

Quantum Condensed Matter

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Contents

1	Optical Properties	3
1.1	Insulators	3
1.1.1	Lorentz Model	3
1.1.2	Link to quantum mechanics	4
1.2	Metals	4
1.3	Drude Model	4
1.3.1	Frequency-dependent Connectivity	4
1.3.2	Results from Drude Model	4
1.3.3	Relaxation-time approximation	5
1.3.4	Validity of Drude Model	5
1.3.5	Summary of key results in Drude Theory	5
1.4	Sommerfeld Model	5
1.4.1	Density of states	5
1.4.2	Screening and the Tomas-Fermi approximation	5
2	Electrons and phonons in periodic solids	6
2.0.1	Binding of crystals	7
2.1	Complex materials	7
2.2	Description of periodic materials	7
2.2.1	Index system for lattice	7
2.2.2	Reciprocal Lattice and Diffraction	7
2.2.3	Diffraction Condition	7
2.3	Lattice dynamics and phonons	7
2.4	Density of states	7
2.5	Heat Capacity	7
2.5.1	Debye Model	8
2.5.2	Heat capacity due to lattice vibration and electrons	8
2.5.3	Compare Einstein and Debye models	8
2.6	Thermal Conductivity of insulators	8
3	Electrons in periodic potential	9
3.1	Schrodinger equation in a periodic table	9
3.2	Bloch theorem from discrete translational symmetry	9
3.3	Tight banding	9
3.3.1	Two Bands	9
3.4	Band Structure and Brillouin Zone	9
3.4.1	Example of Band Structures	10
3.5	Semiclassical Model of electron dynamics	10
4	Experimental Probe of the band structure	10
4.1	Photon Absorption	10
4.1.1	Transition rates	10
4.1.2	GaAs band structure	10
4.1.3	Transition rate- joint density of states	11
4.1.4	Transition rate in direct semiconductors	11
4.1.5	Transition rate in Indirect semiconductors	11
4.2	Photoemission	11
4.3	STM	12
4.4	Cyclotron Resonance	12
5	Scattering in metals	12
5.1	Matthiessen's rule	12

5.2	Emission and absorption of phonons	12
5.2.1	Electron-phonon scattering at room temperature	12
5.2.2	Electron-phonon scattering at low temperature	12
5.2.3	Electron-electron scattering	13
6	Quantum Oscillations	13
6.1	Size of Cyclotron orbits	13
6.2	Density of states	13
6.3	De-Hass Van-Alphen effect	13
6.4	De-Hass Van-Alphen effect in Sr ₂ RuO ₄	13
6.5	Tunneling	13
6.6	Cyclotron Resonance	13
7	Semiconductor band structure	13
7.1	Intrinsic carrier concentration	14
7.2	Doped Semiconductors	14
7.3	Hall effect	15
7.4	Semiconductor devices	15
7.5	Metal	15
7.6	P-N Junction	15
7.7	Band-bending	16
7.8	LED, Solar, TFT, MFT. etc	17
7.9	Two-dimensional electron gas	17
7.10	The Quantum Hall effect	17
8	Electronic Instabilities	17
8.1	Curie law of susceptibility	17
9	Fermi-Liquid Theory	18
9.1	Band Magnetism in metals	18

Abstract

Abstract of this course

1 Optical Properties

We studied the optical properties of materials, including insulators (Using the Lorentz Model) and metals (Using the Drude Model).

We also discussed the thermal properties.

Finally, In metals, one of the most important is screening. Note screening is different from dielectric.

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 the displacement of the electron cloud.

1.1.1 Lorentz Model

Electrons now behave as a 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. N.B. γ is the damping rate.

The flow of work: 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

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

- Permittivity, ϵ_ω

$$\epsilon_\omega = 1 + \chi_\omega$$

- Reflectivity between media of different permittivity, power reflection coefficient .etc.

At low frequencies, we study the permittivity of the 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 the entire metal. Natural frequency $\omega_T \approx 0$.

1.3 Drude Model

We used Drude Model to study the connectivity of metals (while the Lorentz model to study insulators) Drude model is that the electrons are free to move around the metal, and the current is proportional to the electric field. Natural frequency is therefore 0. Also, there is one extra ϵ_∞ term in the permittivity.

$$\epsilon_\omega = \epsilon_\infty - \frac{N}{V} \frac{q^2}{m\epsilon_0(\omega^2 + i\omega\gamma)} = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\gamma}$$

This is not the correct model (See the real one with drift velocity)

1.3.1 Frequency-dependent Connectivity

- Both current density $\mathbf{j} = nq\mathbf{\dot{u}}$, and polarisation $\vec{\mathbf{P}} = nq\vec{\mathbf{u}}$.
- For conduction electrons $\dot{\mathbf{P}}_c = \mathbf{j}$.
- The polarization is comprised of core electrons and conduction:
- ** Solve PDE $\dot{\mathbf{P}} = \mathbf{j} + \epsilon_0\chi_\infty\dot{\mathbf{E}}$ and solution with $\mathbf{E} = \mathbf{E}_0e^{-i\omega t}$ **
- 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 is linked to the real part of frequency-dependent conductivity.

