = \int E g(E) \frac{\partial f(E)}{\partial T} dE$
- Since the Fermi function  $f$  is a step function,  $\frac{\partial f(E)}{\partial T}$  is sharply peaked at the chemical potential  $\mu$ 
  - contributions to the specific heat only come from states within  $k_B T$  of the chemical potential, with each state having specific heat  $\sim k_B$
- We can guess that  $c_V \approx n \frac{k_B T}{E_F} k_B$

# Sommerfeld Model – electronic specific heat

- To calculate this more accurately.... We take the density of states as a constant (slowly varying over scale of  $k_B T$ ) so

$$c_V = \int E g(E) \frac{\partial f(E)}{\partial T} dE \approx g(E) \int E \frac{\partial f(E)}{\partial T} dE$$

- Changing variables,  $x = \frac{E-\mu}{k_B T} \Rightarrow \frac{\partial f}{\partial T} = \frac{e^x}{(e^x+1)^2} \times \left[ \frac{x}{T} + \frac{1}{k_B T} \frac{\partial \mu}{\partial T} \right]$

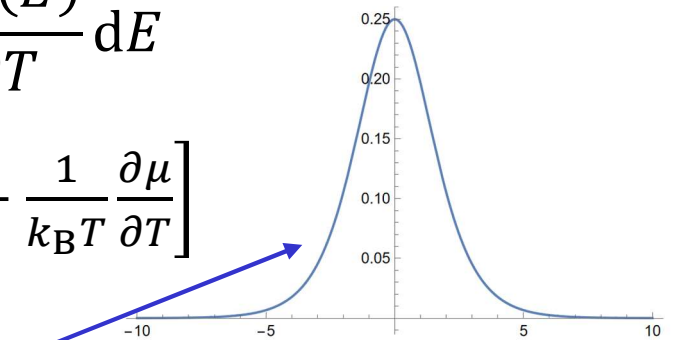
- The number of particles is conserved so

$$\frac{dn}{dT} = 0 = g(E_F) \int \frac{\partial f(E)}{\partial T} dE = g(E_F) k_B T \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2} \times \left[ \frac{x}{T} + \frac{1}{k_B T} \frac{\partial \mu}{\partial T} \right] dx$$

- The first term in the square brackets is odd,  $\frac{e^x}{(e^x+1)^2}$  is even, so  $\frac{\partial \mu}{\partial T} \simeq 0$

- To the same level of accuracy:

$$\begin{aligned} c_V &= g(E_F) \int E \frac{\partial f(E)}{\partial T} dE = g(E_F) k_B T \int_{-\infty}^{\infty} (\mu + k_B T x) \frac{e^x}{(e^x+1)^2} \frac{x}{T} dx \\ &= g(E_F) k_B^2 T \int_{-\infty}^{\infty} \frac{x^2 e^x}{(e^x+1)^2} dx = \frac{\pi^2}{3} k_B^2 T g(E_F) \end{aligned}$$



# Sommerfeld Model – electronic specific heat

- Since  $g(E_F) = \frac{3}{2} \frac{n}{E_F}$  we can write

$$c_V = \frac{\pi^2}{3} k_B^2 T g(E_F) = \frac{\pi^2}{3} k_B^2 T \frac{3}{2} \frac{n}{E_F} = \frac{\pi^2}{2} \frac{k_B T}{E_F} n k_B = \frac{\pi^2}{2} \frac{T}{T_F} n k_B$$

- This result is of the same form as the equation above obtained from a simple argument but with a different prefactor –  $\pi^2/2$  as opposed to 1
- This calculation is the leading-order term in an expansion of  $\mu$  in powers of  $(k_B T/E_F)^2$
- To next order the chemical potential is temperature-dependent (see below) but because for metals  $k_B T \ll E_F$  we can usually ignore it:

$$\mu = E_F \left[ 1 - \frac{1}{3} \left( \frac{\pi k_B T}{2 E_F} \right)^2 + O \left( \frac{k_B T}{E_F} \right)^4 \right]$$

