Phys 672

Advanced Solid State Physics

Physics & Astronomy

King Saud University

First Term: 2025/2024

Lecture No. 01

Review of free electron theory

Prof. Nasser S. Alzayed

Syllabus of the Course

1- Review of free electron theory (Chapter 6 + 7)

2- electron – electron interaction (Chapter 14)

3- electron –phonon interaction (Chapter 14)

4- Magnetic materials :

- diamagnetic (Chapter 11)
- paramagnetic (Chapter 11)
- ferromagnetic materials (Chapter 12)

5- magnetic resonance (Chapter 13)

6- Introduction to Superconductivity and its magnetic properties (Chapter 10)

7-Dielectric and optical properties of solid

A Review of Thermal Properties

Thermal Property is a major one when it comes to materials:

① in 1819: Dulong Petit: Constant Heat Capacity $\approx 3R$

② low T Crisis: it was found that C_v at low T → drops sharply

⇒ Classical equipartition fails.

③ Boltzmann established his statistical framework → But C_v is independent of T.

④ in 1907: Einstein model: atoms work as identical oscillators

A Review of Thermal Properties

⇒ explained the drop of C_v with T

But failed at very low T.

(5) 1912: Debye model: used acoustic phonons

→ T^3 low (agree with exp.)

note: notice that Einstein & Debye use quantum principles:

Einst: all atoms oscillate at same freq.

Debye: " " produce phonons.

Remember: at 1900 plank quantization was established.

A Review of Thermal Properties

⑥ in 1920s: Sommerfeld introduced the Role of electrons in metals $\propto T$

$C_{el} = \text{constant} \cdot T$

⑦ $\Rightarrow$ we have at least Two Terms in C_v:

$$C = \gamma T + A T^3$$

γT: electronic; $A T^3$: phononic

⑧ Simply Quantization was the solution

"phonons + electrons"

$\rightarrow$ agreement with experiment

A Review of Thermal Properties

- **Dulong–Petit (1800s):** Early calorimetry → nearly constant C_V for solids.
- **Crisis at low T:** High-precision cryogenic data showed C_V drops sharply → classical equipartition fails.
- **Stat mech limits:** Boltzmann gave the framework but still predicted T-independent C_V for solids.
- **Quantum turn (1900):** Planck's energy quanta opened the door to discrete vibrational modes.
- **Einstein model (1907):** Identical oscillators explain the drop in $C_V(T)$ but miss the T^3 law.
- **Debye model (1912):** Continuum of acoustic phonons with linear dispersion ⇒ $C_V \propto T^3$ at low T.
- **Experimental push:** Kamerlingh Onnes's liquefaction of He; Nernst & Grüneisen's measurements validated quantum models.
- **Metals clarified:** Sommerfeld's electron theory adds a linear-in-T term; lattice + electrons unify the picture.
- **In short:** Quantized phonons (and electrons) finally explain how matter stores and transports heat.

A Review of Thermal Properties

- We shall discuss only Volume Heat Capacity C_V
- C_V is defined as: *Amount of Heat Energy per unit volume that is required to raise the temperature of one cubic meter of the substance 1 K*.
- We have 3 famous models for C_V:
  - Debye Model
  - Einstein Model
  - Fermi Free Electron Model

Debye Model, Einstein Model → Depend on Phonons

Fermi Free Electron Model → Depends on Electrons

- At High T, Debye & Einstein → $3NK_B$ (Classical Limit)
- At Low T, Debye → T^3 (In agreement with Experiment)
- At low T, only long-wavelength (low-frequency) acoustic phonons are thermally excited, and their number grows as T^3 in three dimensions.

$$C_V \approx \frac{12\pi^4}{5} N k_B \left(\frac{T}{\Theta_D}\right)^3, \qquad T \ll \Theta_D.$$

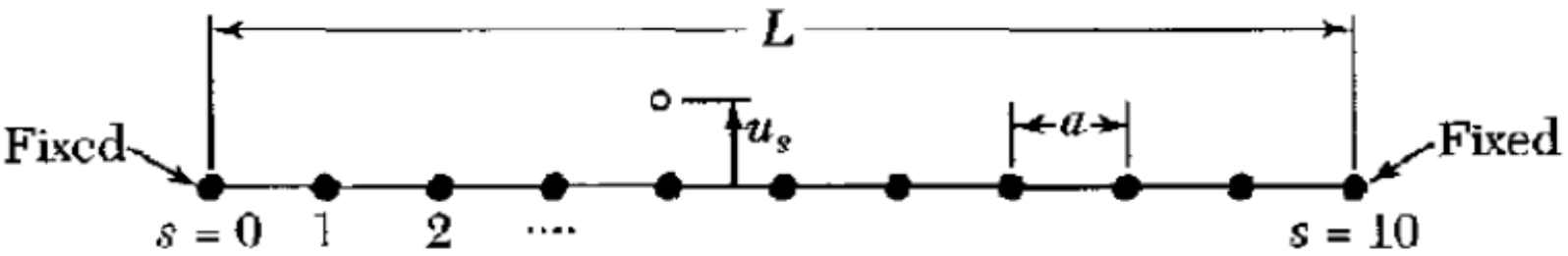
Modeling in Physics

- Modeling in physics is crucial because it provides a bridge between abstract physical laws and real-world phenomena.
- By constructing mathematical or computational models, scientists can simplify complex systems into manageable forms, reveal underlying principles, and make quantitative predictions.
- Models not only guide experimental design and interpretation but also expose limitations of existing theories—driving the development of new physics.
- In essence, modeling is the language through which theory, experiment, and application communicate.

Major Models in this Course

1. Einstein Model: Atoms modeled as independent quantum oscillators of a single frequency.
2. Debye Model: Continuum of acoustic phonon modes with linear dispersion
3. Fermi Gas Model : Conduction electrons treated as a classical or quantum gas.
4. Nearly Free Electron Model: Weak periodic potential modifies free electrons → energy gaps at Brillouin zone boundaries.
5. Tight-Binding Model: Electrons strongly bound to atoms with overlap of atomic orbitals forming bands.
6. Bloch's Theorem: Wavefunctions in a periodic potential modeled as plane waves times periodic functions.
7. Density of States Models: Model for distribution of electronic states in free, nearly free, or tight-binding cases.
8. Band Model of Solids: Classification into metals, semiconductors, and insulators based on band filling.
9. Effective Mass Model: Approximation where electrons in bands behave as free particles with renormalized mass.

Classical Heat Capacity



$$D(\omega) = \left(\frac{VK^2}{2\pi^2}\right)\left(\frac{dK}{d\omega}\right) \quad \text{- - - (1)}$$

Total Energy in 1-D:

$$U = \sum_{n=1}^{N} \frac{\hbar\omega_n}{e^{\frac{\hbar\omega_n}{K_B T}} - 1} \quad \text{- - - (2)}$$

$$\therefore C = \frac{\partial U}{\partial T} :$$

at high T : each mode → k_B

∴ $C \tilde{=} N k_B$ (1-D)

at low T ∴ only long λ modes are Important

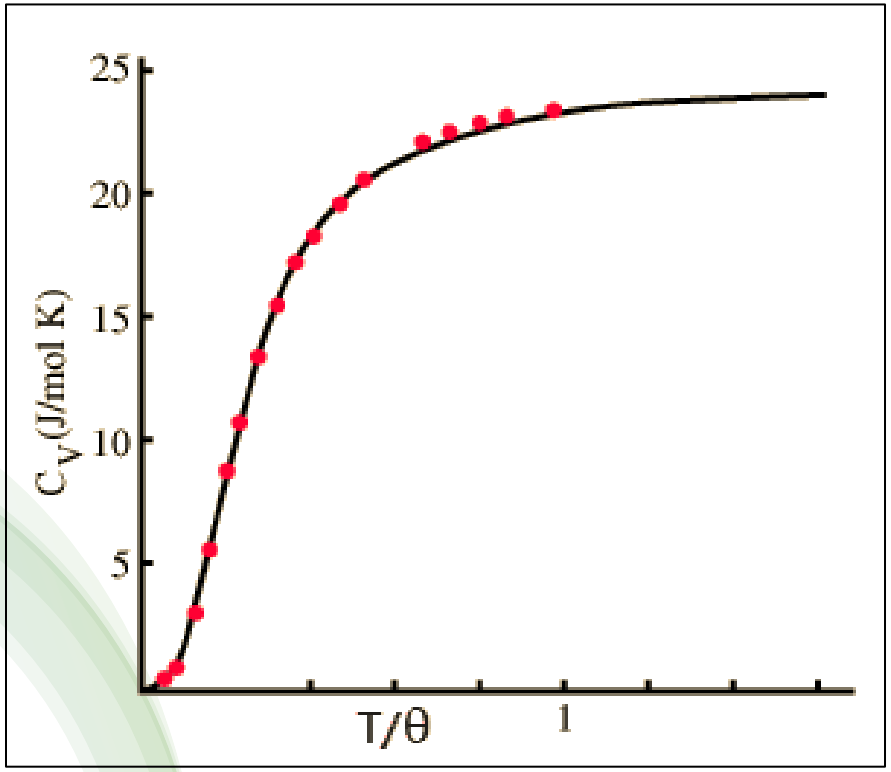
1-D density of states $\Rightarrow C \propto T$

in 3-D " " " $\Rightarrow C \propto T^3$

Debye Model for Density of States

$$\omega = vK$$

$$C_v = Cons. \int_0^{\omega_D} d\omega \frac{\omega^4 e^{\hbar\omega/\tau}}{\left(e^{\hbar\omega/\tau} - 1\right)^2}$$



Debye T^3 Law

In the figure:

① low T : $\frac{T}{\theta_D} \ll 1$ $\quad C_v \propto T^3$

② T → higher: → more phonone modes

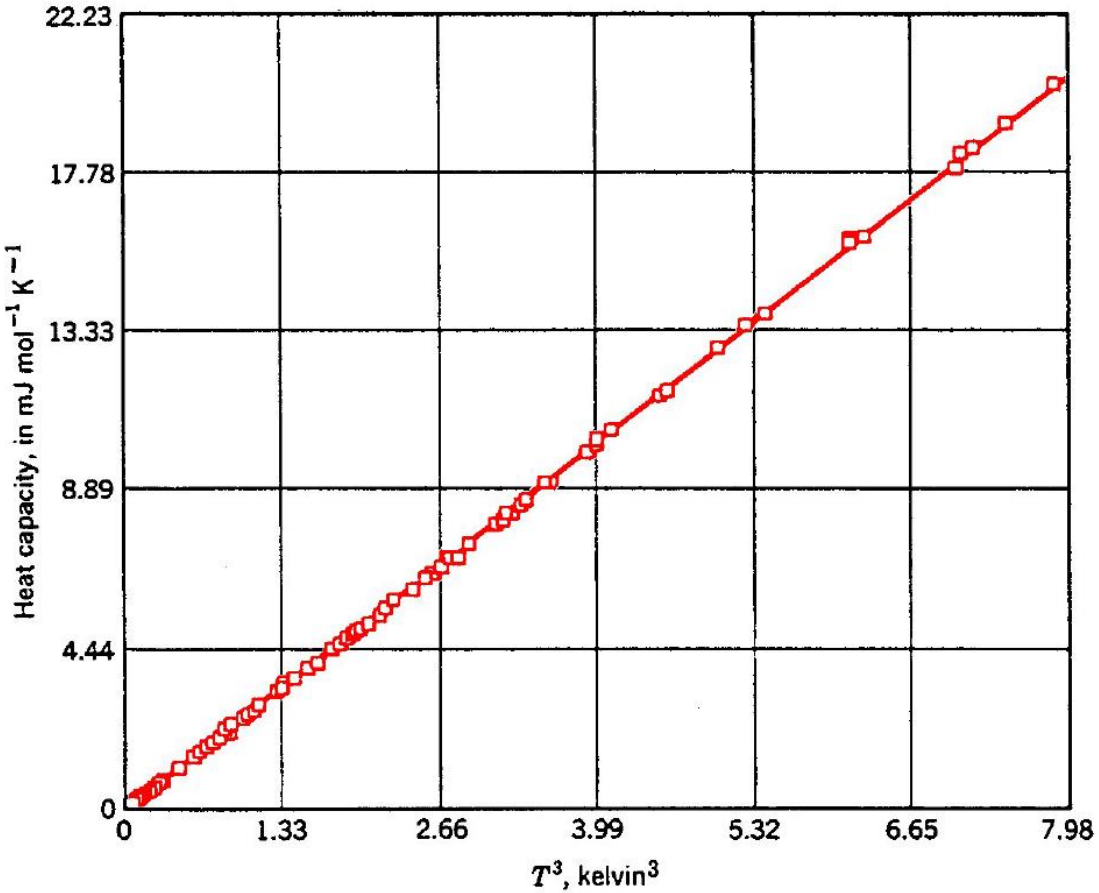
③ $\frac{T}{\theta_D} \gg 1$: very high T

$C_v \rightarrow 3R \quad (3NK)$

∴ Debye model is good in all T Range and it only Rely on θ_D.