1.3.2 Results from Drude Model

Plasma frequency

$$\omega_p^2 = \frac{ne^2}{\epsilon_0 m}$$

Frequency dependence of the relative permittivity and electrical conductivity (taking into account the polarisability of the atomic cores, $\chi_\infty = \epsilon_\infty - 1$ causes slight modifications):

Note that high permittivity means high reflection. Low permittivity means absorption (Highly imaginary ϵ) or transmission (Low ϵ)

$$\begin{aligned}\epsilon(\omega) &= 1 - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} \xrightarrow{\epsilon_\infty \neq 1} \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\gamma} \\ \sigma(\omega) &= -i\omega\epsilon_0(\epsilon(\omega) - 1) \xrightarrow{\epsilon_\infty \neq 1} -i\omega\epsilon_0(\epsilon(\omega) - \epsilon_\infty)\end{aligned}$$

Useful expressions for electrical conductivity and Hall coefficient:

$$\begin{aligned}\sigma(\omega) &= \frac{ne^2\tau}{m(1 - i\omega\tau)} \xrightarrow{\omega \rightarrow 0} \frac{ne^2\tau}{m} = ne\mu \\ R_H &= \frac{E_y}{j_x B} = \frac{1}{nq}\end{aligned}$$

(q is carrier charge, n is carrier density, τ is relaxation time = $1/\gamma$)

1.3.3 Relaxation-time approximation

We denote relaxation time as τ , and 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:

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

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 $\approx \mathbf{f}(\mathbf{t})\delta t$, as a result, the contribution to the average momentum is of order $(\delta t)^2$: **negligible**

Non-collided electrons:

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

1.3.4 Validity of Drude Model

1.3.5 Summary of key results in Drude Theory

1.4 Sommerfeld Model

Both Lorentz and Drude's theories fail dramatically to describe thermodynamic properties. Now we apply the equipartition theorem to the dipole model, expecting a contribution of k_B to the 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. Number density of electrons $n = \int_0^\infty g(E)f(E)dE$
5. Internal energy density is $U = \int_0^\infty g(E)Ef(E)dE$
6. $C_v = \frac{dU}{dT} = \int_0^\infty g(E)E\frac{df}{dT}dE$
7. Note that C_v due to electrons is usually much smaller than lattice-specific heat capacity.
8. 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 fields. Compare to dielectric material with electrons are not free to move and have potential reduced by ϵ
2. A balance is reached between minimizing potential and kinetic energy, screening over a short but finite range.
3. In order to study the effect of introducing external potential. We study the 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} , change density will redistribute and we have a perturbing 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 density, n : Recall 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}

2 Electrons and phonons in periodic solids

In this section, we discuss the type of bonds: "Van der Waal", ionic, covalent. Crystal structure This is like a section that dedicated to material science

2.0.1 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

2.1 Complex materials

2.2 Description of periodic materials

2.2.1 Index system for lattice

2.2.2 Reciprocal Lattice and Diffraction

2.2.3 Diffraction Condition

The spacing

$$2d \sin \theta = n\lambda \quad (15)$$

2.3 Lattice dynamics and phonons

1D monatomic chain

1D diatomic chain

1D different spring constant

1D different mass

3D crystal In 3D crystal, there are always 3 acoustic modes and $3(m-1)$ optical modes where m is the number of atoms per unit cell.

2.4 Density of states

2.5 Heat Capacity

When studying heat capacities, we discuss the optical branch (Einstein Model) and acoustic model (Debye model)

2.5.1 Debye Model

2.8 Lattice-specific heat Phonons obey Bose-Einstein statistics, but their number is not conserved and so the chemical potential is zero, leading to the Planck distribution

$$n(\omega) = \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$

The internal energy is

$$U = \int d\omega D(\omega) n(\omega) \hbar\omega$$

For the Einstein model

$$U_E = \frac{N\hbar\omega_o}{e^{\hbar\omega_o/k_B T} - 1}$$

and the heat capacity is

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = Nk_B \left(\frac{\hbar\omega_o}{k_B T} \right)^2 \frac{e^{\hbar\omega_o/k_B T}}{(e^{\hbar\omega_o/k_B T} - 1)^2}$$

At low temperatures, this grows as $\exp -\hbar\omega_o/k_B T$ and is very small, but it saturates at a value of Nk_B (the Dulong and Petit law) above the characteristic temperature $\theta_E = \hbar\omega_o/k_B$.⁶

At low temperatures, the contribution of optical modes is small, and the Debye spectrum is appropriate. This gives

$$U_D = \int_0^{\omega_D} d\omega \frac{V\omega^2}{2\pi^2 v^3} \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$$

Defining the Debye temperature $\theta_D = \hbar\omega_D/k_B T$ and using $\omega_D^3 = 6\pi^2 v^3 N/V$ from above, we obtain $\theta_D = (6\pi^2 N/V)^{1/3} \hbar v/k_B$.