- Examples:
  - electron gas in solids –  $c_V$  often much smaller than lattice specific heat
  - liquid-helium mixture of  $^3\text{He}$  in  $^4\text{He}$  – near-ideal Fermi gas of *atoms* (next slide)



# Specific Heat of mixtures of $^3\text{He}$ and $^4\text{He}$

- Experimental procedure:
- Cool helium mixtures to mK temperatures
- Isolate from surroundings
- Input heat for given time
- Measure temperature rise
- Calculate specific heat at particular temperatures and pressures

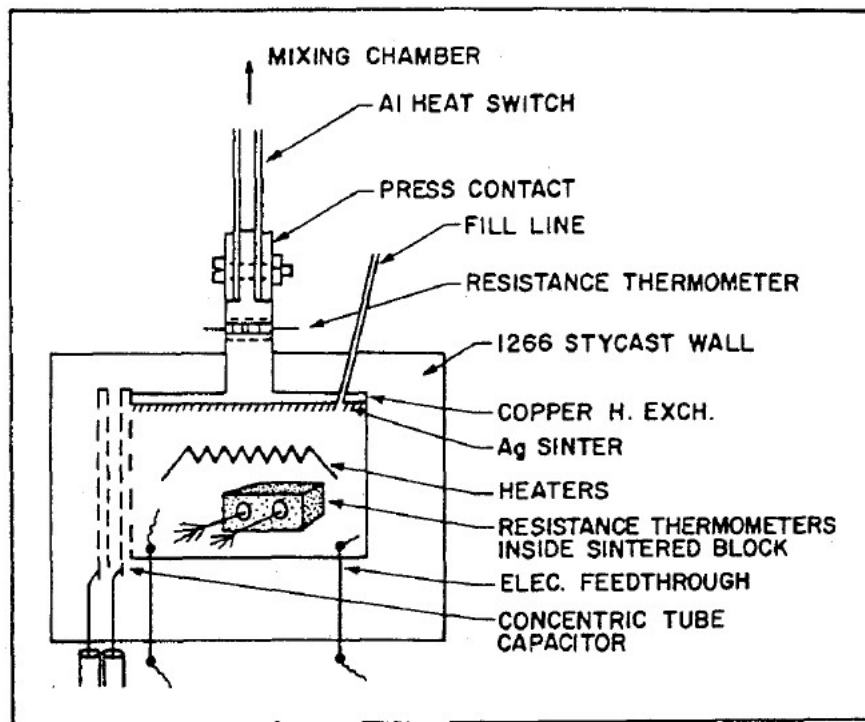
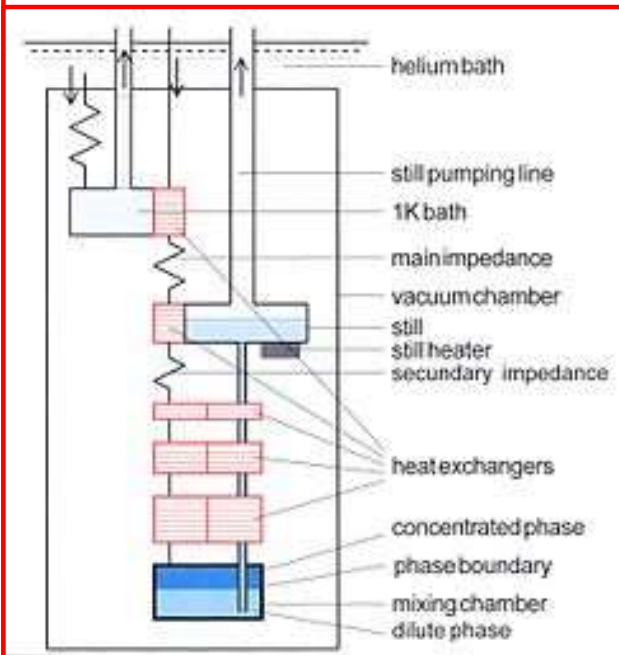
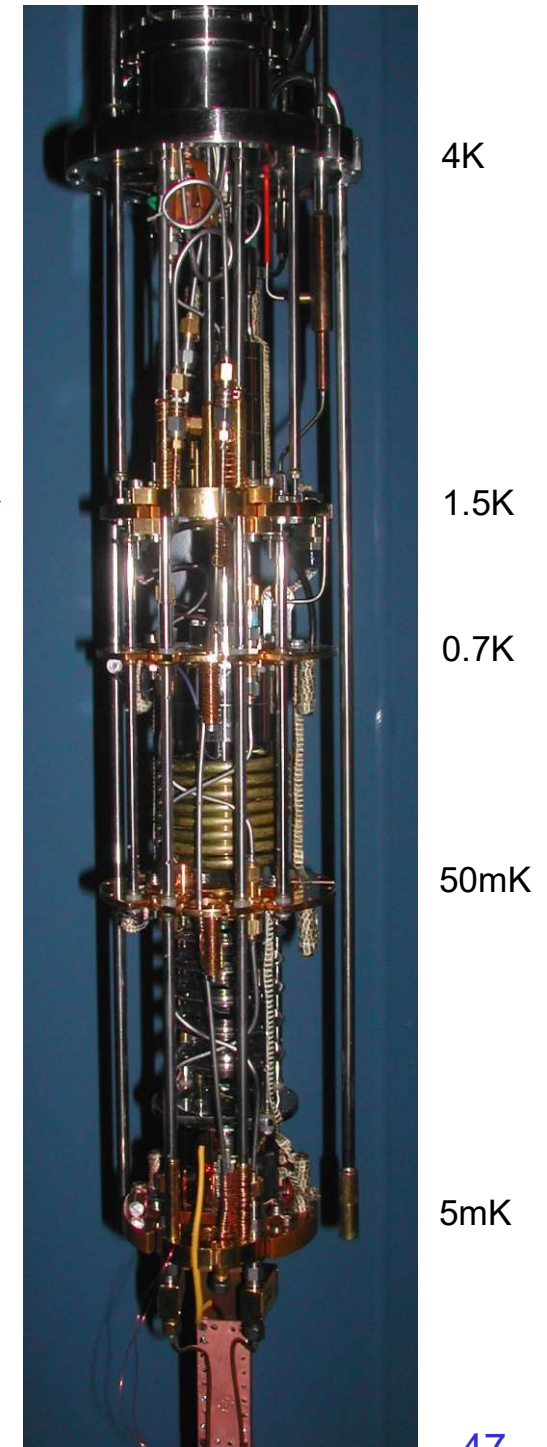