Debye T^3 La

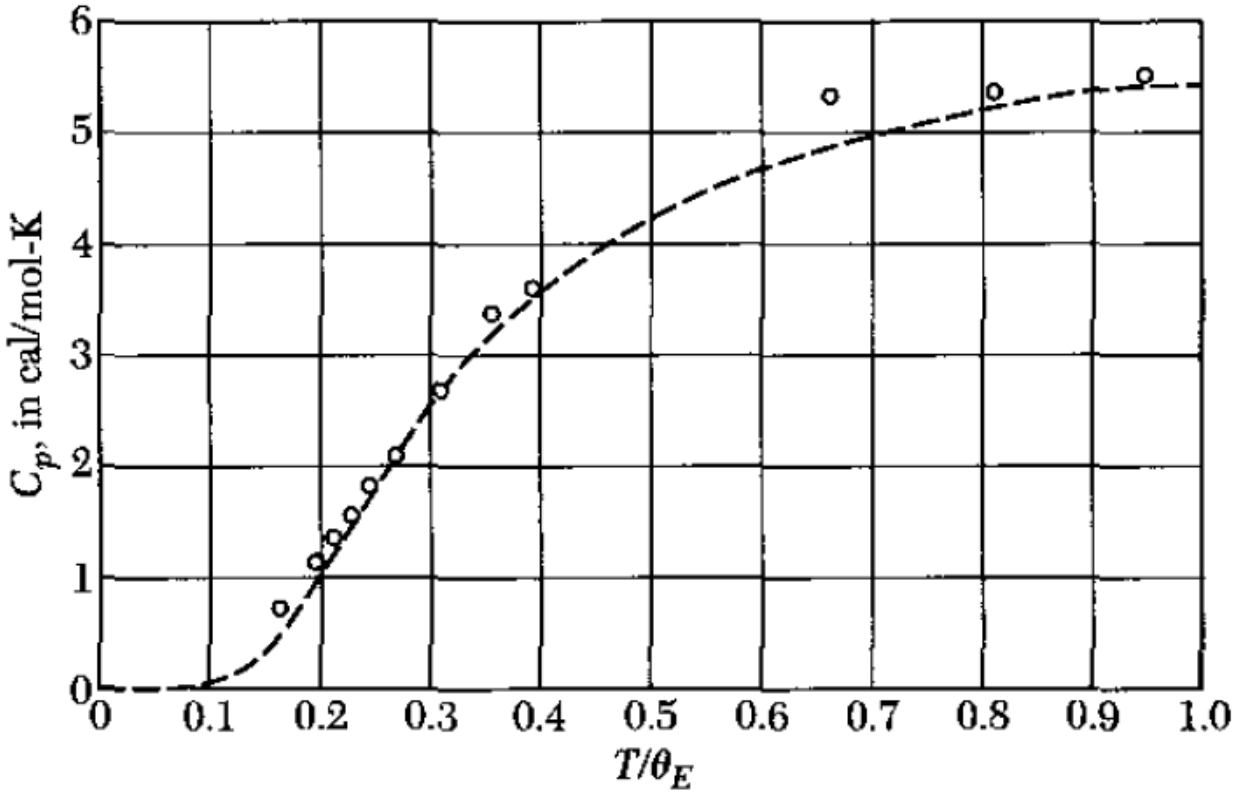
$$C_v \cong cons.T^3$$



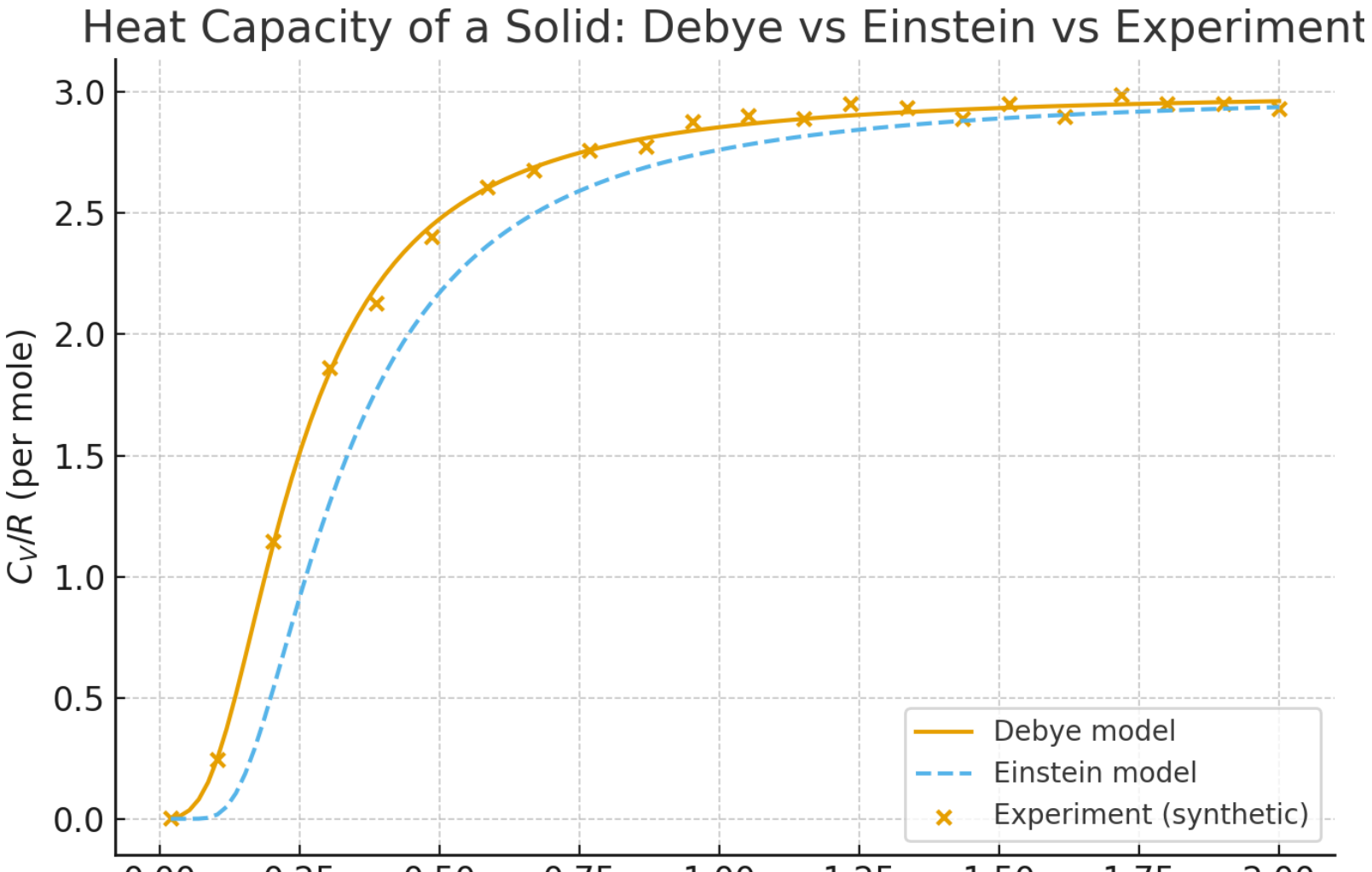
Einstein Model of the Density of States

$$D(\omega) = N\delta(\omega - \omega_o)$$

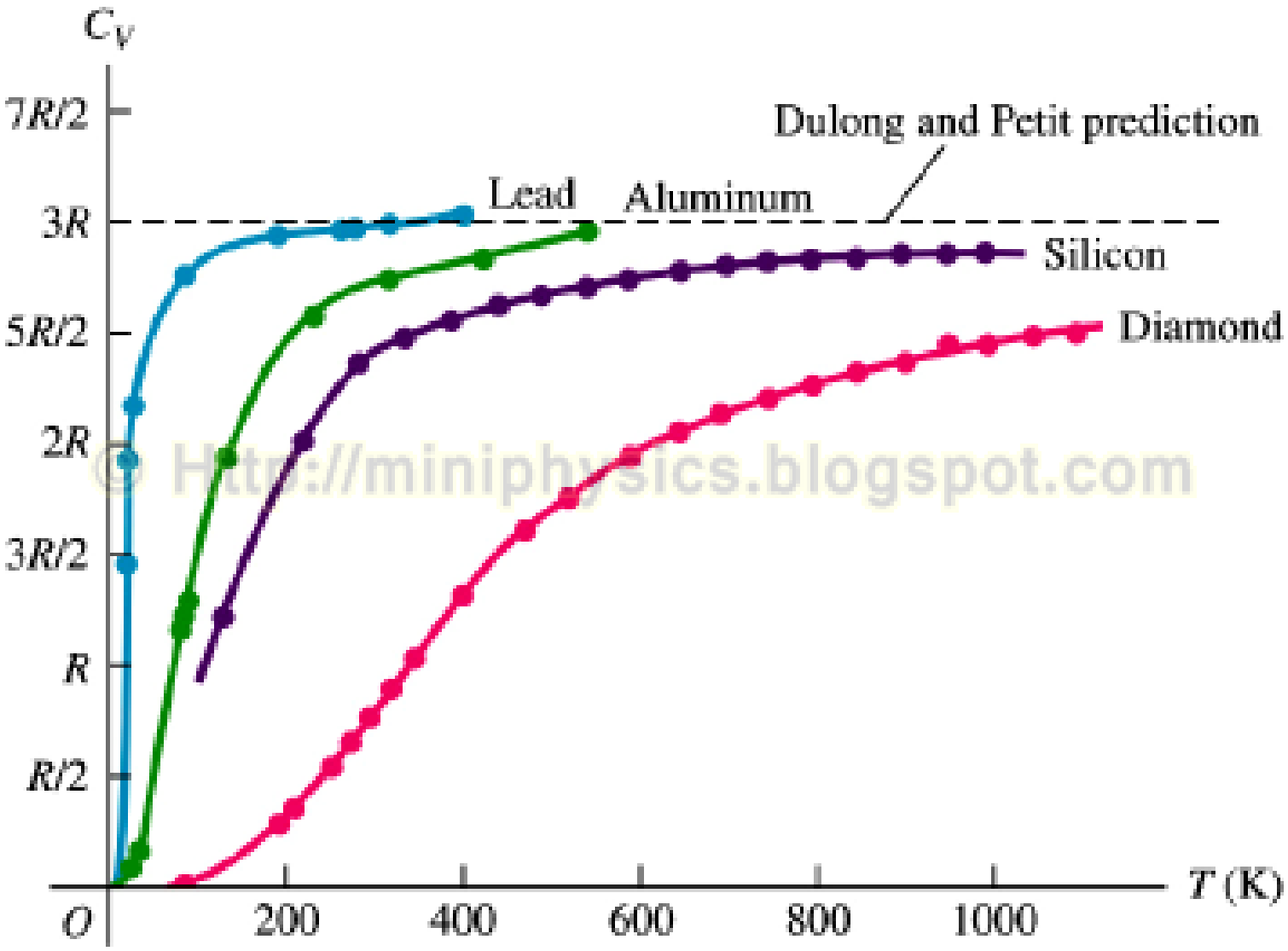
$$C_v = Nk_B \left(\frac{\hbar\omega}{\tau}\right)^2 \frac{e^{\hbar\omega/\tau}}{\left(e^{\hbar\omega/\tau} - 1\right)^2}$$