By writing $x = \hbar\omega/k_B T$ and including a factor of 3 for different modes, we obtain for the internal energy

$$U_D = \frac{3V\hbar}{2\pi^2 v^3} \int_0^{\omega_D} d\omega \frac{\omega^3}{e^{\hbar\omega/k_B T} - 1} = 9Nk_B T \frac{T}{\theta_D} \int_0^{\theta_D/T} dx \frac{x^3}{e^x - 1}$$

and by differentiating the middle expression with respect to temperature, the heat capacity (see Fig. 2.29) is

$$C_V = 9Nk_B \left(\frac{T}{\theta_D} \right)^3 \int_0^{\theta_D/T} dx \frac{x^4 e^x}{(e^x - 1)^2}$$

where the Debye temperature is $\theta_D = \hbar\omega/k_B$. We have multiplied by 3 to account for the three acoustic branches.

2.5.2 Heat capacity due to lattice vibration and electrons

Two major contributions to heat capacity: electrons and lattice vibrations. Electron heat capacity is linear to T ??? while lattice vibration heat capacity is $\propto T^3$

2.5.3 Compare Einstein and Debye models

Why we are comparing these two models???

2.6 Thermal Conductivity of insulators

1. The thermal conductivity, κ is defined by $\mathbf{J}_q = -\kappa \nabla T$, where \mathbf{J}_q is the flux of heat (energy per unit area per unit time).
2. Kinetic theory gives $\kappa = \frac{1}{3} C_V \ell v = \frac{1}{3} C_V v^2 \tau$, where C_V is the phonon specific heat per unit volume, v is the phonon velocity, $\ell = v\tau$ is the mean free path and τ is the scattering time.

3. Debye theory predicts that $C_V \propto T^3$ **at low** T and that it is constant at high T (While in reality, at high temperature, thermal conductivity is dominated by scattering).
4. v , the velocity of sound, is almost constant, but τ depends on several scattering mechanisms.
5. Scattering Mechanisms include normal, Umklapp, points defects sample boundaries and crystal dislocations.
6. At high temperature κ falls rapidly due to rapid fall in τ , the scattering time.

3 Electrons in periodic potential

By solving Hamiltonian's equation, we conclude Bloch's theorem: Eigenstates of the 1D Hamiltonian can be chosen to be a plane wave multiplied by a function with the periodicity of the Bravais lattice. We consider first a formal treatment in terms of a complete set of basis functions, namely the set of all plane-wave states which satisfy the periodic boundary conditions. The results from this treatment can be used to obtain Bloch's theorem, which is one of the cornerstones of electronic structure in solids. Next, we will approach Bloch's theorem from a more abstract but also more elegant direction, which uses the translational symmetry of the lattice directly.

3.1 Shrodinger equation ina periodic table

3.2 Bloch theorem from discrete translational symmetry

Another way to think about Bloch theorem, consider what happens to eigenstate of Hamiltonian.

The underlying reason is that if an operator is unchanged under a change of coordinate system, then applying a symmetry operation on the eigenstate of such an operator produces another eigenstate of the operator, with the same eigenvalue as the original one.

For two commuting operators H and T , we can always choose simultaneous eigenstates of both H and T

Two forms of Bloch theorem:

$$\psi_{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{G}} c_{\mathbf{q}-\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} = e^{i\mathbf{q}\cdot\mathbf{r}} u_{j,\mathbf{q}}(\mathbf{r})$$

$$\psi_{\mathbf{k}}^{(n)}(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}} \psi_{\mathbf{k}}^{(n)}(\mathbf{r})$$

3.3 Tight banding

A tight band is also called a linear combination of atomic orbitals.

3.3.1 Two Bands

In this section, we consider tight binding - two bands. For example, s-band or d-band. We approach this problem by forming two Bloch states, one from each set of atomic orbital

3.4 Band Structure and Brillouin Zone

Brillouin Zone We found that the energy eigenstates formed discrete bands $E_n(\mathbf{k})$, which are continuous functions of the momentum \mathbf{k} and are additionally labeled by a band index n . The bandstructure is

periodic in the reciprocal lattice $E_n(\mathbf{k} + \mathbf{G}) = E_n(\mathbf{k})$ for any reciprocal-lattice vector \mathbf{G} . It is sometimes useful to plot the bands in repeated zones, but remember that these states are just being relabelled and are not physically different.

