

Quantum Condensed Matter

Xinyu Zhong
Wolfson College

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Abstract

Abstract of this course

1 Optical Properties**1.1 Insulators**

The model we used here is Lorentz or dipole oscillator model.

Oscillation of charges around their average position.

Model atoms as nucleus and electron cloud and an applied E-field will lead to displacement of electron cloud.

1.1.1 Lorentz Model

Electrons now behave as damped harmonic oscillator.

$$m\ddot{u} + m\gamma\dot{u} + m\omega_T^2 u = qE \quad (1)$$

Natural frequency ω_T is determined by force constant and mass.

γ is damping rate.

Flow: for a certain frequency ω_T , we can obtain

- dipole moment per atom, p_ω
- Polarisation (dipole moment per unit volume), P_ω
- Susceptibility, χ_ω
- Permittivity, ϵ_ω
- Reflectivity between media of different permittivities, power reflection coefficient .etc.

At low frequencies, we study the permittivity of material

$$\epsilon(\omega \approx 0) = 1 + n_v \frac{q^2}{m\epsilon_0\omega_T^2} \quad (2)$$

This explains the different static permittivity of different materials.

Example: Atomic absorption

?? [Something about line width](#)

1.1.2 Link to quantum mechanics**1.2 Metals**

Inner electrons closely bounded, contribute to permittivity according to Lorentz oscillator metals. Outer electrons have cut loss from ions, now free to roam around entire metal. Natural frequency $\omega_T \approx 0$

1.3 Drude Model

We used Drude Model to study the connectivity of metals

1.3.1 Frequency-dependent Connectivity

- Both current density $\mathbf{j} = nq\dot{\mathbf{u}}$, and polarisation $\vec{\mathbf{P}} = nq\vec{\mathbf{u}}$.
- For conduction electrons $\dot{\mathbf{P}}_c = \mathbf{j}$.
- The polarisation is comprised of core electrons and conduction:
- $\dot{\mathbf{P}} = \mathbf{j} + \epsilon_0\chi_\infty\dot{\mathbf{E}}$
- From this differential equation we have $\mathbf{j}_\omega = -i\omega\epsilon_0\mathbf{E}_\omega(\chi_\omega - \chi_\infty)$
- Imaginary part of the permittivity can be derived from here

1.3.2 Relaxation-time approximation

We denote relaxation time as τ , the probability of collision during δt is $\delta t/\tau$. Now consider the change in **momentum** change after δt , by considering electrons collided and not collided during that δt :
The current J due to electrons of number density n , mass m of average (drift velocity) \mathbf{v} and momentum \mathbf{p} is given as:

$$\mathbf{j} = -n e \mathbf{v} = -\frac{ne}{m} \mathbf{p} \quad (3)$$

Note that \mathbf{J} is proportional to \mathbf{v} and \mathbf{p} .

The evolution of \mathbf{p} in time δt under the action of external force \mathbf{f} , e.g. $\mathbf{f} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$

Collided electrons has a fraction $\delta t/\tau$ and momentum is acquired is $\approx \mathbf{f}(t)\delta t$, as a result, the contribution to the average momentum is of order $(\delta t)^2$:**negligible**

Non-collided electrons:

$$\mathbf{p}(t + \delta t) = (1 - \delta t/\tau)(\mathbf{p}(t) + \mathbf{f}(t)\delta t + O(\delta t)^2) \quad (4)$$

1.3.3 Validity of Drude Model

1.4 Sommerfeld Model

Both Lorentz and Drude theories fails dramatically describing thermodynamic properties. Now we apply equipartition theorem to the dipole model, expect contribution of k_B to heat capacity of each oscillator, and $3/2k_B$ per atom. Also we consider quantum static effects.

1.4.1 Density of states

1. Fermi sphere
2. Note spin degeneracy
3. $g(E) \equiv$ number of states per unit energy per unit volume.
4. Note that C_v due to electrons is usually much smaller than lattice specific heat capacity.
5. This is seen in the liquid helium mixture of ^3He and ^4He

Example: Specific heat of mixture of ^3He and ^4He

We see that at low temp limit, C_v is linear to T

1.4.2 Screening and the Tomas-Fermi approximation

1. Screening: placing positive charges in metal will result in electrons moving around to screen its potential resulting in zero electric field. Compare to dielectric material with electrons are not free to move and have potential reduced by ϵ
2. A balance is reached between minimising potential and kinetic energy, screening over a short but finite range.
3. In order to study the effect of introducing external potential. We study response of a free electron in a perturbing potential. Free electron in **METAL**, without external potential, gives potential in the metal to be:

$$\nabla^2 V_0(r) = -\frac{\rho_0(r)}{\epsilon} \quad (5)$$

indicating that potential is linked to charge distribution. In plasma or Jellium model. $\rho_0 = 0$

4. In the presence of perturbing potential V_{ext} , chaneg density will redistribute and we have a per-turbing potential in the metal, its correction is :

$$\nabla^2 \delta V_0(r) = -\frac{\delta \rho_0(r)}{\epsilon} \quad (6)$$

d

Slowly varying potential The approximation is: Slowly varying potential, and only shifts the free electron.

Constant chemical potential keeping the electrons states filled up to a constant energy μ requires we adjust local Fermi energy $E_F(\mathbf{r})$:

$$\mu = E_F(\mathbf{r}) - eV_{tot}(\mathbf{r}) \quad (7)$$

Local density approximation Small shift in the Fermi energy $\delta E_F(\mathbf{r})$ will give rise to a change in number densit, n : Recalll the then relationship:

$$\int^{E_F} g_v(E) dE = n \quad (8)$$

we obtain:

$$\delta n = e g_V(E_F)(\delta V + V_{ext}) \quad (9)$$

Linearised Thomas Fermi now we know the small change in ρ , as $\rho = en$ We obtain:

$$\nabla^2 \delta V(\mathbf{r}) = \frac{e^2 g_V(E_F)}{\epsilon_0} (\delta V + V_{ext}) \quad (10)$$

Density Response Solve the Equation above, by Fourier Transformation, we obtain:

$$\delta V(\mathbf{q}) = -\frac{q_{TF}^2}{q^2 + q_{TF}^2} V_{ext}(\mathbf{q}) \quad (11)$$

Here q_{TF} is the *Thomas-Fermi Wave vector* The number density, as now we know δV ,

Dielectric permittivity the dielectric permittivity $\epsilon_{TF}(q)$

$$\epsilon_{TF}(q) = 1 + \frac{q_{TF}^2}{q^2} \quad (12)$$

Screening *At small q , long distance, ϵ_{TF}*

1.5 Electrons and phonons in periodic solids

In this section, we discuss the type of bonds: "Van der Waal", ionic, covalent. Crystal structure

1.5.1 Binding of crystals

Inert gas

1. Filled electron shells and large ionization energies.
2. Interaction between neutral atoms is weak, and leading attractive force is van der Waals interaction, which gives potential proportional to $1/R^6$.
3. Lennard-Jones potential:

$$U(R) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right] = \epsilon\left[\left(\frac{R_{min}}{r}\right)^{12} - 2\left(\frac{R_{min}}{r}\right)^6\right] \quad (13)$$

Ionic Crystals

1. Electrostatic energy for a regular lattice:

$$U_{electrostatic} = -\frac{1}{2} \frac{\alpha_M q^2}{4\pi\epsilon_0 R} \quad (14)$$

where α_M is a dimensionless constant that depends only on the crystal structure