Einstein VS. Debye Model

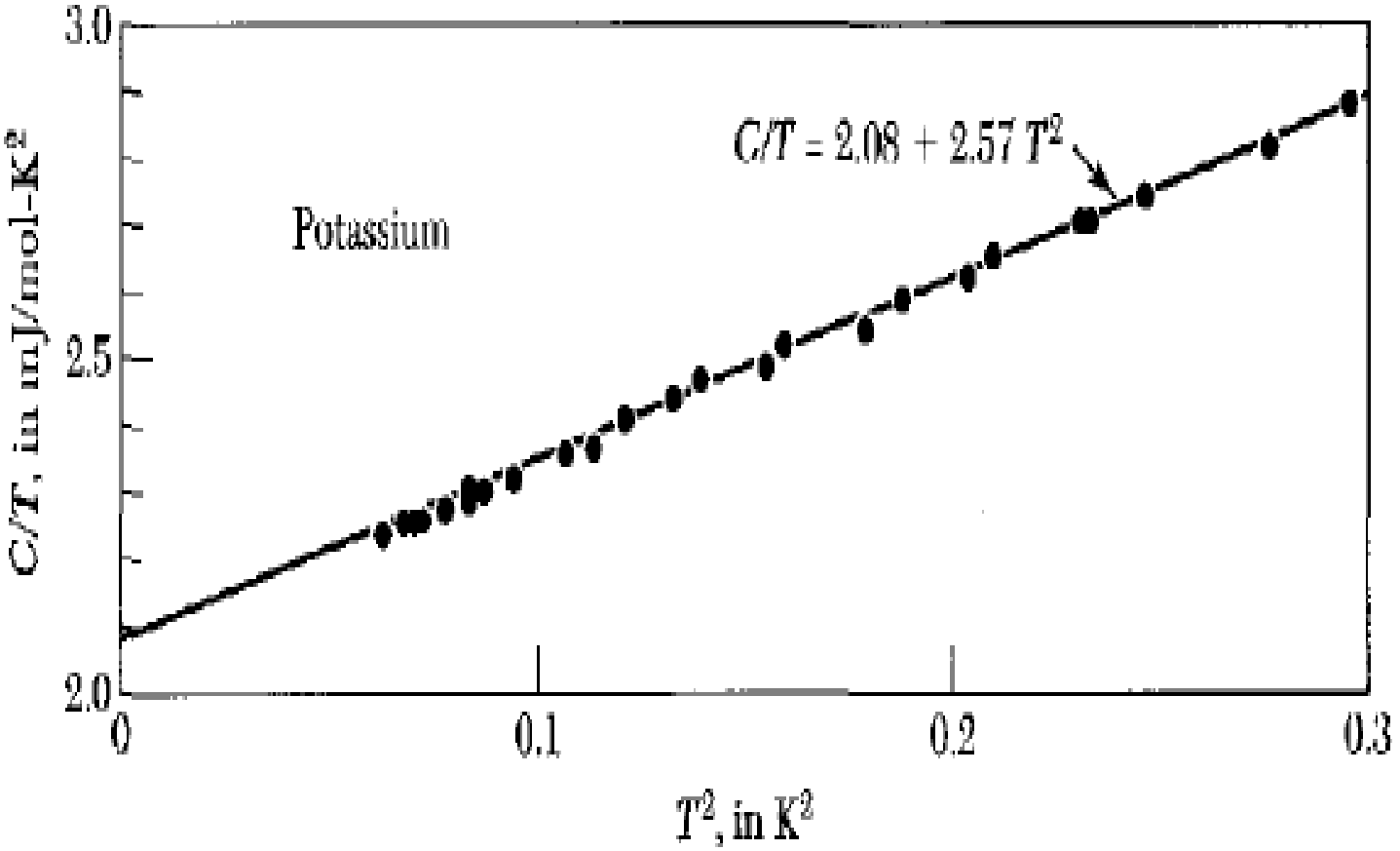


Experimental data



Total Heat Capacity

$$C = \gamma T + AT^3$$



Free Electron Fermi Gas

- **Free Electron Model has a good agreement with experiment for the full range of temp.**

1. Energy Levels in 1-D
2. Effect of Temperature on the Fermi-Dirac Distribution
3. Free Electron Gas in 3-D
4. Heat Capacity of the Electron Gas
5. Electrical Conductivity and Ohm's Law
6. Motion in Magnetic Fields
7. Thermal Conductivity of Metals
8. Nanostructures

Free Electron Fermi Gas

- Classically: $C_{v,e} \approx \frac{3}{2} N K_B$
- **Problem**: Experiment shows the electronic contribution is tiny compared to lattice heat capacity.
- Need a quantum model: Sommerfeld's Fermi Gas Model (1928).
- Key idea: electrons obey Pauli exclusion and Fermi–Dirac statistics

Free Electron Fermi Gas

- **Fermi–Dirac Distribution:**
- Occupation probability:

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

- At T= 0: all states filled up to Fermi energy E_F
- At low T: only electrons within $\sim k_B T$ of E_F can be thermally excited.

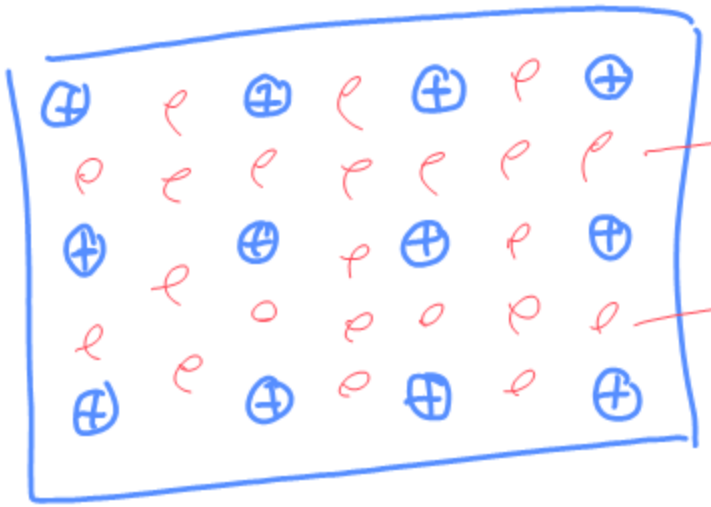
Total Heat Capacity

$$C = \gamma T + AT^3 + \cdots$$

(1) e (2) phon.

The first one who put his model for the metals was Drud ← 100%

Sommerfeld ← 50% + 50%



electrons are like a sea:

sea of electrons

∴ All electrons are FREE to move and don't Interact with: neither atoms nor each

Simply they behave like (Gases)

∴ + ive Ions (Fixed)

- Give electrons → sea of electrons
- they are subject to Pauli ex. prine.

$J = \sigma E$ ← Elec. Field.

J: current density

σ: conductivity → $\rho = \frac{1}{\sigma}$

Free Electron Fermi Gas

Introduction:

According to this model; the valence electrons become conduction electrons and move freely through the metal.

Example: Na^{11}: *1s, 2s,2p* ➔ 10 e (bound)

3s ➔ 1 free electron

Hence, we have ***3s*** conduction band.

For N atoms: we have N free electrons

Free Electron Fermi Gas

Introduction (Continued):

- **Free Electron Fermi Gas**: *A collection of large no. of electrons that are free to move and subject to Pauli Ex. Principle* (**Fermi See**)
- **Free to move**: *Because of the periodicity of the lattice.*
- **Pauli Ex. Principle**: *Means that few scattering could happen to electrons from other electrons (not from ions).*

Quantum Mechanics Role:

(1) Free Electron model

(2) Nearly free E. M.

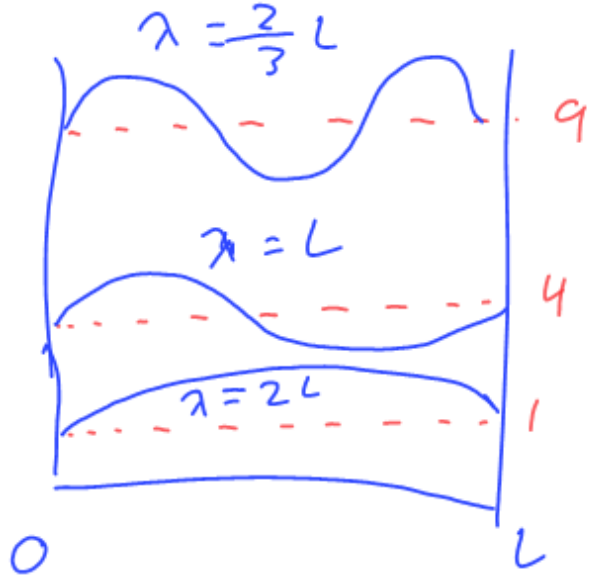
(3) Bloch Theorm

in F.E.m.: $V = 0$

electrons move under no potential at all.

solving for this uses easiest Q.M. method

a particle in a box.



$\psi_n(0) = \psi_n(L)$

Boundary Conditions

Schrödinger Eq for 1 electron: $V = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = \epsilon_n \psi_n \quad \text{---} \quad (1)$$

with $\psi_n = A\sin\left(\frac{n\pi}{L}x\right) = A\sin\left(\frac{2\pi}{\lambda_n}x\right)$ .. (2)

$n = 1, 2, 3 \cdots$ $\lambda_n = \frac{2}{n}L$ ----- (3)

put (2) in (1) and take 2nd derivative.

$$\Rightarrow \varepsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2 \quad \text{------ (4)}$$

$$= \frac{\hbar^2 \pi^2}{2mL^2} \cdot n^2 \quad \text{------ (5)}$$

$\because n_F = \frac{N}{2}$, let $n \rightarrow n_F$

$$\therefore \varepsilon_F = \frac{\hbar^2 \pi^2}{2mL^2}\left(\frac{N}{2}\right)^2 \quad \text{------ (6)}$$

N = No. of electrons.

Free Electron Fermi Gas

Energy Levels in 1-D:

Schrödinger Eq. of 1 electron: $H\psi_n = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = \varepsilon_n\psi_n$ *(1)*

ε_n *is the energy of the e in orbital.*

We then apply the bound. Cond.: $\psi_n(0) = \psi_n(L) = 0$

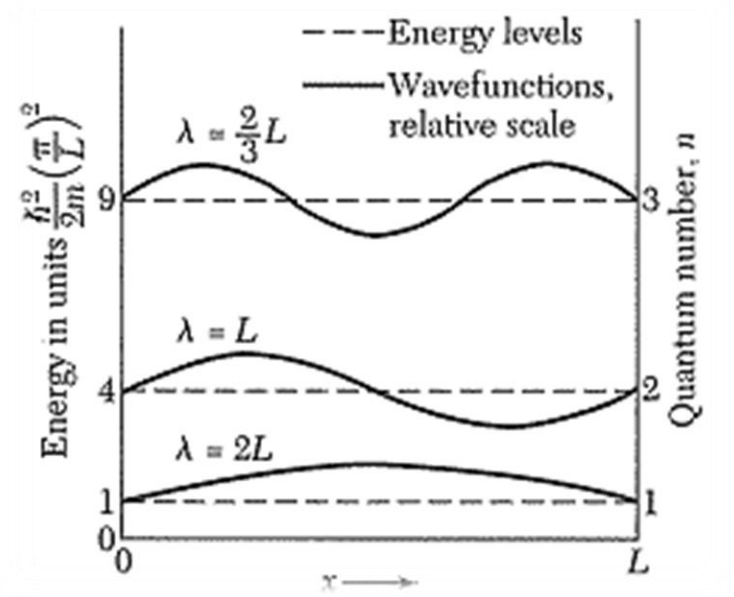
Solution is of the form:

$$\psi_n = A\sin\left(\frac{n\pi}{L}x\right) = A\sin\left(\frac{2\pi}{\lambda_n}x\right)$$

Where: $n = 1, 2, \cdots$ and: $\lambda_n = \frac{2}{n}L$

We feed this wave function back in eq. (1)

$$\frac{d\psi_n}{dx} = A\left(\frac{n\pi}{L}\right)\cos\left(\frac{n\pi}{L}x\right)$$



Free Electron Fermi Gas

Energy Levels in 1-D (continued):

Hence, 2nd derivative:

$$\frac{d^2\psi_n}{dx^2} = -A\left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi}{L}x\right)$$

Energy Levels are thus given by:

$$\varepsilon_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

But this is for (1 e). We need to work out the energy levels for N e's. Pauli Ex. Principle does not allow any two e's to have same set of quantum numbers.

In our case (linear solid) these quantum numbers are n & m_s

Hence, if n is the same, m_s must be different.

Ex. n = 2 ➔ $m_s = \pm ½$ (2 electrons)

Energy, however, could be the same for more than one orbital (this is called *degeneracy*)

Free Electron Fermi Gas

Energy Levels in 1-D (continued):

Fermi Energy ε_F is the energy of the Last FULL level at 0 K.

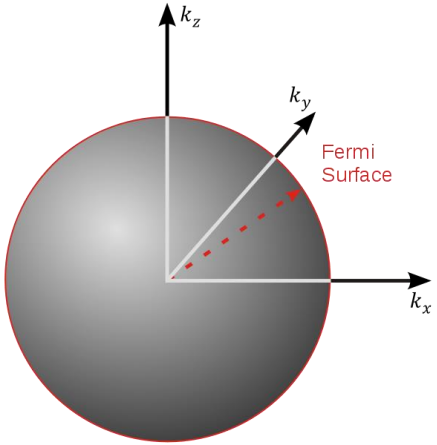
Last FULL energy level is n_F.