Fig. 1. A schematic view of the calorimeter. The internal parts are spaced from the walls and from each other by layers of nylon lace (not shown).

Helium dilution  
refrigerator



From Wikipedia



# Specific heat of mixtures of liquid $^3\text{He}$ and $^4\text{He}$

- From above,  $c_V = \frac{\pi^2}{2} \frac{T}{T_F} n k_B$ ,  $T_F = \frac{E_F}{k_B} = \frac{\hbar^2}{2m k_B} (3\pi^2 n)^{2/3}$
- Linear behaviour in Fermi-gas regime  $T \ll T_F$

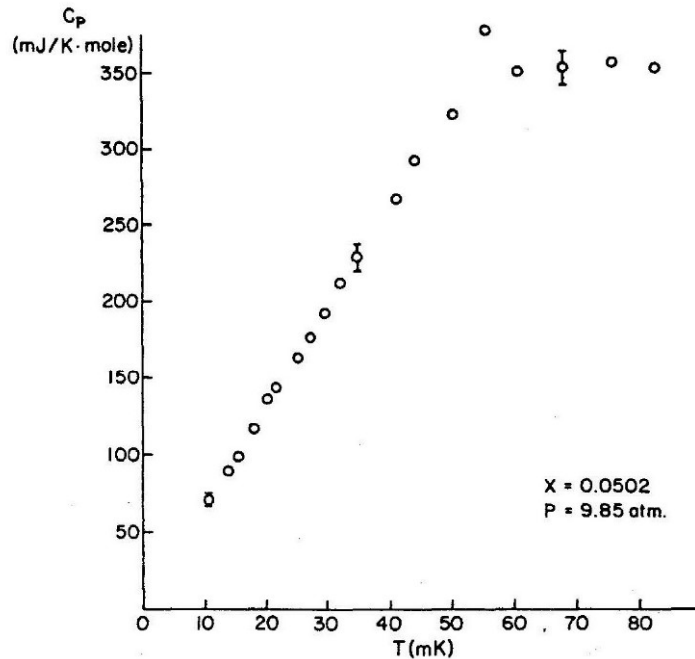


Fig. 2. Specific heat per mole of solution for  $X = 0.0502$  at 10 atm. Error bars represent the experimental uncertainties.

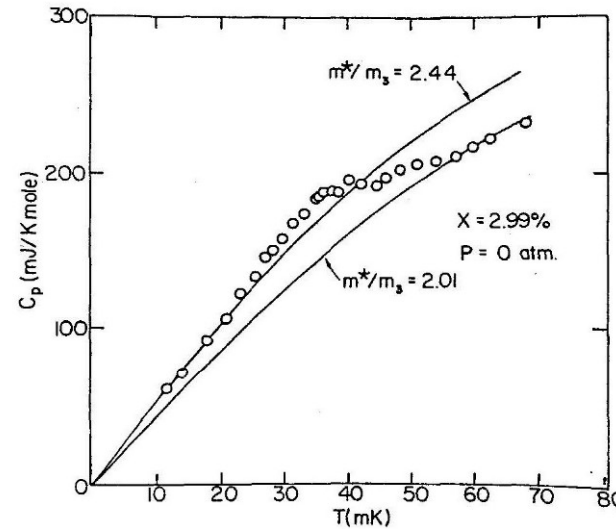


Fig. 3. Specific heat per mole of solution for  $X = 0.0299$  at zero pressure. Error bars represent experimental uncertainties. The upper line is the specific heat of a free Fermi gas of the same number density having an effective mass determined by the low-temperature slope of the data ( $T_F^* = 235$  mK,  $m^*/m_3 = 2.44$ ). The lower curve was fitted to the higher temperature data above 50 mK by adjusting  $m^* = 2.01m_3$ .

TABLE II

Experimental Values of the Effective Fermi Temperature  $T_F^*$  and the Specific Heat Effective Mass  $m^*$

$X$	$P$ , atm	$T_F^*$ , mK	$m^*/m_3$
0.0502	0	$330 \pm 16$	$2.45 \pm 0.12$
0.0502	9.85	$314 \pm 13$	$2.74 \pm 0.12$
0.0502	20.00	$292 \pm 13$	$3.07 \pm 0.13$
0.0299	0	$235 \pm 9$	$2.44 \pm 0.09$
0.0299	10.00	$203 \pm 10$	$3.02 \pm 0.14$

Polturak and Rosenbaum  
JLTP, **43**, 477 (1981)

- So, knowing  $c_V$ ,  $T$ ,  $n$ , we can calculate the Fermi temperature  $T_F$  and the effective mass  $m^*$
- Effective mass 2.44 to 3.07 times bare  $^3\text{He}$  mass – due to interactions
- We can't reach the Fermi temperature with electrons!