Crystal Momentum The quantity $\hbar\mathbf{k}$ is the crystal momentum, and it enters conservation laws for scattering processes. For example, if an electron absorbs the momentum of a phonon of wavevector \mathbf{q} , the final state will have a Bloch wavevector $\mathbf{k}' = \mathbf{k} + \mathbf{q} + \mathbf{G}$, where \mathbf{G} is whatever reciprocal lattice vector necessary to keep \mathbf{k}' inside the Brillouin zone. Physical momentum can always be transferred to the lattice in arbitrary units of $\hbar\mathbf{G}$. Notice that depending on the energy conservation, processes can thus lead to transitions between bands.

title

3.4.1 Example of Band Structures

3.5 Semiclassical Model of electron dynamics

4 Experimental Probe of the band structure

The system can be excited in different ways: absorption of photon/ or photon + phonon. Photons will appear vertically and phonons are horizontal on plots of energy against k .

The minimum gap in a semi-conductor is the energy difference between the highest occupied state and the lowest unoccupied state, and this is the threshold for optical absorption.

Maximum valence band states and the minimum band state can occur at the same or different momentum.

Examples of the indirect band gap is Si and Ge. A **Phonon-mediated** transition is required and

4.1 Photon Absorption

4.1.1 Transition rates

Fermi's Golden Rule: $W_{i \rightarrow f} = \frac{2\pi}{\hbar} |M|^2 g(\hbar\omega)$ which depends on the dipole matrix element M and the density of states g .

The matrix element is calculated using the initial and final states and the perturbation due to interaction of electric field of the photon and the electric dipole moment P **Why there is a dipole moment:**

We calculate the matrix element by integrating over the whole crystal:

$$M = \frac{e}{V} \int u_f^*(\mathbf{r}) e^{i\mathbf{k}_f \cdot \mathbf{r}} (\mathbf{E}_0 \cdot \mathbf{r} e^{i\mathbf{k} \cdot \mathbf{r}}) u_i(\mathbf{r}) e^{i\mathbf{k}_i \cdot \mathbf{r}} d^3\mathbf{r}.$$

This expression is simplified as conservation of momentum so the phase factor must be zero.

Photon absorption is vertical on the E-K diagram as the wavevector of photon is much lower than the wavevector of electron states.

4.1.2 GaAs band structure

As

4.1.3 Transition rate- joint density of states

Back to the Transition rate, the factor g that appears in Fermi golden rule is the joint density of states, due to the fact that both initial and final states lie in continuous bands.

$$\begin{aligned}\hbar\omega < E_g &= g(\hbar\omega) = 0 \\ \hbar\omega > E_g &= g(\hbar\omega) = \left(\frac{1}{2\pi^2}\right) \left(\frac{2\mu}{\hbar^2}\right)^{3/2} \sqrt{\hbar\omega - E_g}\end{aligned}$$

4.1.4 Transition rate in direct semiconductors

$\alpha \propto \sqrt{\hbar\omega - E_g}$ is the theoretical rate of absorption while in reality it is hardly obeyed.

1. Coulomb attraction between electrons and holes, which enhances absorption and leading to formation of a bound pair - exciton.
2. Impurities and defects with energies within the bandgap.

Excitons An exciton is a bound electron-hole pair analogous to the hydrogen atom. In an exciton, electron and heavy-hole masses are combined in a reduced effective mass

$$\frac{1}{\mu^*} = \frac{1}{m_e^*} + \frac{1}{m_{hh}^*}$$

GaAs has permittivity $\varepsilon = 12.8$. We can use a modified equation for the energy levels of a hydrogen atom to calculate energy levels of excitons:

$$E_n = -\frac{\mu^*}{m_e \varepsilon^2} \cdot \frac{13.6\text{eV}}{n^2} = -\frac{R_x}{n^2}$$

The energy ε_n of an exciton is equal to the energy required to create an electron-hole pair, minus the binding energy or

$$\varepsilon_n = E_g - \frac{R_x}{n^2}$$

4.1.5 Transition rate in Indirect semiconductors

Semiconductors like Si and Ge have their conduction band minimum away from the BZ center and the valence band maximum. A transition between band edges needs a big change in electron wavevector.

Transition from electron $((\varepsilon_i, k_1))$ to

The absorption rate is a second order process, meaning that the rate for indirect semiconductors is much smaller. absorption coefficient $\alpha(\hbar\omega) \propto (\hbar\omega - E_g \mp \hbar\Omega)^2$ has a frequency (of Phonon) dependency, which is not seen in direct bandgap semiconductors.

4.2 Photoemission

Most direct way to measure electron spectral function.

1. Photon incident on a solid, causes transitions from occupied states to plane-wave-like states.
2. excited electrons leave the crystal and are collected by the detector to analyze its energy and momentum.
3. Determine the band structure directly.

Note that momentum parallel to the surface is conserved.

4.3 STM

4.4 Cyclotron Resonance

5 Scattering in metals

We consider the scattering in metal with isotropic bands characterized by an effective mass and a spherical Fermi surface.