For N electrons; $n_F = N/2$

Thus, for N electron system:

$$\varepsilon_F = \frac{\hbar^2}{2m}\left(\frac{n_F\pi}{L}\right)^2 = \frac{\hbar^2}{2m}\left(\frac{N\pi}{2L}\right)^2$$

The free fermions that occupy the lowest energy states form a sphere in **k** space. The surface of this sphere is the ***Fermi surface***



Free Electron Fermi Gas

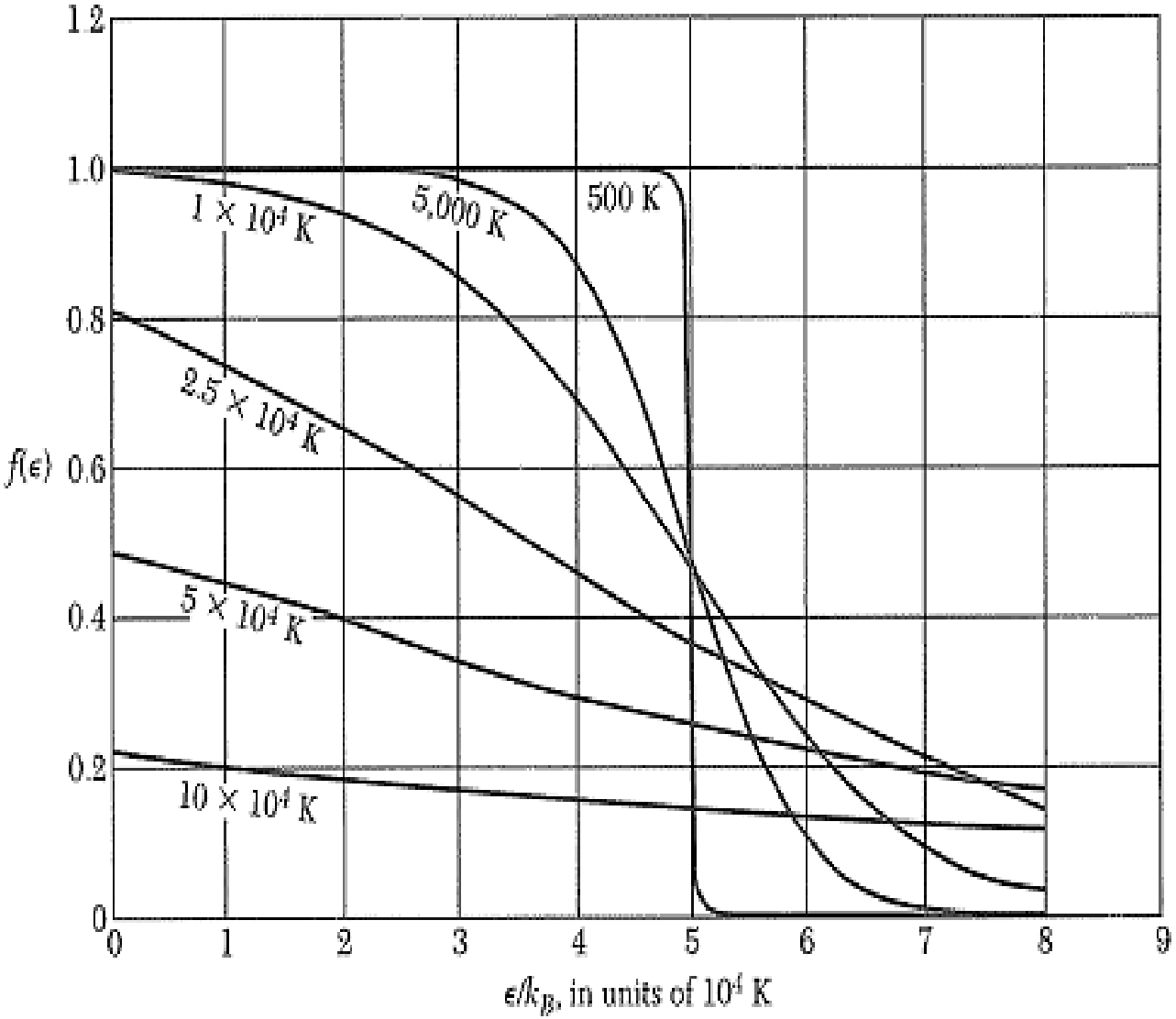
Effect of T on Fermi-Dirac Distribution

- System of N e's is at Ground State if T = 0 K
- As T increase ➔ Kinetic Energy of e's increase
- ➔ Higher Levels are occupied
- Since No. of e's is fixed ➔ other levels get vacant.

Fermi-Dirac Distribution Function $f(\varepsilon)$ gives the **probability** that an orbital (level) of energy ε is occupied at temp. T:

$$f(\varepsilon) = \frac{1}{e^{\left(\frac{\varepsilon-\mu}{K_B T}\right)} + 1}$$

μ is the chemical potential. At T = 0 : $\mu = \varepsilon_F$



Free Electron Fermi Gas

Free Electron Gas in 3-D (continued):

- Wave Eq. in 3-D takes the form

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_k(\mathrm{r})=\varepsilon_k\psi_k(\mathrm{r}) \qquad (6)$$

- Hence, wave function inside a box of *L* x *L* x *L*:

$$\psi_n(\mathrm{r})=A\sin\left(\frac{\pi n_x x}{L}\right)\sin\left(\frac{\pi n_y y}{L}\right)\sin\left(\frac{\pi n_z z}{L}\right) \qquad (7)$$

- Periodicity of the wave leads to: $\psi_n(x+L,y,z)=\psi(x,y,z)$ (8)

With same results for *y* and *z*. In other words, value of the function at the left side of the cube is the same at the right side.

Free Electron Fermi Gas

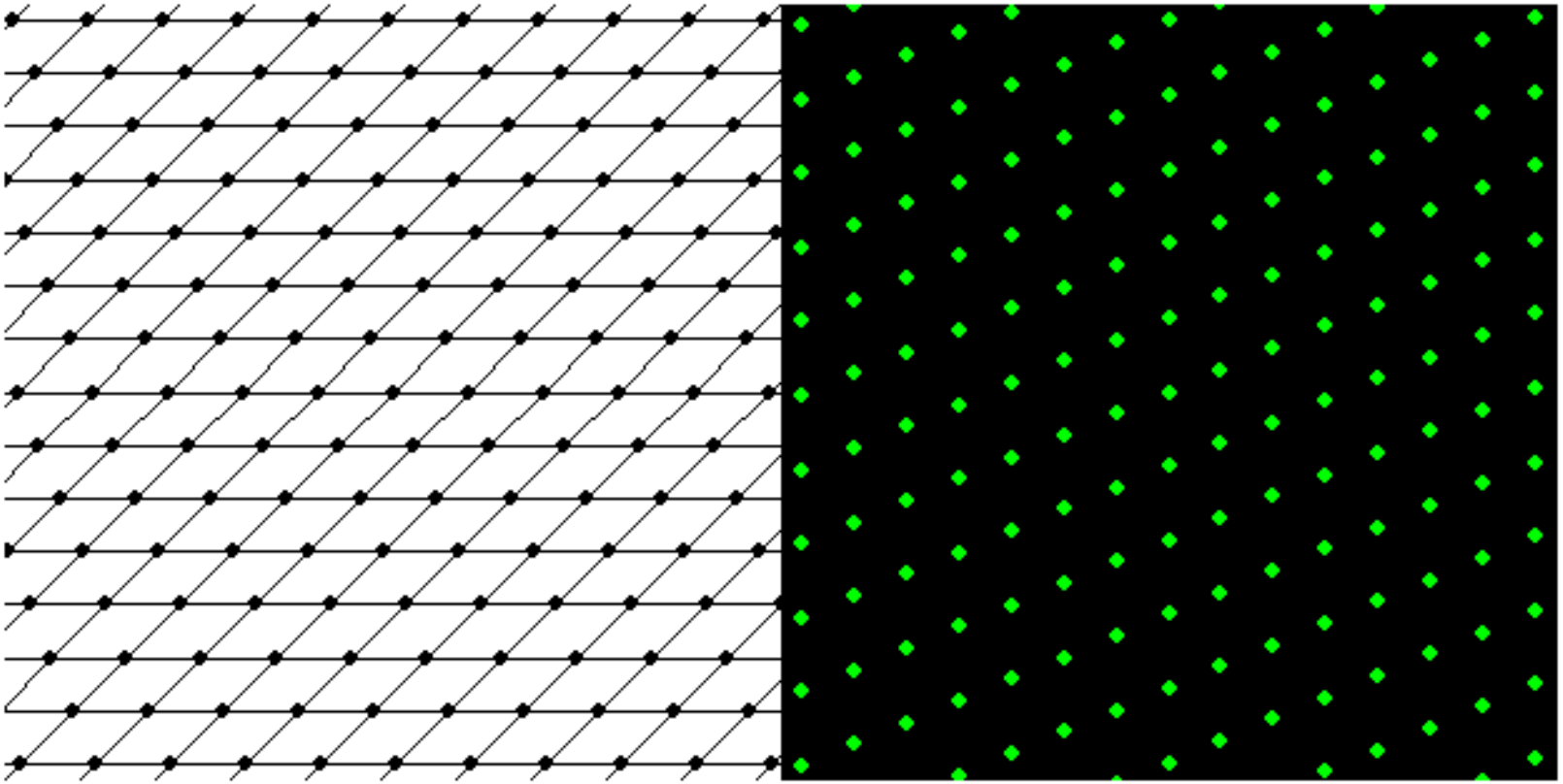
Free Electron Gas in 3-D (continued):

- Eq. (9) in (6) we have the energy levels:

$$\varepsilon_k = \frac{\hbar^2}{2m} k^2 = \frac{\hbar^2}{2m}\left(k_x{}^2 + k_y{}^2 + k_z{}^2\right) \qquad (12)$$

- Wavevector k and wavelength λ are related as: $k = 2\pi / \lambda$
- Momentum p in Q.M. is given by: $\mathbf{p} = -i\hbar\nabla$
- When this momentum (operator) applied to the wavefunction in Eq. (9), we get the eigenfunction ψ_k with eigenvalue: $\hbar\mathbf{k}$
- For a system of N e's in G.S. the occupied orbitals are represented by as points inside a sphere in k space.

Free Electron Fermi Gas



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Free Electron Fermi Gas

Free Electron Gas in 3-D (continued):

- Sphere surface represents Fermi Energy ε_F expressed as:

$$\varepsilon_F = \frac{\hbar^2}{2m} k_F{}^2 \qquad (14)$$

- Since Volume element in k space is $(2\pi / L)^3$ (volume of 1 state) while the total volume of the sphere is: $\frac{4}{3}\pi k_F{}^3$ we can find total no. of states (orbitals) for this system as:

$$\frac{4}{3}\pi k_F{}^3 \div \left(\frac{2\pi}{L}\right)^3 \times 2 = \frac{V}{3\pi^2} k_F{}^3 = N \qquad (15)$$

The x 2 in L.H.S. is because of 2 e's for every Q.N. m_s

Phys 672

Advanced Solid State Physics

Physics & Astronomy
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First Term: 2025

Lecture No. 02

Review of free electron theory

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Free Electron Fermi Gas

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- **Problem**: Experiment shows the electronic contribution is tiny compared to lattice heat capacity.
- Need a quantum model: **Sommerfeld's Fermi Gas Model** (1928).
- Key idea: electrons obey Pauli exclusion and Fermi–Dirac statistics

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1-Introduction

Sommerfeld critical ideas in Q.M.

(1) He is the first to Introduce angular Q. N. l

(2) He is the first to Introduce spin Q. N. S

(3) He was the first to call "e" an Quantum particle.

(4) He was the first to prpose that electrons inside a solid $\Longrightarrow$ F. D. distrib

2-Energy Levels in 1-D:

Schrödinger Eq. of 1 electron:

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We then apply the bound. Cond.: $\psi_n(0) = \psi_n(L) = 0$

Solution is of the form:

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Where: $n = 1, 2, \cdots$ and: $\lambda_n = \frac{2}{n}L$

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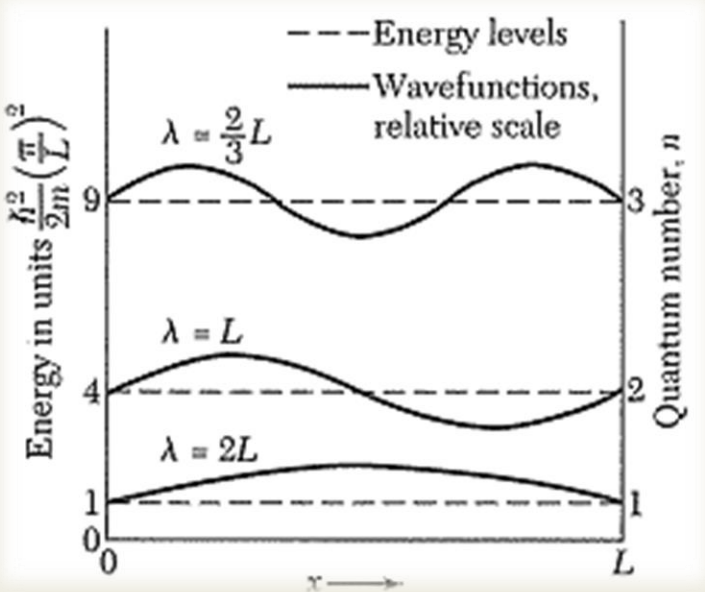

2-Energy Levels in 1-D:

Hence, 2nd derivative:

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Energy Levels are thus given by:

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Hence, if n is the same, m_s must be different.