# Screening and the Thomas–Fermi approximation

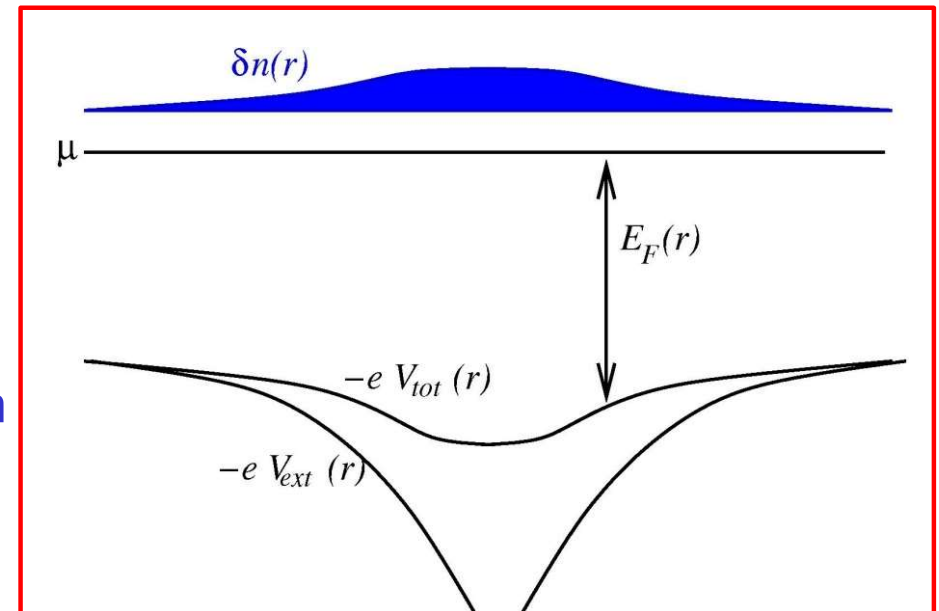
- Placing a positive charge in a metal will result in electrons moving around to screen its potential, resulting in zero electric field
- This is quite different from a dielectric, where electrons are not able to move freely and the potential is reduced by dielectric constant  $\epsilon$
- In a classical picture electrons can move anywhere, but quantum mechanics dictates this is not possible – an electron cannot sit right on top of a nucleus – zero-point energy would be too great if it were trapped there
- In metals a balance is reached between minimising potential and kinetic energy, screening over a short but finite distance
- We estimate the response of a free-electron gas to a perturbing potential:  $V_0(\mathbf{r})$  is the electrostatic potential,  $\rho_0(\mathbf{r})$  the charge distribution

$$\nabla^2 V_0(\mathbf{r}) = -\frac{\rho_0(\mathbf{r})}{\epsilon_0}$$

- Consider the positive background charge to be homogeneous with the electron gas moving around – plasma or “Jellium” model – and in this case  $\rho_0(\mathbf{r}) = 0$  everywhere (this does not include the charges used to set up the perturbing potential)

# Screening and the Thomas–Fermi approximation

- In the presence of a perturbing potential  $V_{\text{ext}}(\mathbf{r})$  the electron charge density redistributes,  $\rho(\mathbf{r}) = \rho_0(\mathbf{r}) + \delta\rho(\mathbf{r})$ , which *by itself* would change the potential to  $V(\mathbf{r}) = V_0(\mathbf{r}) + \delta V(\mathbf{r})$ . Changes are related by  $\nabla^2 \delta V(\mathbf{r}) = -\frac{\delta\rho(\mathbf{r})}{\epsilon_0}$
- We link the charge redistribution to the applied potential by assuming the perturbing potential is slowly varying and so only shifts *free-electron* energy levels
  - uses DOS  $g(E)$  at each point
  - the same as assuming a spatially varying Fermi energy
  - this is the “**Thomas–Fermi**” approximation
- The potential is the total produced by the added external charge and the induced “screening” charge



$V_{\text{tot}} = V_{\text{ext}} + \delta V$  hence:

$$-\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}) + (-e)(\delta V(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}))\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