1. Electrical conductivity
2. thermal conductivity (dependent on T)
3. electronic specific heat capacity

Wiedemann-Franz law:

The ratio of the thermal conductivity and the electrical conductivity is proportional to the temperature. We further discuss this issue with electrical and thermal transport.

1. electrical transport
2. thermal transport: Long arrow
3. Long arrow means changed direction of electrons which both affect thermal and electrical transport
4. Short arrow only appears for short arrow in the low temperature

5.1 Matthiessen's rule

The scattering process with the shortest scattering time will dominate. An application for the Matthiessen's rule is the calculation of electron mobility in 2D electron gases for different scattering processes

5.2 Emission and absorption of phonons

Phonons, we picture them as propagating local distortion of the crystal, which may scatter an electron in two different ways: elastic and inelastic (Conservation of momentum). So far we assumed the positions of ions are not affected, while it is not true in general. Electrons can distort the lattice – as if they emitted a phonon. Phonons have blackbody distribution with energy of order $k_B T$

5.2.1 Electron-phonon scattering at room temperature

A phonon can scatter electron to the other side of Fermi surface (Recall the long arrow in the electrical and thermal transport)

5.2.2 Electron-phonon scattering at low temperature

Energy of phonon is too little to change direction. In this case electrical scattering rate is much less than the thermal scattering rate. Hence we have $\tau_\sigma^{-1} \propto T^5$ and $\tau_\kappa^{-1} \propto T^3$ and so $\tau_\sigma^{-1} \ll \tau_\kappa^{-1}$ at low T .

Umklapp Scattering into the neighboring Brillouin Zone.

Temperature (scatterer)	Scattering times	$-1 + 2$ σ σ	W-F ratio
Very low (impurities)	$\tau_\kappa \approx \tau_\sigma$ $\sim \text{const}$	$\kappa \propto T$ $\sigma \sim \text{const}$	L_0
$T \sim \theta_D/10$ (phonons)	$\tau_\kappa \propto T^{-3}$ $\tau_\sigma \propto T^{-5} \rightarrow e^{-\theta_F/T}$	$\kappa \propto T^{-2},$ $\sigma \propto T^{-5} \rightarrow e^{-\theta_F/T}$	$< L_0$
$T > \sim \theta_D$ (phonons)	$\tau_\kappa \approx \tau_\sigma$ $\propto T^{-1}$	$\kappa = \text{const},$ $\sigma \propto T^{-1}$	L_0

5.2.3 Electron-electron scattering

Relatively Unimportant Conservation of energy/momentum

6 Quantum Oscillations

6.1 Size of Cyclotron orbits

The flux threading the real space Area enclosed by the k-space orbital:

$$A_k = \left(\frac{e}{\hbar}\right)^2 B^2 A_r$$

$$A_k = \frac{2\pi e}{\hbar} B \left(n + \frac{1}{2}\right)$$

6.2 Density of states

Period of Oscillation:

$$\Delta\left(\frac{1}{B}\right) = \frac{1}{B_{n+1}} - \frac{1}{B_n} = \frac{2\pi e}{\hbar} \frac{1}{A_k}$$

This links the period of quantum oscillations to the cross-sectional area of Fermi Surface.

6.3 De-Hass Van-Alphen effect

6.4 De-Hass Van-Alphen effect in Sr2RuO4

6.5 Tunneling

I will not study this part

6.6 Cyclotron Resonance

7 Semiconductor band structure

Direct gap vs Indirect gap

1. Direct gap: $k = 0$
2. Indirect gap: $k \neq 0$, local minimum at the origin of the reciprocal lattice. Global minimum at $k = \eta$

7.1 Intrinsic carrier concentration

Semiconductors are material with small energy gap. So small that the thermal energy is large enough to excite electrons from the valence band to the conduction band.

1. Dispersion relationship
2. Density of states for conduction band and valence band:
3. Carrier density:

$$n = \int_{E_c}^{\infty} dE g_e(E) f(E)$$

with Fermi function

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

4. Concentration of electrons

$$n \approx 2 \left(\frac{m_e^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{E_c - \mu}{k_B T}}$$

the concentration of holes

$$p \approx 2 \left(\frac{m_h^* k_B T}{2\pi \hbar^2} \right)^{3/2} e^{-\frac{\mu - E_v}{k_B T}}$$

5. define n_c and p_c :

$$n = n_c(T) e^{-\frac{E_c - \mu}{k_B T}}$$

$$p = p_v(T) e^{-\frac{\mu - E_v}{k_B T}}$$

6. Note that np is constant

$$np = n_c(T) p_v(T) e^{-\frac{E_g}{k_B T}}$$

7. Energy gap = $E_c - E_v$

$$E_g = E_c - E_v \simeq 1\text{eV}$$

where E_g is size of the energy gap law of mass action

The only assumption made is that the distance of the Fermi level from the edge of both bands is large in comparison to $k_B T$, this is true in the presence of impurities and dopants.