Example: n = 2 ➔ $m_s = \pm ½$ (2 electrons)

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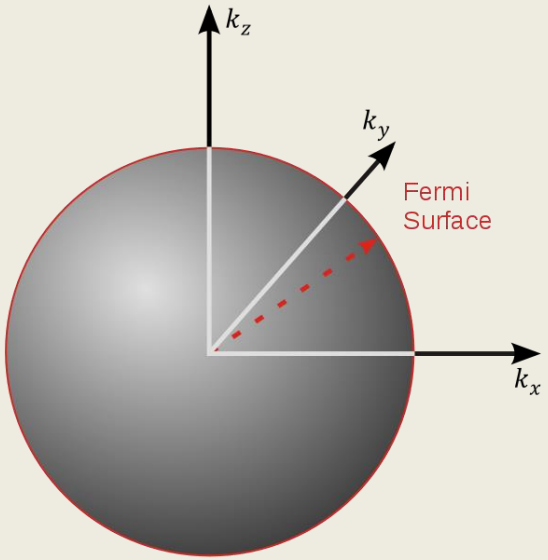

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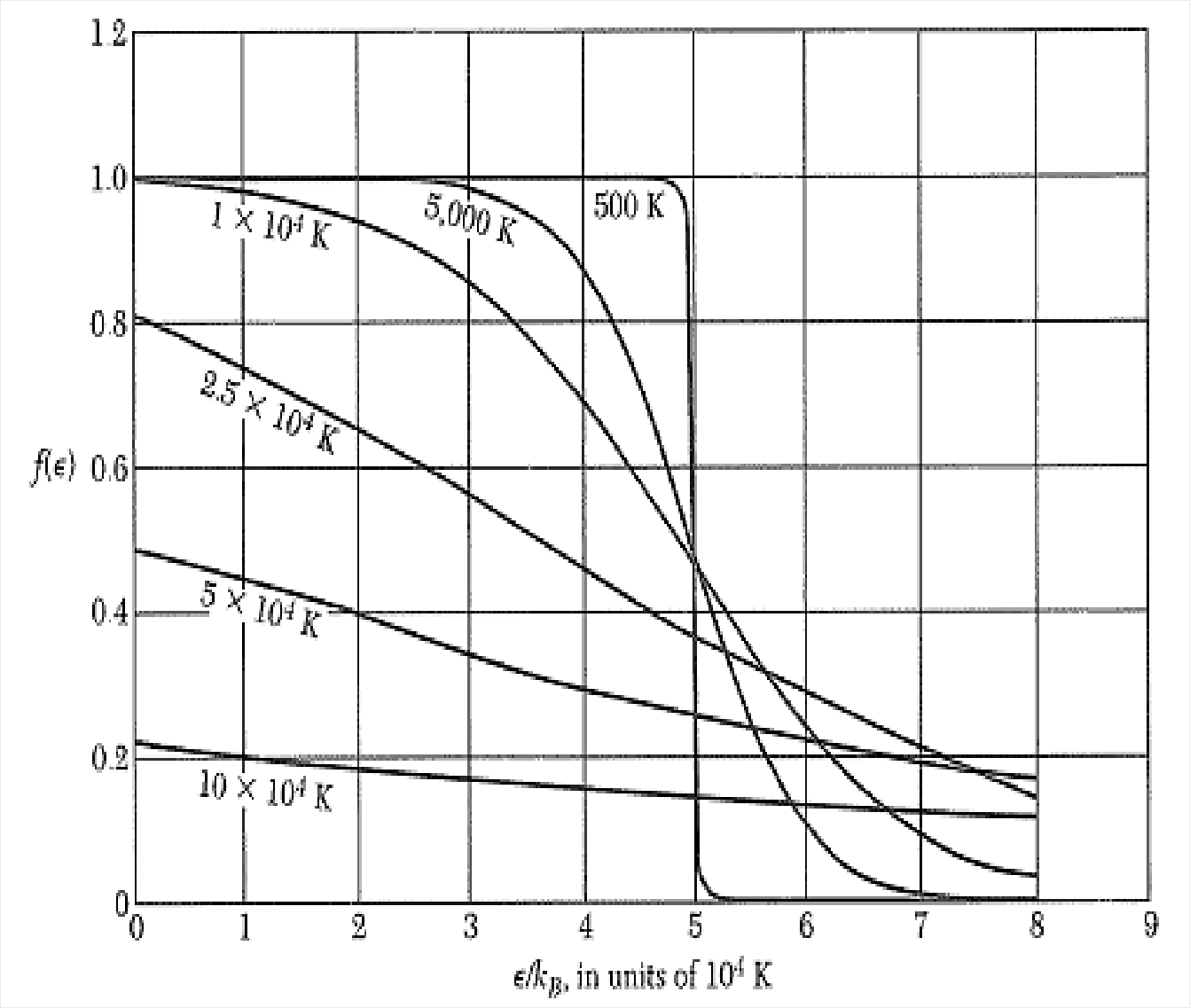
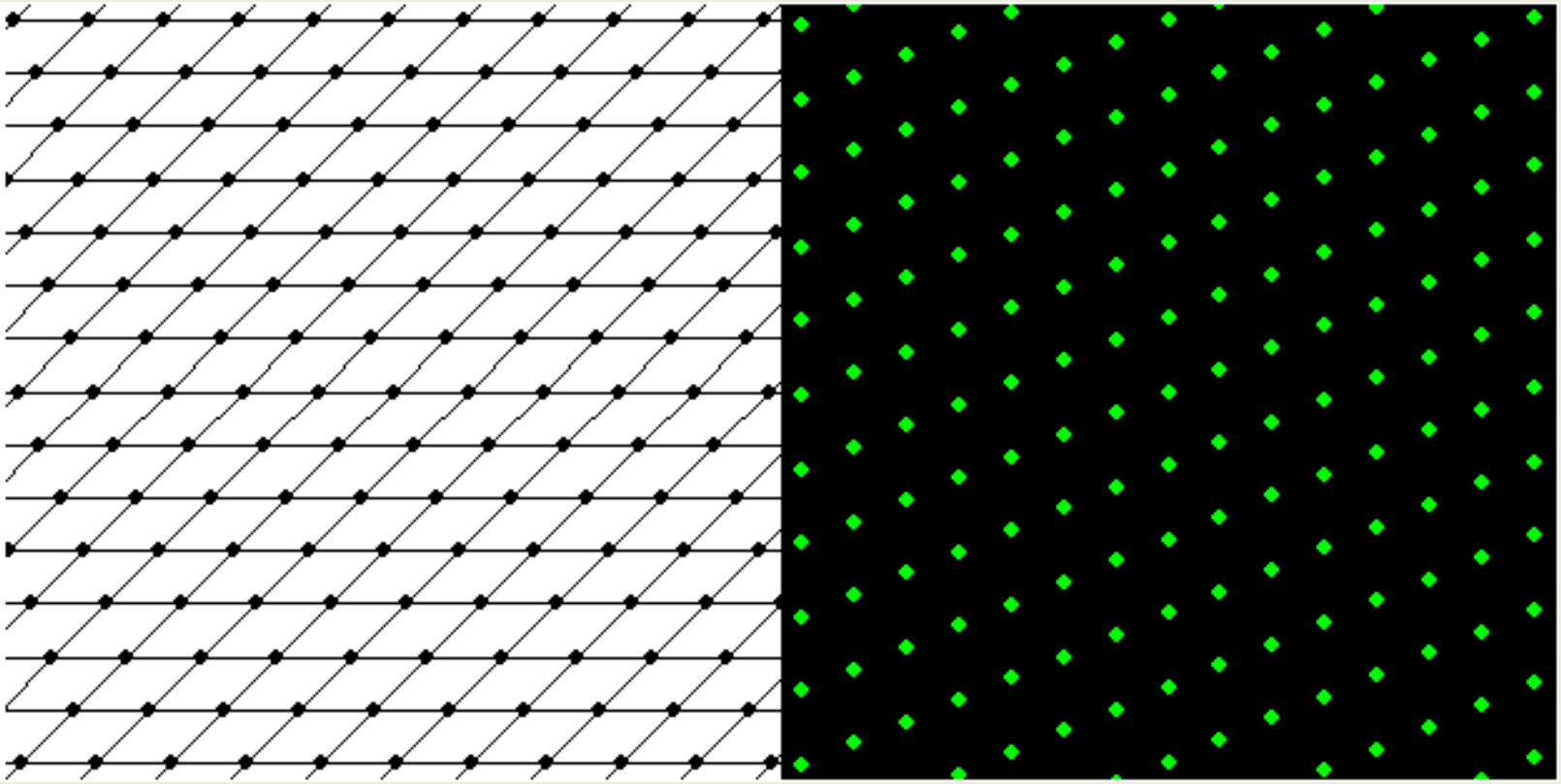
$$f(\varepsilon) = \frac{1}{e^{\left(\frac{\varepsilon-\mu}{K_B T}\right)} + 1} \qquad (5)$$

μ is the chemical potential. At T = 0 : $\mu = \varepsilon_F$

Energy Levels in 1-D (continued):



Free Electron Fermi Gas



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The figure:

① Left side: Real space (atomic in 2-D)

② Lines represent periodic arrangement (lattice)

③ we consider $V = 0$ (Free electrons)

④ Right side: Reciprocal space

⑤ green dots ≡ reciprocal lattice points

Q. How to get ⑤ out of ①?

A. using Fourier transform

⑥ How to get ⑤? from XRD

⑤ is used to construct Brillouin Zones

⑦ ① is lattice in normal space → ⑤ momentum space

EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

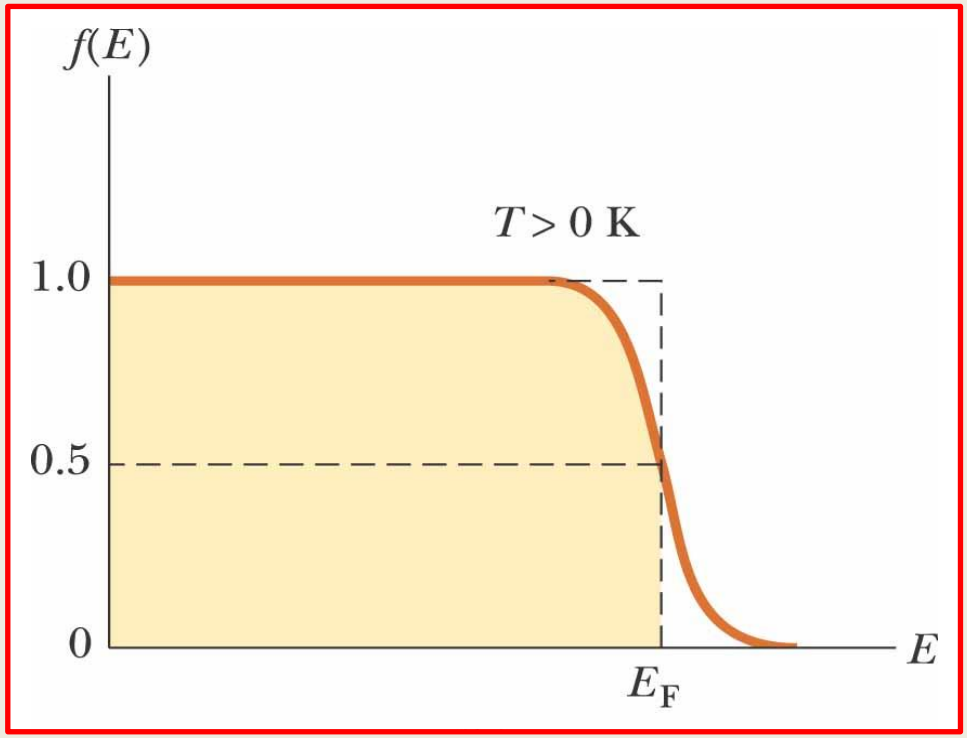
- *The ground state is the state of the N electron system at absolute zero*. What happens as the temperature is increased? The solution is given by the Fermi-Dirac distribution function.
- The kinetic energy of the electron gas increases as the temperature is increased: some energy levels are occupied which were vacant at absolute zero, and some levels are vacant which were occupied at absolute zero .The **Fermi-Dirac distribution gives the probability that an orbital at energy ε** will be occupied in an ideal electron gas in thermal equilibrium.