# Screening and the Thomas–Fermi approximation

- Assume the induced potential is slowly varying on the scale of the Fermi wavelength  $2\pi/k_F$  so the energy eigenvalues are just shifted by potential as a function of position:

$$E(\mathbf{k}, \mathbf{r}) = E_0(\mathbf{k}) - eV_{\text{tot}}(\mathbf{r})$$

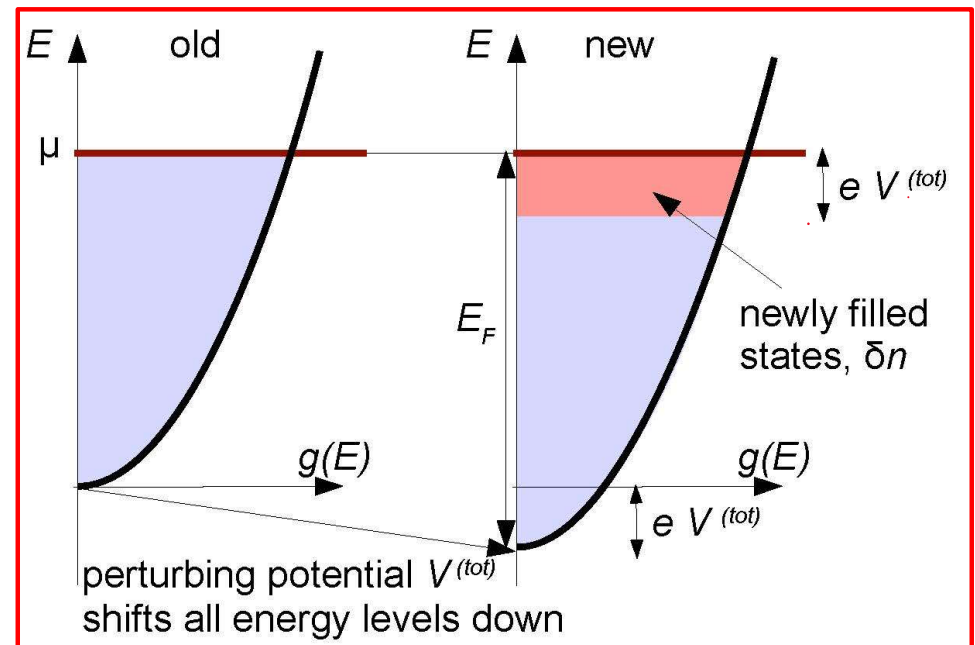
where  $E_0(\mathbf{k})$  has the free-electron parabolic dispersion  $\frac{\hbar^2 k^2}{2m}$

- Keeping the electron states filled up to a constant energy  $\mu$  means we adjust the local Fermi energy  $E_F(\mathbf{r})$  as measured from the bottom of the band so

$$\mu = E_F(\mathbf{r}) - eV_{\text{tot}}(\mathbf{r})$$

- A small shift in the local Fermi energy leads to a change in the local electron number density,  $n$ :  
 $\delta n = g_V(E_F)\delta E_F = e g_V(E_F)V_{\text{tot}}$
- And from above,  $V_{\text{tot}} = V_{\text{ext}} + \delta V$  so we have

$$\delta n = e g_V(E_F)(V_{\text{ext}} + \delta V)$$



# Screening and the Thomas–Fermi approximation

- Since the added potential and induced electron number density are small we can use Poisson's equation to write

$$\nabla^2 \delta V(\mathbf{r}) = \frac{e}{\epsilon_0} \delta n = \frac{e^2 g_V(E_F)}{\epsilon_0} (\delta V(\mathbf{r}) + V_{\text{ext}}(\mathbf{r}))$$

- We can calculate the induced potential and density response using Fourier transformation: assume an oscillatory perturbing potential

$V_{\text{ext}} = V_{\text{ext}}(\mathbf{q}) \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}$  and a resulting oscillatory induced potential

$\delta V = \delta V(\mathbf{q}) \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}$ , and substitute into the equation above:

$$\nabla^2 (\delta V(\mathbf{q}) \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}) = -q^2 \delta V(\mathbf{q}) \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}} = \frac{e^2 g_V(E_F)}{\epsilon_0} (\delta V(\mathbf{q}) + V_{\text{ext}}(\mathbf{q})) \mathbf{e}^{i\mathbf{q}\cdot\mathbf{r}}$$

$$\Rightarrow \delta V(\mathbf{q}) [q^2 + e^2 g_V(E_F)/\epsilon_0] = -V_{\text{ext}}(\mathbf{q}) e^2 g_V(E_F)/\epsilon_0$$

$$\Rightarrow \delta V(\mathbf{q}) = -V_{\text{ext}}(\mathbf{q}) \frac{e^2 g_V(E_F)/\epsilon_0}{q^2 + e^2 g_V(E_F)/\epsilon_0} = -\frac{q_{\text{TF}}^2}{q^2 + q_{\text{TF}}^2} V_{\text{ext}}(\mathbf{q})$$