7.2 Doped Semiconductors

Carriers can also be created in semiconductors by adding impurity atoms in a process called doping. The binding energy of the impurity level:

$$\Delta_d = \frac{e^4 m_c^*}{2 (4\pi\epsilon\epsilon_0 \hbar)^2} = \frac{m_c^*/m_e}{\epsilon^2} \times 13.6\text{eV}$$

which can be very small compared to the band gap, and often comparable or smaller than thermal energies. Such donor impurities readily donate electrons to the conduction band.

7.3 Hall effect

Relaxation time approximation:

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

Therefore, in the steady state, for electrons,

$$\mathbf{j}_e = \frac{ne^2\tau_e}{m_e}(\mathbf{E}(t) + \mathbf{v}_e \times \mathbf{B}) = ne\mu_e(\mathbf{E}(t) + \mathbf{v}_e \times \mathbf{B})$$

If both electrons and holes are present, we have

$$\mathbf{j}_e = ne\mu_e(\mathbf{E} + \mathbf{v}_e \times \mathbf{B}) + pe\mu_h(\mathbf{E} + \mathbf{v}_h \times \mathbf{B})$$

If we choose the current to be flowing in the x -direction, and \mathbf{B} to be in the z -direction, then v_x^e and v_x^h have opposite signs and, using $\mu = v/E$, we have

$$\begin{aligned} j_x &= eE_x(n\mu_e + p\mu_h) \\ 0 &= eE_y(n\mu_e + p\mu_h) - eB(n\mu_e v_x^e + p\mu_h v_x^h) \end{aligned}$$

Eliminating E_x we get

$$E_y = \frac{j_x B (n\mu_e^2 - p\mu_h^2)}{e(n\mu_e + p\mu_h)^2}$$

Now, we can define the Hall coefficient:

$$R_H = \frac{E_y}{j_x B} = \frac{(n\mu_e^2 - p\mu_h^2)}{e(n\mu_e + p\mu_h)^2}$$

7.4 Semiconductor devices

For bulk devices we will use the semiclassical approximation, treating electrons as classical particles governed by the Hamiltonian

$$H = E_n(\mathbf{k}) - e\phi(\mathbf{r})$$

with the momentum $\mathbf{p} = \hbar\mathbf{k}$ and a spatially varying electrostatic potential $\phi(\mathbf{r})$. The potential will arise from externally applied fields, from charges induced by doping, and from changes in the material composition.

For an isolated solid in equilibrium, the energy difference between the chemical potential μ and the vacuum level is the work function Φ . This is the energy required to remove an electron from the Fermi level and place it in a state of zero kinetic energy in free space.

Two different isolated materials with different work functions will then have different chemical potentials. If these two materials are placed in contact, their chemical potentials must equalise, which is accomplished by electron flow to the more electronegative material; this material becomes charged, its potential ϕ changes, and an overall balance will be established. But in general, there will be as a result internal inhomogeneous electric fields.

7.5 Metal

7.6 P-N Junction

A pn junction is formed by inhomogeneous doping: a layer of n-type placed near p-type. Joining two regions gives a step in chemical potential μ , causing the current to flow.

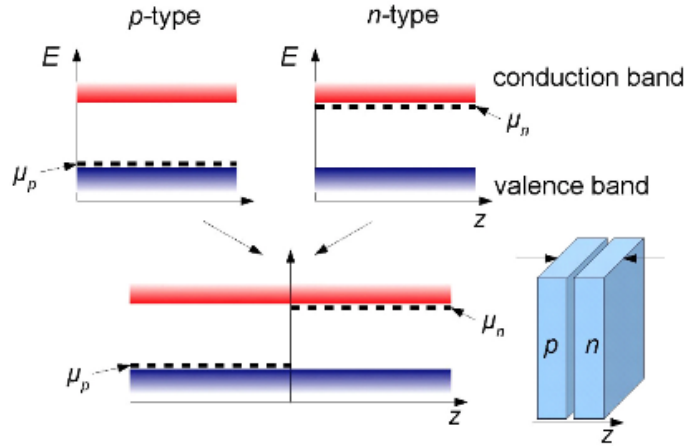


Figure 4.9: Two separate p- and n-type regions being combined to form a p-n junction.