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/k_B T} + 1} \qquad (5)$$

μ is a function of temperature; it is to be chosen in such a way that the total number of particles = *N. At absolute zero* $\mu = \varepsilon_F$

EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

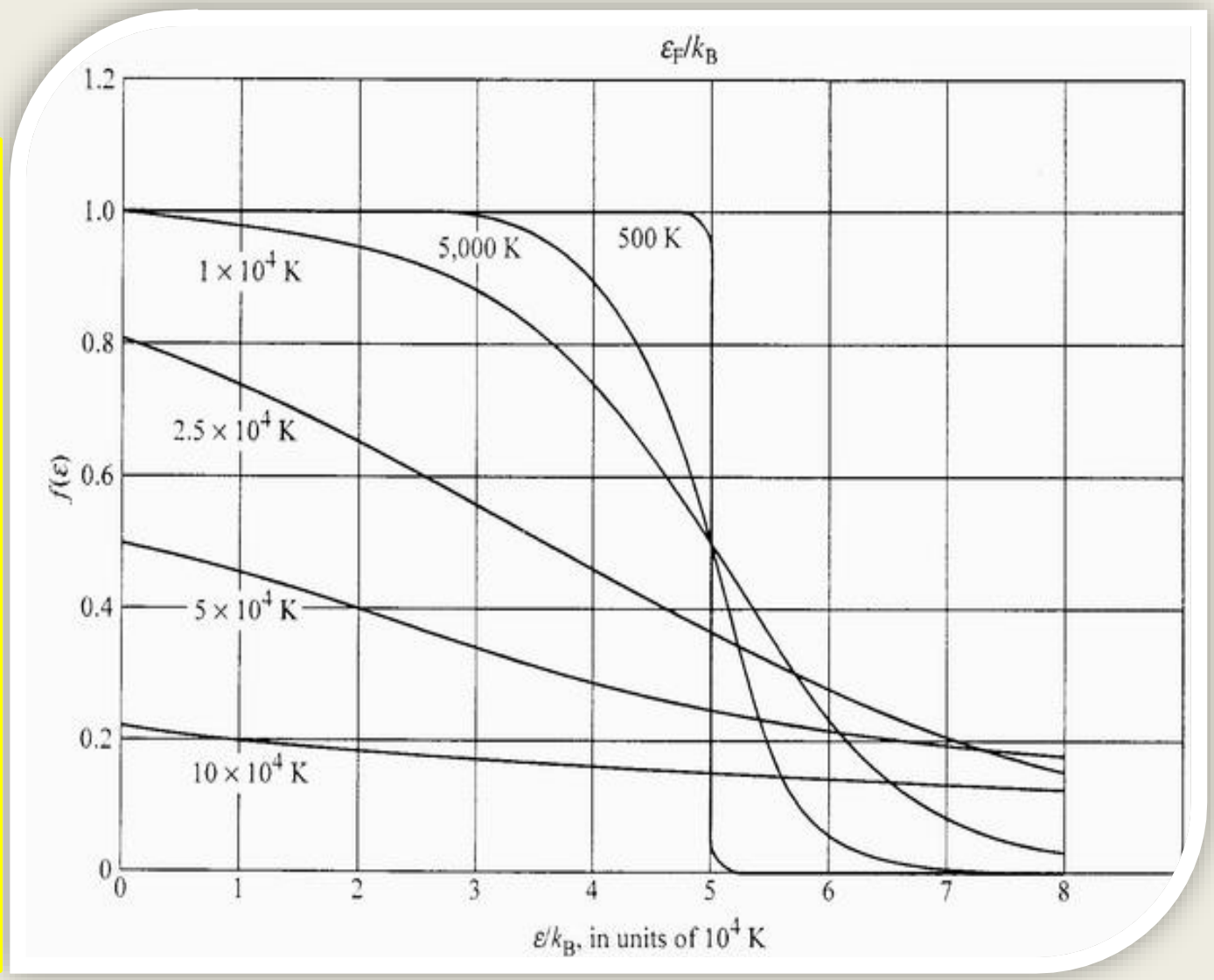
because in the limit $T \rightarrow 0$ *the function* $f(\varepsilon)$ *changes discontinuously from the value 1 (filled) to* the value 0 (empty) at $\varepsilon = \varepsilon_F = \mu$. *At all temperatures* $f(\varepsilon)$ *is equal to ½ when* $\varepsilon = \mu$, for then the denominator of (5) has the value 2.



f(ε) = 1 (means full)
f(ε) = 0 (means vacant)
At very low temp. f(ε) becomes similar to Boltzmann or Maxwell Distribution.

EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

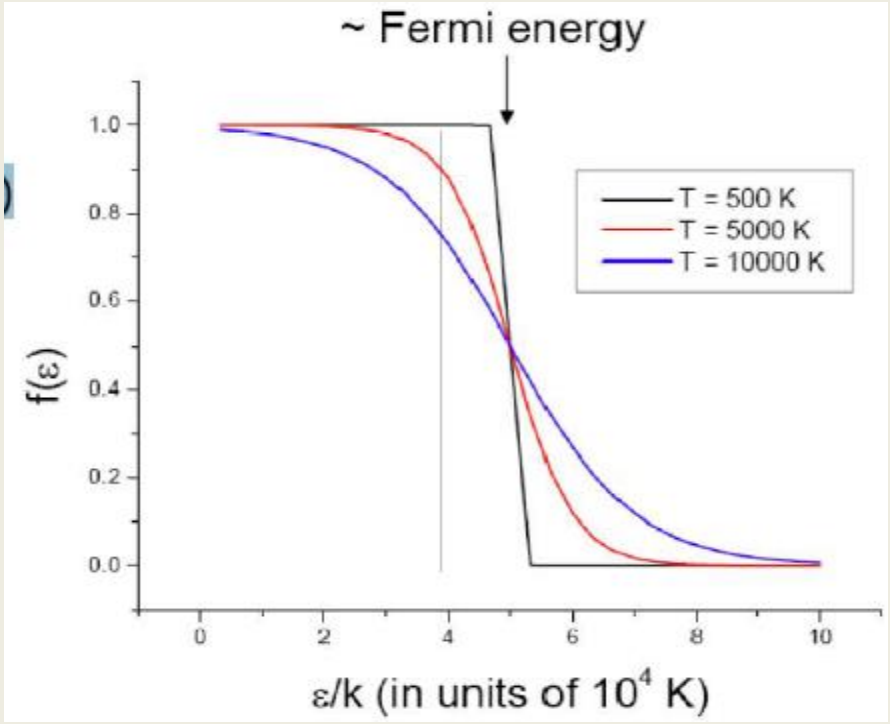
f(ε) at the various temperatures, for $T_\varepsilon = \varepsilon_F/K_BT =$ *50,000 K. The total number of particles* is constant, independent of temperature.



EFFECT OF TEMPERATURE ON THE FERMI-DIRAC DISTRIBUTION

This is what the *f(ε)* looks like at different Temperatures

- As T → 0 K, it becomes a step function
- Note that the lower energy levels are usually filled first, and as temperature increases; no of electrons at higher energy levels increases.



Fermi energy changes as the temperature changes because it is defined as: $\mu = F_{n+1} - F_n$ (n= no. of particles, electrons)
Where F is the Helmholtz Free Energy: F=U-TS
U: System energy, S: Entropy (Increases as T increase)

Different DISTRIBUTION Systems

Distribution System	Notes	
Maxwell-Boltzmann distribution	•identical particles •distinguishable •wave function : not overlap	$f(\varepsilon) = Ae^{-\varepsilon/k_B T}$
Bose-Einstein distribution	•Identical particles •indistinguishable •wave function : overlap •spin quantum number = 0,1,2, …	$f(\varepsilon) = \frac{1}{e^{\alpha} e^{\varepsilon/k_B T} - 1}$
Fermi-Dirac distribution	•Identical particles •indistinguishable •wave function: overlap •spin quantum number = 1/2,3/2,5/2 …..	$f(\varepsilon) = \frac{1}{e^{\alpha} e^{\varepsilon/k_B T} + 1}$

FREE ELECTRON GAS IN THREE DIMENSIONS

We just need to extend our results for 1-D.

$$\frac{-\hbar^2}{2m}\left(\frac{\partial^2}{dx^2}+\frac{\partial^2}{dy^2}+\frac{\partial^2}{dz^2}\right)\psi_k(r)=\varepsilon_k\psi_k(r) \qquad (6)$$

for a cube of length L we have:

$$\psi_n(r)=A\sin\left(\frac{\pi n_x x}{L}\right)\sin\left(\frac{\pi n_y y}{L}\right)\sin\left(\frac{\pi n_z z}{L}\right) \qquad (7)$$

n_x, n_y, n_z are all positive intigers.

ψ is periodic in x, y, z with period L. Thus:

$$\psi(x+L,y,z)=\psi(x,y,z) \qquad (8)$$

$$\psi(x,y+L,z)=\psi(x,y,z),\quad \psi(x,y,z+L)=\psi(x,y,z)$$

FREE ELECTRON GAS IN THREE DIMENSIONS

Wave functions satisfying the free particle Schrodinger equation and the periodicity condition are of the form of a traveling planave:

$$\psi_k(r) = e^{ik.r} \tag{9}$$

$$\text{with: } k_x, k_y, k_z = 0; \pm\frac{2\pi}{L}; \pm\frac{4\pi}{L}; \ldots\ldots \tag{10}$$

Any component of k of the form *2nπlL will satisfy the periodicity* condition over a length L, where *n is a positive or negative integer.* these values of k_x satisfy (8), for:

$$e^{ik_x(x+L)} = e^{i\frac{2n\pi}{L}(x+L)} = e^{i\frac{2n\pi}{L}x}.e^{i2n\pi} = e^{i\frac{2n\pi}{L}x} = e^{ik_x x} \tag{11}$$

Differentiate (9) twice then put it back in Eq. (6):

$$\varepsilon_k = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}(k_x^2 + k_x^2 + k_x^2) \tag{12}$$

FREE ELECTRON GAS IN THREE DIMENSIONS

The energy at the surface of the sphere is the Fermi energy:

$$\varepsilon_F = \frac{\hbar^2}{2m} k_F^2 \qquad (14)$$

We can calculate the total No. of states inside Fermi Sphere from dividing the total Fermi sphere volume on the volume of one state

Volume of one state: $\left(\frac{2\pi}{L}\right)^3$

Total volume of Fermi Sphere: $\frac{4}{3}\pi k_F^3$

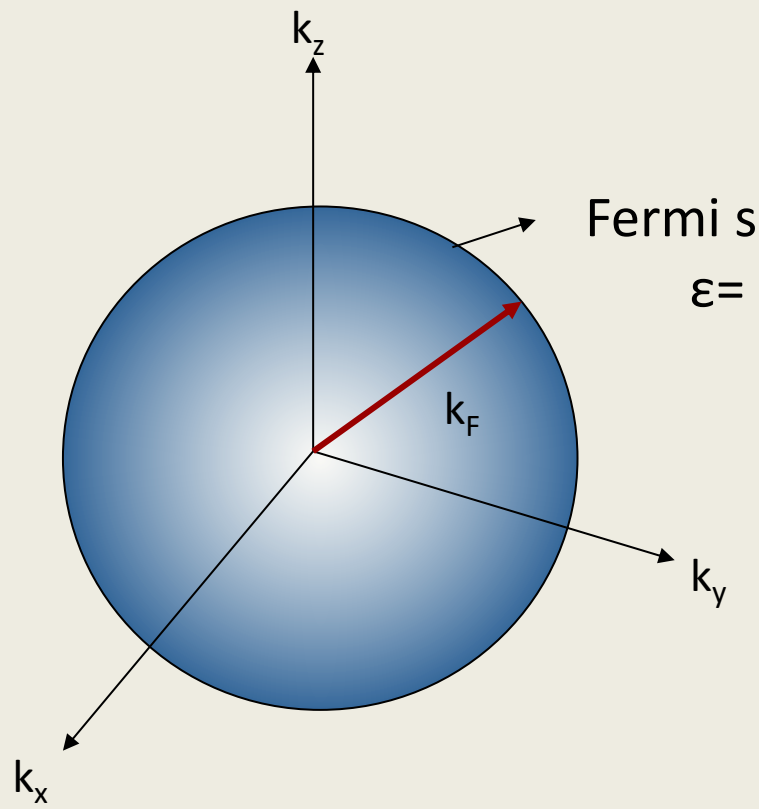
$$\therefore N = 2.\frac{4}{3}\pi k_F^3 \Big/ \left(\frac{2\pi}{L}\right)^3 = \frac{V}{3\pi^2} k_F^3 \quad \text{(Total No. of states)} \qquad (15)$$

$$\Rightarrow k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} \qquad (16)$$

Hencem k_F depends only on particle concentration

FREE ELECTRON GAS IN THREE DIMENSIONS – Fermi Sphere

The occupied states are inside the Fermi sphere in *k*-space as shown below; the radius is Fermi wave number k_F



$$\varepsilon_F = \frac{\hbar^2}{2m} k_F^2$$

$$= \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$

The surface of the Fermi sphere represents the boundary between occupied & unoccupied k states at absolute zero for the free electron gas.

FREE ELECTRON GAS IN THREE DIMENSIONS

Calculated values of $\mathbf{k_F}$, $\mathbf{v_F}$ and $\mathbf{E_F}$ are given in Table 1 for selected metals.