- Here we define the Thomas–Fermi wavevector  $q_{\text{TF}} \equiv (e^2 g_V(E_F)/\epsilon_0)^{1/2}$

# Screening and the Thomas–Fermi approximation

- The Thomas-Fermi wavevector  $q_{\text{TF}} = (e^2 g_V(E_F)/\epsilon_0)^{1/2}$ , and, given that for the free-electron gas

$$g_V(E) = \frac{1}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} E^{1/2}, \quad E_F = \frac{\hbar^2 k_F^2}{2m} \Rightarrow g_V(E_F) = \frac{m}{\pi^2 \hbar^2} k_F$$

we obtain  $q_{\text{TF}}^2 = \frac{1}{\pi^2} \left( \frac{me^2}{\epsilon_0 \hbar^2} \right) k_F = \frac{4}{\pi} \frac{k_F}{a_B} = \left( \frac{2.95}{r_s^{1/2}} \right) \text{\AA}^{-1}$

where the Bohr radius is  $a_B = \frac{4\pi\hbar^2\epsilon_0}{me^2} \simeq 0.53\text{\AA}$

and the Wigner–Seitz radius  $r_s$  is defined by  $(4\pi/3)r_s^3 = n^{-1}$

- To find the induced electron number density  $n_{\text{ind}}(\mathbf{q})$ , we have from above

$$\delta n = e g_V(E_F)(V_{\text{ext}} + \delta V), \quad \delta V(\mathbf{q}) = -\frac{q_{\text{TF}}^2}{q^2 + q_{\text{TF}}^2} V_{\text{ext}}(\mathbf{q}), \quad q_{\text{TF}}^2 = e^2 g_V(E_F)/\epsilon_0$$

$$\Rightarrow \delta n(\mathbf{q}) \equiv n_{\text{ind}}(\mathbf{q}) = \frac{q_{\text{TF}}^2 \epsilon_0}{e} V_{\text{ext}}(\mathbf{q}) \left( 1 - \frac{q_{\text{TF}}^2}{q^2 + q_{\text{TF}}^2} \right) = \frac{\epsilon_0}{e} V_{\text{ext}}(\mathbf{q}) \left( \frac{q^2}{q^2/q_{\text{TF}}^2 + 1} \right)$$

# The Thomas–Fermi dielectric function

- The wavevector-dependent dielectric function  $\epsilon(\mathbf{q})$  relates the electric displacement  $\mathbf{D}$  to the electric field  $\mathbf{E}$  by  $\epsilon_0 \epsilon(\mathbf{q}) \mathbf{E}(\mathbf{q}) = \mathbf{D}(\mathbf{q})$
- Given  $\nabla V_{\text{ext}} = -\mathbf{D}(\mathbf{q})/\epsilon_0$ ,  $\nabla V_{\text{tot}} = -\mathbf{E}(\mathbf{q})$   
 $\Rightarrow \nabla V_{\text{ext}} = \epsilon(\mathbf{q}) \nabla V_{\text{tot}}$
- Since, from above,  $V_{\text{tot}} = V_{\text{ext}} + \delta V$

$$\Rightarrow V_{\text{ext}}(\mathbf{q}) = \epsilon(\mathbf{q}) \underbrace{(\delta V(\mathbf{q}) + V_{\text{ext}}(\mathbf{q}))}_{V_{\text{tot}}}$$