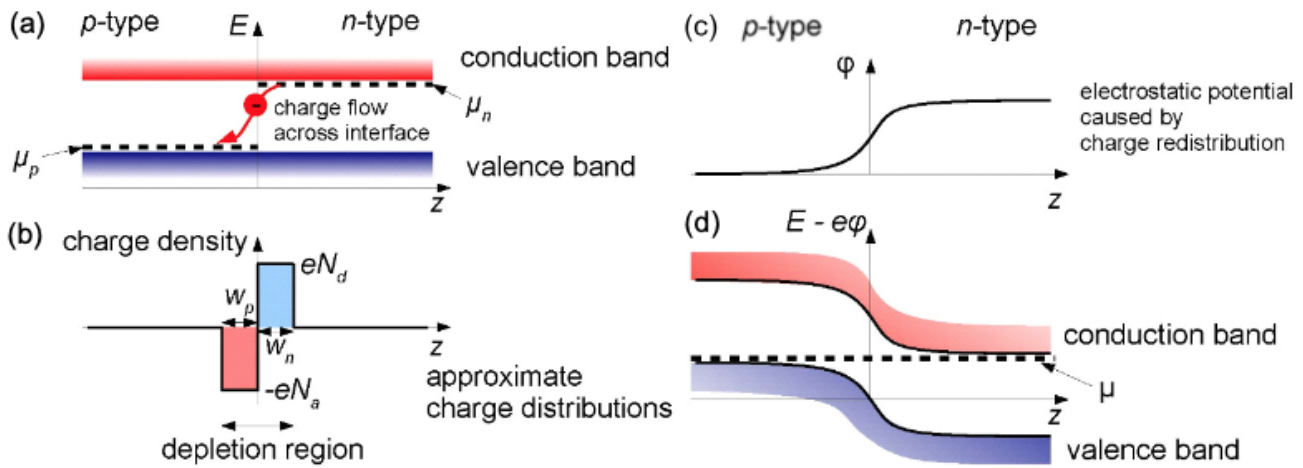


Figure 4.10: (a) Charge flow when p-type and n-type regions are brought together. (b) Charge in the depletion region formed by the charge transfer in (a). (c) Potential ϕ resulting from the charge in the depletion region. (d) Band-bending caused by the depletion-region charge.

Figure 1:

7.7 Band-bending

Charge redistribution causes a spatial varying electrostatic potential, energy level shifts from E to $E - e\phi$. The potential satisfies Poisson's equation:

$$\nabla^2 \phi = \frac{\partial^2 \phi}{\partial z^2} = -\frac{\rho}{\epsilon \epsilon_0}$$

with boundary condition: Far away from the junction in the n-type region, μ is close to the top of the bandgap and in the p-type region it is close to the bottom of the bandgap. The junction potential ϕ_j (often called V_b) is defined via $e\phi_j = \mu_n - \mu_p = E_g$. From charge neutrality, i.e., the requirement that there is as much negative charge on one side of the depletion region as a positive charge on the other side, we have

$$N_A w_p = N_D w_n$$

where N and w are thickness and doping densities.

7.8 LED, Solar, TFFT, MFFT. etc

7.9 Two-dimensional electron gas

Electrons will fill the state up to Fermi Energy

When applying magnetic field, it splits into Landau levels, and the energy of the Landau levels is given by

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega_c$$

, where ω_c is the cyclotron frequency. Each LL has the same degeneracy. The average density of states per unit area per Landau Level is given by

$$g = \frac{2n_L}{\hbar \omega_c}$$

, 2 is from spin degeneracy. This is the same for $B = 0$:

$$g(E) = \frac{m}{\pi \hbar^2}$$

We solve for n_L

$$n_L = \frac{eB}{h}$$

If there are ν filled Landau levels at a field B , the total density of electrons per unit area is given by

$$n_e = \frac{\nu eB}{h}$$

Suppose there are ν occupied Landau levels at field B_1 . Then $n_e = \frac{\nu eB_1}{h}$. If the field is increased from B_1 to B_2 and the highest Landau level is depopulated, the electrons are redistributed among $\nu - 1$ levels. Hence $n_e = \frac{\nu eB_1}{h} = \frac{(\nu-1)eB_2}{h}$. On eliminating ν

$$n_e = \frac{e}{h} \left(\frac{1}{B_1} - \frac{1}{B_2} \right)^{-1}.$$

This means that the depopulation of the Landau levels is periodic in $1/B$, as in 3D.

7.10 The Quantum Hall effect

8 Electronic Instabilities

8.1 Curie law of susceptibility

$$\chi = \frac{n\mu_0\mu^2}{3k_B T}$$

We consider a local moment \mathbf{m} of fixed magnitude $\mu = |\mathbf{m}|$, in a small applied magnetic field $\mathbf{H} \rightarrow \mathbf{0}$. The dipole energy of this moment is given by $E = -\mu_0 \mathbf{m} \cdot \mathbf{H}$. There are no discrete states, so this corresponds to $J = \infty$, but the system still relies on QM, as one can only have fixed moments in QM.