Table 1 Calculated free electron Fermi surface parameters for metals at room temperature

(Except for Na, K, Rb, Cs at 5 K and Li at 78 K)

Valency	Metal	Electron concentration, in cm^{-3}	Radius[a] parameter r_s	Fermi wavevector, in cm^{-1}	Fermi velocity, in cm s^{-1}	Fermi energy, in eV	Fermi temperature $T_F = \epsilon_F/k_B$, in deg K
1	Li	4.70×10^{22}	3.25	1.11×10^8	1.29×10^8	4.72	5.48×10^4
	Na	2.65	3.93	0.92	1.07	3.23	3.75
	K	1.40	4.86	0.75	0.86	2.12	2.46
	Rb	1.15	5.20	0.70	0.81	1.85	2.15
	Cs	0.91	5.63	0.64	0.75	1.58	1.83
	Cu	8.45	2.67	1.36	1.57	7.00	8.12
	Ag	5.85	3.02	1.20	1.39	5.48	6.36
	Au	5.90	3.01	1.20	1.39	5.51	6.39
2	Be	24.2	1.88	1.93	2.23	14.14	16.41
	Mg	8.60	2.65	1.37	1.58	7.13	8.27
	Ca	4.60	3.27	1.11	1.28	4.68	5.43
	Sr	3.56	3.56	1.02	1.18	3.95	4.58
	Ba	3.20	3.69	0.98	1.13	3.65	4.24
	Zn	13.10	2.31	1.57	1.82	9.39	10.90
	Cd	9.28	2.59	1.40	1.62	7.46	8.66
3	Al	18.06	2.07	1.75	2.02	11.63	13.49
	Ga	15.30	2.19	1.65	1.91	10.35	12.01
	In	11.49	2.41	1.50	1.74	8.60	9.98
4	Pb	13.20	2.30	1.57	1.82	9.37	10.87
	Sn(w)	14.48	2.23	1.62	1.88	10.03	11.64

[a]The dimensionless radius parameter is defined as $r_s = r_0/a_H$, where a_H is the first Bohr radius and r_0 is the radius of a sphere that contains one electron.

FREE ELECTRON GAS IN THREE DIMENSIONS – Fermi Sphere

The number of orbitals per unit energy range: D(ϵ) = density of states.

$$N = \frac{V}{3\pi^2}\left(\frac{2m\varepsilon}{\hbar^2}\right)^{3/2} \qquad (19)$$

This leads to:

$$D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{V}{2\pi^2}.\left(\frac{2m}{\hbar^2}\right)^{3/2}.\varepsilon^{1/2} \quad (20)$$

Equation (19):

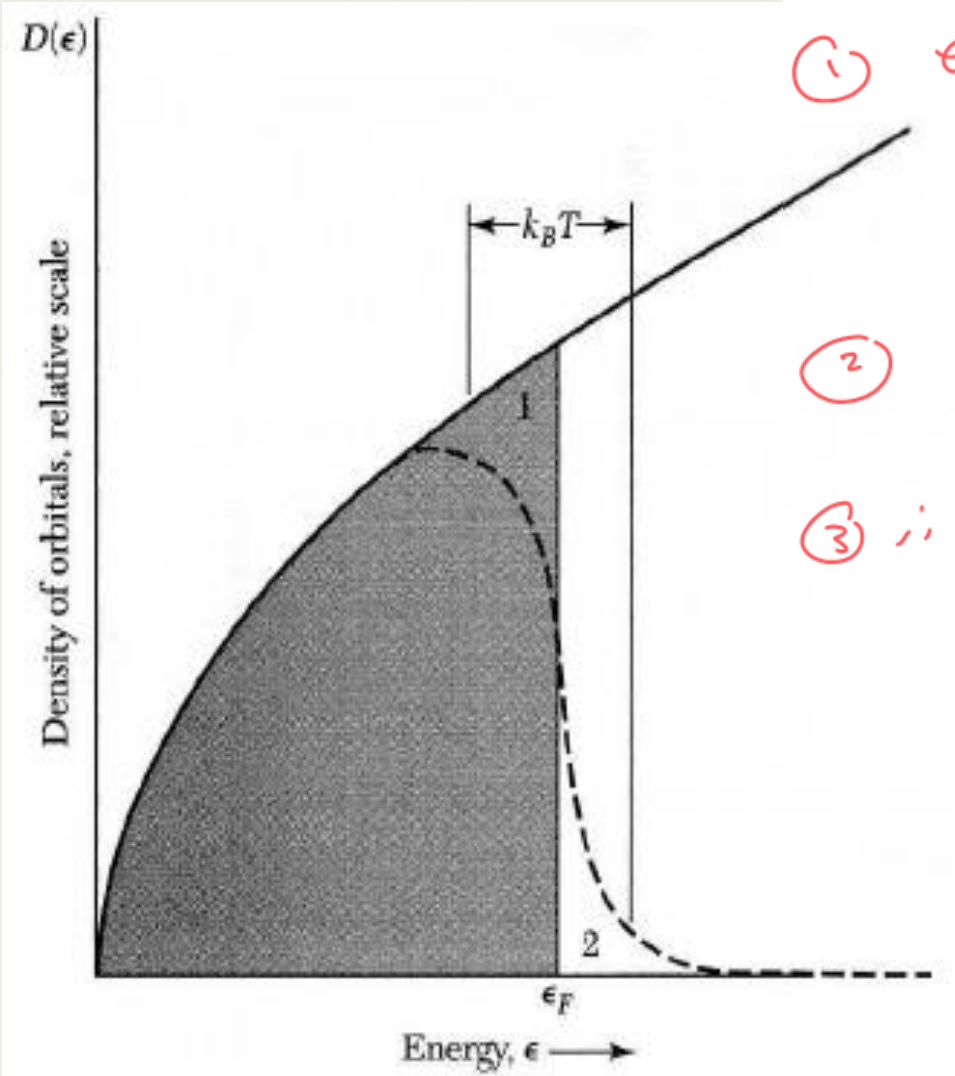
$$\ln N = \frac{3}{2}\ln \varepsilon + const.$$

Hence:

$$\frac{dN}{N} = \frac{3}{2}.\frac{d\varepsilon}{\varepsilon} \Rightarrow D(\varepsilon) = \frac{dN}{d\varepsilon} = \frac{3N}{2\varepsilon} \quad (21)$$

Within a factor of the order of unity, the number of orbitals per unit energy range at the Fermi energy is the total number of conduction electrons divided by the Fermi energy.

FREE ELECTRON GAS IN THREE DIMENSIONS



① electrons move from ① ⟶ ② when Thermally excited.

② only electrons within k_BT can do that.

③ ∴ only small fraction of electrons are thermally excited.

Figure 5 Density of single-particle states as a function of energy, for a free electron gas in three dimensions. The dashed curve represents the density $f(\epsilon, T)D(\epsilon)$ of filled orbitals at a finite temperature, but such that k_BT is small in comparison with ϵ_F. The shaded area represents the filled orbitals at absolute zero. The average energy is increased when the temperature is increased from 0 to T, for electrons are thermally excited from region 1 to region 2.

HEAT CAPACITY OF THE ELECTRON GAS

④ this small fraction of electrons dominate:

* thermal properties
* electrical ..
* magnetic ..

} of metals.

example. $C_e \propto T$

HEAT CAPACITY OF THE ELECTRON GAS

The question that caused the greatest difficulty in the early development of the electron theory of metals concerns the heat capacity of the conduction electrons. *Classical statistical mechanics predicts that a free particle should have a heat capacity of* $\frac{3}{2}k_B$ where k_B *is the Boltzmann constant.*

If N atoms each give one valence electron to the electron gas, and the electrons are freely mobile, then the electronic contribution to the heat capacity should be $\frac{3}{2}Nk_B$, just as for the atoms of a monatomic gas. *But the observed electronic contribution at room temperature is usually less than 0.01 of this value*.

When we heat the specimen from absolute zero, not every electron gains an energy $\sim k_BT$ as expected classically, *but only those electrons in orbitals within an energy range* k_BT *of the Fermi level are excited thermally*

HEAT CAPACITY OF THE ELECTRON GAS

If N is the total number of electrons, only a fraction of the order of T/T_F *can be excited thermally at temperature T.*
Each of these NT/T_F *electrons has a thermal energy of the order of* k_BT. The total electronic thermal kinetic energy *U is of the order of:*

$$U_{el} \approx N \frac{T}{T_F} k_B T \qquad (22)$$

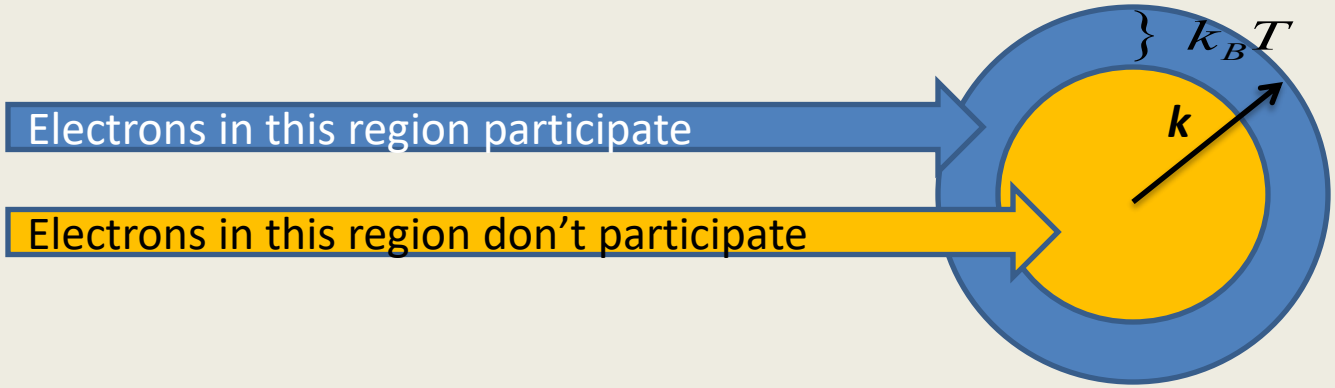
The electronic heat capacity is given by:

$$C_{el} = \frac{\partial U}{\partial T} \approx N k_B \frac{T}{T_F} \qquad (23)$$

C_{el} is directly proportional to *T, in agreement with the experiment*.
At room temperature C_{el} *is smaller* than the classical value $\frac{2}{3}Nk_B$ *by a factor of the order of 0.01 or less, for* $T_F \sim 5 \times 10^4$ *K.*
Hence: Classical value does not agree with experiment

HEAT CAPACITY OF THE ELECTRON GAS

- Classical Statistical Physics heat capacity of one electron: C= $\frac{2}{3}k_B$
- Classical Statistical Physics heat capacity of N electrons: C = $\frac{2}{3}Nk_B$
- Experimental result of C = 1% of this value only
- Error in Classical theory was due to considering all electrons that participate in conductivity as *Free electrons*.
- Fermi solved this puzzle: Only electrons that have energies of ~ k_BT below Fermi Surface or higher participate in Heat Capacity.
- Hence: only NT/T_F of electrons is important.
- All other electrons are not useful.



HEAT CAPACITY OF THE ELECTRON GAS

- ⇨ *All Free electrons participate in Electrical Conductivity*
- *But only T/T_F fraction participate in Heat Capacity*
- *This conclusion is a major indication of the success of the Fermi Free Electron Gas.*

HEAT CAPACITY OF THE ELECTRON GAS

- We want to derive an expression for the ***electronic heat capacity***:

The increase $\Delta U \equiv U(T) - U(0)$ in the total cnergy of a system of N electrons when heated from 0 to T is:

$$\Delta U \equiv \int_0^\infty \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon - \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon \qquad (24)$$

Total No of electrons inside Fermi sphere (or including outside where no electros):

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon \qquad (25)$$

we can write (then multply both sides by ε_F:)

$$\int_0^\infty d\varepsilon = \int_0^{\varepsilon_F} d\varepsilon + \int_{\varepsilon_F}^\infty d\varepsilon$$

$$\left(\int_0^{\varepsilon_F} + \int_{\varepsilon_F}^\infty \right) D(\varepsilon) f(\varepsilon) \varepsilon_F d\varepsilon = \int_0^{\varepsilon_F} \varepsilon_F D(\varepsilon) d\varepsilon \qquad (26)$$

HEAT CAPACITY OF THE ELECTRON GAS

(26) & (24): 6 terms:

$$\Delta U = \int_{\varepsilon_F}^{\infty} (\varepsilon - \varepsilon_F) D(\varepsilon) f(\varepsilon) d\varepsilon + \int_{0}^{\varepsilon_F} (\varepsilon_F - \varepsilon)\left[1 - f(\varepsilon)\right] D(\varepsilon) d\varepsilon \qquad (27)$$

The *first integral* on the right-hand side of (27) gives the energy needed to take electrons from ε_F to the orbitals of energy $\varepsilon > \varepsilon_F$, and the *second integral* gives the energy needed to bring the electrons to ε_F from orbitals below ε_F .

The product $f(\varepsilon)D(\varepsilon)d\varepsilon$ in the first integral of (27) is the number of electrons elevated to orbitals in the energy range $d\varepsilon$ at an energy ε. The factor $[1 - f(\varepsilon)]$ in the second integral is the probability that an electron has been removed from an orbital ε.