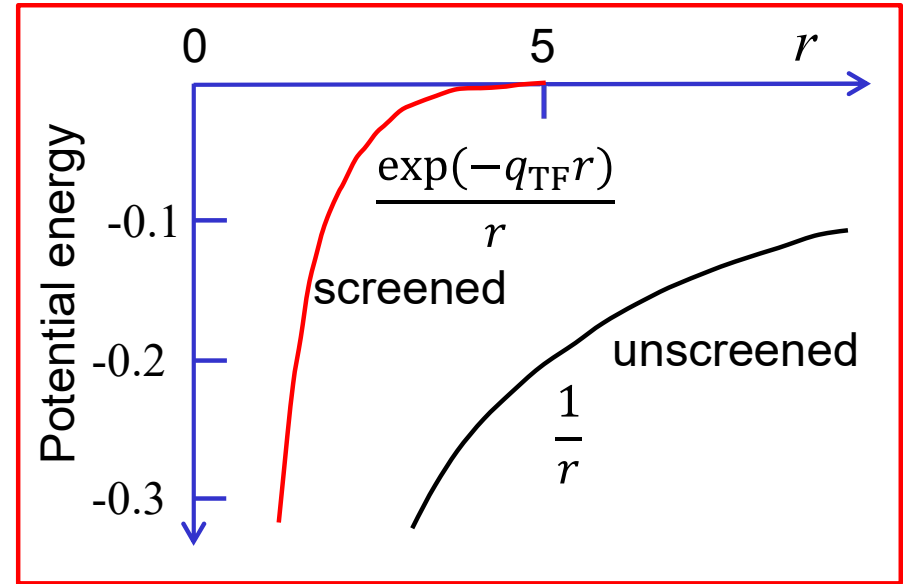
- Using  $\delta V(\mathbf{q}) = -\frac{q_{\text{TF}}^2}{q^2 + q_{\text{TF}}^2} V_{\text{ext}}(\mathbf{q}) \Rightarrow V_{\text{tot}}(\mathbf{q}) = V_{\text{ext}}(\mathbf{q}) \frac{q^2}{q^2 + q_{\text{TF}}^2}$
- And hence the “Thomas–Fermi dielectric function” is given by

$$\epsilon^{\text{TF}}(\mathbf{q}) = 1 + \frac{q_{\text{TF}}^2}{q^2}$$

- $q_{\text{TF}}^{-1}$  is the Thomas–Fermi screening length
  - for copper, where the electron density  $n = 8.5 \times 10^{22} \text{cm}^{-3}$ , we have  $1/q_{\text{TF}} = 0.055 \text{ nm}$

# Thomas–Fermi screening

- From last slide,  $\epsilon^{\text{TF}}(\mathbf{q}) = 1 + \frac{q_{\text{TF}}^2}{q^2}$
- For small  $q$  (long distances),  $\epsilon^{\text{TF}} \propto q^{-2}$
- Long-range part of Coulomb potential also  $\propto q^{-2}$  so it is exactly cancelled
- In real space, if  $V_{\text{ext}} = Q/r$  (Coulombic and long range) then  $V(r) = (Q/r)e^{-q_{\text{TF}}r}$  is the short-range screened potential (problem sheet 1 question 6)
- The screened potential is known as the “Yukawa potential” in particle physics
- Exponential factor reduces range of Coulomb potential – screened over distances comparable to inter-particle spacing (for metals, with  $r_s/a_B \sim 2 - 6$ )
- Mobile electron gas highly effective at screening external charges
- Application to resistivity of alloys – atoms of Zn (valency 2) added substitutionally to metallic copper (valency 1) have an excess charge
- Foreign atom scatters conduction electrons with interaction given by screened Coulomb potential – scattering contributes to increase in resistivity; theory and experiment in agreement



# Summary

- Problems with Drude theory
- The Sommerfeld model – electrons in a degenerate Fermi gas
- Free-electron gas in three dimensions
- Fermi surface and density of states
- Thermal properties of the Fermi gas – specific heat
- Experimental measurements of specific heat in liquid helium
- Screening and the Thomas–Fermi approximation
- Thomas–Fermi wavevector and dielectric function
- Effect of screening on a Coulomb potential