Consider magnetic moments μ at an angle θ to the applied field. The energy $E = -\mu \cdot \mathbf{B} = -\mu B \cos \theta$, and the Boltzmann factor is $\exp \frac{\mu B \cos \theta}{k_B T}$. The probability of the angle lying between θ and $\theta + d\theta$ is proportional to

$$\exp \frac{\mu B \cos \theta}{k_B T} \times \frac{1}{2} \sin \theta d\theta \quad (\text{including the fraction of solid angle}).$$

The average moment parallel to \mathbf{B} is given by

$$\langle \mu_z \rangle = \frac{\int_0^\pi \mu \cos \theta \exp(\mu B \cos \theta / k_B T) \frac{1}{2} \sin \theta d\theta}{\int_0^\pi \exp(\mu B \cos \theta / k_B T) \frac{1}{2} \sin \theta d\theta} = \frac{\int_{-1}^1 x \exp(yx) dx}{\int_{-1}^1 \exp(yx) dx}$$

This gives the Langevin function (see Fig. 5.9)

$$\frac{\langle \mu_z \rangle}{\mu} = \coth y - \frac{1}{y} = \frac{M}{M_s}.$$

The saturation magnetization $M_s = n\mu$ occurs when all n moments per unit volume are aligned, which will happen when $\mu B / k_B T \gg 1$. As $y = \frac{\mu B}{k_B T} \rightarrow 0$

$$\coth y \approx \frac{1}{y} + \frac{y}{3} \implies \coth y - \frac{1}{y} \approx \frac{y}{3}$$

Hence

$$\frac{M}{M_s} = \frac{\langle \mu_z \rangle}{\mu} \approx \frac{y}{3} = \frac{\mu B}{3k_B T}$$

Since, in small magnetic fields,

$$\chi = M/H \approx (\mu_0 M) / B \quad \text{and} \quad M_s = n\mu$$

9 Fermi-Liquid Theory

9.1 Band Magnetism in metals

Let us start with Pauli paramagnetism-the response of a metal to an applied magnetic field. We consider a Fermi gas with energy dispersion $\epsilon_{\mathbf{k}}$ in a magnetic field H . In a magnetic field, the spin-up and spin-down bands will be Zeeman-split (see Fig. 5.17):

$$\begin{aligned} \epsilon_{\mathbf{k}\uparrow} &= \epsilon_{\mathbf{k}} - \mu_B B_a \\ \epsilon_{\mathbf{k}\downarrow} &= \epsilon_{\mathbf{k}} + \mu_B B_a \end{aligned}$$

Since the chemical potential must be the same for both spins, there must be a transfer of carriers from the minority spin band to the majority spin band:

$$n_{\uparrow} - n_{\downarrow} = 2\mu_B B_a \frac{1}{2} g_v(E_F) = \mu_B B_a g_v(E_F)$$

where $g_v(E_F)$ is the density of states at the Fermi level per unit volume..³ We could relate g_v to the density of states per atom as $g_v = \frac{N}{V} g$. The magnetisation is $M = \mu_B (n_{\uparrow} - n_{\downarrow})$, and $B_a = \mu_0 H$, which gives the static spin susceptibility

$$\frac{M}{H} = \chi_\sigma = \mu_0 \mu_B^2 g(E_F)$$

Now let us include in a very simple fashion the effect of interactions. The Stoner-Hubbard model, which provides arguably the simplest way forward, includes an energy penalty U for lattice sites which are doubly occupied, i.e., they hold both an up- and a down-spin electron.

$$\hat{H}_{\text{int}} = \sum_{\text{sites } i} U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

If we treat this interaction in a mean-field approximation, it leads to a shift of the energies of the two spin bands

$$\begin{aligned} \epsilon_{\mathbf{k}\uparrow} &= \epsilon_{\mathbf{k}} + U \bar{n}_{\downarrow} - \mu_0 \mu_B H \\ \epsilon_{\mathbf{k}\downarrow} &= \epsilon_{\mathbf{k}} + U \bar{n}_{\uparrow} + \mu_0 \mu_B H. \end{aligned}$$

We see that the presence of spin-down electrons increases the energy of the spin-up electrons in the same way as a magnetic field pointing down would. Conversely, spin-up electrons cause the energy of spin-down electrons to increase in the same way as a magnetic field pointing up. The interactions between the electrons appear formally in the same way as an additional magnetic field. This so-called exchange field is not physical in the sense that it could deflect a compass needle, it is a book-keeping device to handle the effects of the Coulomb interaction between the electrons.

With the same approximation as before - that the density of states can be taken to be a constant, we can then self-consistently determine the average spin density

$$\frac{N}{V} (\bar{n}_\uparrow - \bar{n}_\downarrow) = [U (\bar{n}_\uparrow - \bar{n}_\downarrow) + 2\mu_0\mu_B H] \frac{1}{2} g_v(E_F)$$

The magnetisation is $M = \mu_B (n_\uparrow - n_\downarrow)$ which then gives us the static spin susceptibility

$$\chi_\sigma = \mu_0 \frac{\mu_B^2 g(E_F)}{1 - \frac{Ug(E_F)}{2}}$$

Here, g denotes the density of states per atom, in contrast to $g_v = \frac{N}{V}g$, which is the density of states per unit volume. In comparison to the non-interacting case, the magnetic susceptibility is enhanced, and will diverge if U is large enough that the Stoner criterion is satisfied

$$\frac{Ug(E_F)}{2} > 1$$