The heat capacity is found on differentiating ΔU with respect to T. The only temperature-dependent term in (27) is $f(\varepsilon)$

HEAT CAPACITY OF THE ELECTRON GAS

The heat capacity of the electron gas is found on differentiating *8U with* respect to *T.*

$$c_{el} = \frac{dU}{dT} = \int_0^\infty d\varepsilon[\varepsilon - \varepsilon_F]\frac{df}{dT}D(\varepsilon) \qquad (28)$$

$$\text{Fermi Dirac: } f(\varepsilon) = \frac{1}{e^{\left(\frac{\varepsilon-\mu}{K_B T}\right)}+1} \qquad (x\,1)$$

Let $D(\varepsilon) \rightarrow D(\varepsilon_F)$ in (28) and $\mu \rightarrow \varepsilon_F$ in Fermi Dirac Function:

$$\therefore c_{el} \cong D(\varepsilon_F)\int_0^\infty d\varepsilon[\varepsilon - \varepsilon_F]\frac{df}{dT} \qquad (29)$$

equation (x1) becomes:

$$f(\varepsilon) = \frac{1}{e^{\left(\frac{\varepsilon-\varepsilon_F}{K_B T}\right)}+1} \qquad (x\,2)$$

HEAT CAPACITY OF THE ELECTRON GAS

let $k_B T \rightarrow \tau$:

$$f(\varepsilon) = \frac{1}{e^{\left(\frac{\varepsilon-\varepsilon_F}{\tau}\right)}+1} \qquad (x\ 3)$$

we then differentiate w.r.t τ:

$$\frac{df(\varepsilon)}{d\tau} = \frac{\left[-\left(\frac{\varepsilon-\varepsilon_F}{\tau^2}\right)e^{\left(\frac{\varepsilon-\varepsilon_F}{\tau}\right)}(-1)\right]}{\left[e^{\left(\frac{\varepsilon-\varepsilon_F}{\tau}\right)}+1\right]^2} = \left(\frac{\varepsilon-\varepsilon_F}{\tau^2}\right)\frac{e^{\left(\frac{\varepsilon-\varepsilon_F}{\tau}\right)}}{\left[e^{\left(\frac{\varepsilon-\varepsilon_F}{\tau}\right)}+1\right]^2} \qquad (x\ 4)$$

$$\because \tau = k_B T \Rightarrow d\tau = k_B dT$$

$$\frac{1}{dT} = k_B \frac{1}{d\tau}$$

HEAT CAPACITY OF THE ELECTRON GAS

Rewriting Eq. (29):

$$c_{el} \cong k_B D(\varepsilon_F) \int_0^{\infty} d\varepsilon [\varepsilon - \varepsilon_F] \left(\frac{\varepsilon - \varepsilon_F}{\tau^2} \right) \frac{e^{\left(\frac{\varepsilon - \varepsilon_F}{\tau} \right)}}{\left[e^{\left(\frac{\varepsilon - \varepsilon_F}{\tau} \right)} + 1 \right]^2}$$

$$\Rightarrow c_{el} = k_B D(\varepsilon_F) \int_0^{\infty} d\varepsilon \left(\frac{\varepsilon - \varepsilon_F}{\tau} \right)^2 \frac{e^{\left(\frac{\varepsilon - \varepsilon_F}{\tau} \right)}}{\left[e^{\left(\frac{\varepsilon - \varepsilon_F}{\tau} \right)} + 1 \right]^2} \qquad (30)$$

$$let: x = \left(\frac{\varepsilon - \varepsilon_F}{\tau} \right) \Rightarrow dx = \frac{d\varepsilon}{\tau} = \frac{d\varepsilon}{k_B T} \Rightarrow d\varepsilon = k_B T dx$$

$\rightarrow$ we have $k_B T$ and k_B in (30) $\Rightarrow k_B^2 T$:

HEAT CAPACITY OF THE ELECTRON GAS

Hence, we have:

$$c_{el} = k_B{}^2 T D(\varepsilon_F) \int_{\frac{-\varepsilon_F}{\tau}}^{\infty} dx \; x^2 \frac{e^x}{\left[e^x + 1\right]^2} \qquad (31)$$

for the lower limit of integral:

$$x = \left(\frac{\varepsilon - \varepsilon_F}{\tau}\right) \Rightarrow x = \frac{0 - \varepsilon_F}{\tau} = \frac{-\varepsilon_F}{\tau} \quad [\text{lower limit in (30)} = \varepsilon = 0]$$

as $T \rightarrow 0$, $x \rightarrow -\infty$

Using table of Integrals:

$$\int_{-\infty}^{\infty} dx \; x^2 \frac{e^x}{\left[e^x + 1\right]^2} = \frac{\pi^2}{3} \qquad (32)$$

(32) in (31): $c_{el} = \frac{\pi^2}{3} k_B{}^2 T D(\varepsilon_F)$ (33)

HEAT CAPACITY OF THE ELECTRON GAS

From eq. (21) above, we have:

$$D(\varepsilon_F) = \frac{3N}{2\varepsilon_F}$$

$$\therefore D(\varepsilon_F) = \frac{3}{2}\frac{N}{k_B T_F}$$

with: $T_F = \frac{\varepsilon_F}{k_B}$, (33) $\rightarrow$:

$$C_{el} = \frac{1}{2}\pi^2 {k_B}^2 \frac{T}{T_F} \qquad (36)$$

$$T_F = Const.$$

Recall that although T_F *is called the Fermi temperature, it is not the electron* temperature, but only a convenient reference notation>
We shall compare this result with experimental data.

Experimental Heat Capacity of Metals:

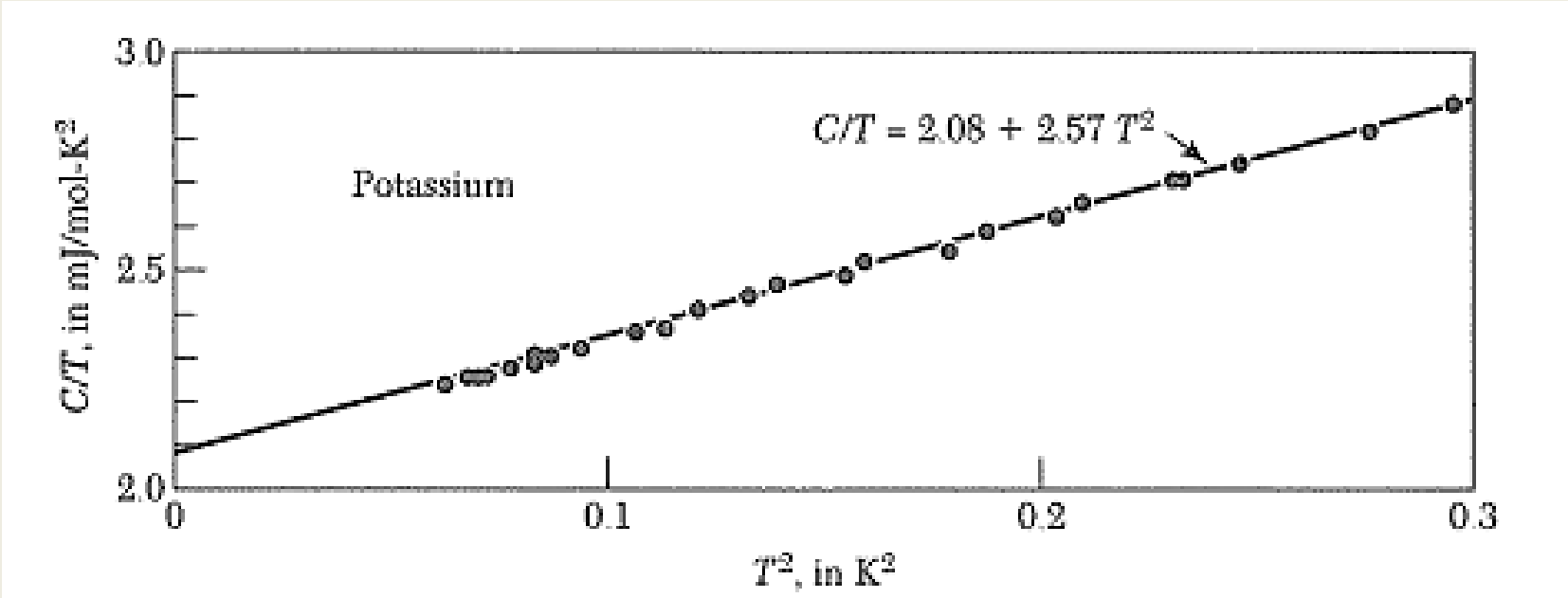
At temperatures much below both the Debye temperature and the Fermi temperature, the heat capacity of metals may be written as the sum of electron and phonon contributions:

$$C = \gamma T + AT^3$$

where γ and A are constants characteristic of the material.

$\therefore$ **Electronic part is Linear to *T*** ***(Agree with Fermi Free Electron Model)***

While Phononic part is αT^3 (Agree with Debye model)



Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 03

Review of free electron theory

Prof. Nasser S. Alzayed

Introduction

- The free electron model of metals gives us good insight into the heat capacity, thermal conductivity, electrical conductivity, magnetic susceptibility, and electrodynamics of metals.
- But the model fails to help us with other large questions:
  - *the distinction between metals, semimetals, semiconductors, and Insulators*
  - *the occurrence of positive values of the Hall coefficient*
  - *the relation of conduction electrons in the metal to the valence electrons of free Atoms*
  - *many transport properties, particularly magneto transport*

- Hence, we need to modify Fermi Electron Model to be able to answer these puzzles. ***We will see that little modification is just adequate.***

Introduction

- The difference between a good conductor and a good insulator is striking. The electrical resistivity of a pure metal may be as low as 10^{-10} Ω.cm at 1 K, apart from the possibility of superconductivity.
- The resistivity of a good insulator may be as high as 10^{22} Ω.cm.
- This range of 10^{32} may be the widest of any common physical property of solids.

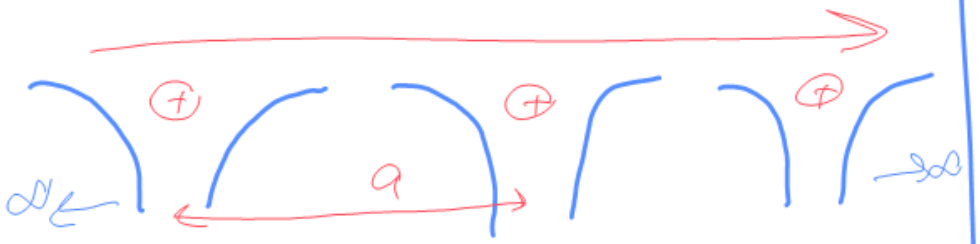
- Every solid contains electrons. The important question for electrical conductivity is how the electrons respond to an applied electric field.
- electrons in crystals are arranged in energy bands.
- Bands are separated by band gaps (Forbidden Regions)
- Source of bands come from the interaction of the conduction electron waves with the ion cores of the crystal

In the Free electron Picture

⇒ no Interaction Between electrons and Ions.

⇒ V = Constant (Potential)

In Reality (nearly Free-E. M)

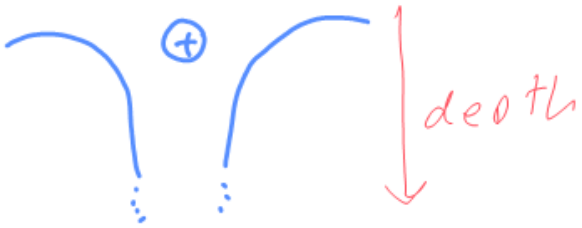


Potential is not Constant

V is Periodic

∴ $V(x+a) = V(x)$

depth of V ↓ depends on the Ions



Periodicity of V

⇒ Periodicity in other Lattice (crystal) properties

e.g.: ρ density

n no. of electrons

Q charge

Also; current-density or Probability & anything is the Periodic in nature

$\Rightarrow |\psi(x)|^2 = |\psi(x+a)|^2$

for a free electron:

$\psi(x) = e^{ikx}$ ⟿

for a nearly free electron

OR: if $N(x)$ is Periodic

$\Rightarrow \psi(x+a) = e^{i\phi(a)}\psi(x)$ ①

Where: $|e^{i\phi(a)}|^2 = 1$

① $\Rightarrow \psi(x+2a) = e^{i\phi(2a)}\psi(x)$

$= e^{2i\phi(a)}\psi(x)$

let $\phi(a) = ka$ $\quad \phi(2a) = 2\phi(a)$

$\therefore \psi(x+a) = e^{ika}\psi(x)$ ... ②

$\Rightarrow \psi(x) = e^{ikx}u_k(x)$ ... ③

Where $u_k(x)$ is periodic function that has same Periodicity of lattice.

③ $\Rightarrow$

$\psi_k(x) = e^{ikx}u_k(x)$ ⁂ ④

Bloch's Theorem

Bloch Theorm says:

if $V(x+a) = V(x)$ Periodic Potential

$$\Rightarrow \psi_k(x) = e^{ikx} u_k(x) \quad \} \sim\sim (5)$$

where: $u_k(x+a) = u_k(x)$

in 3-D:

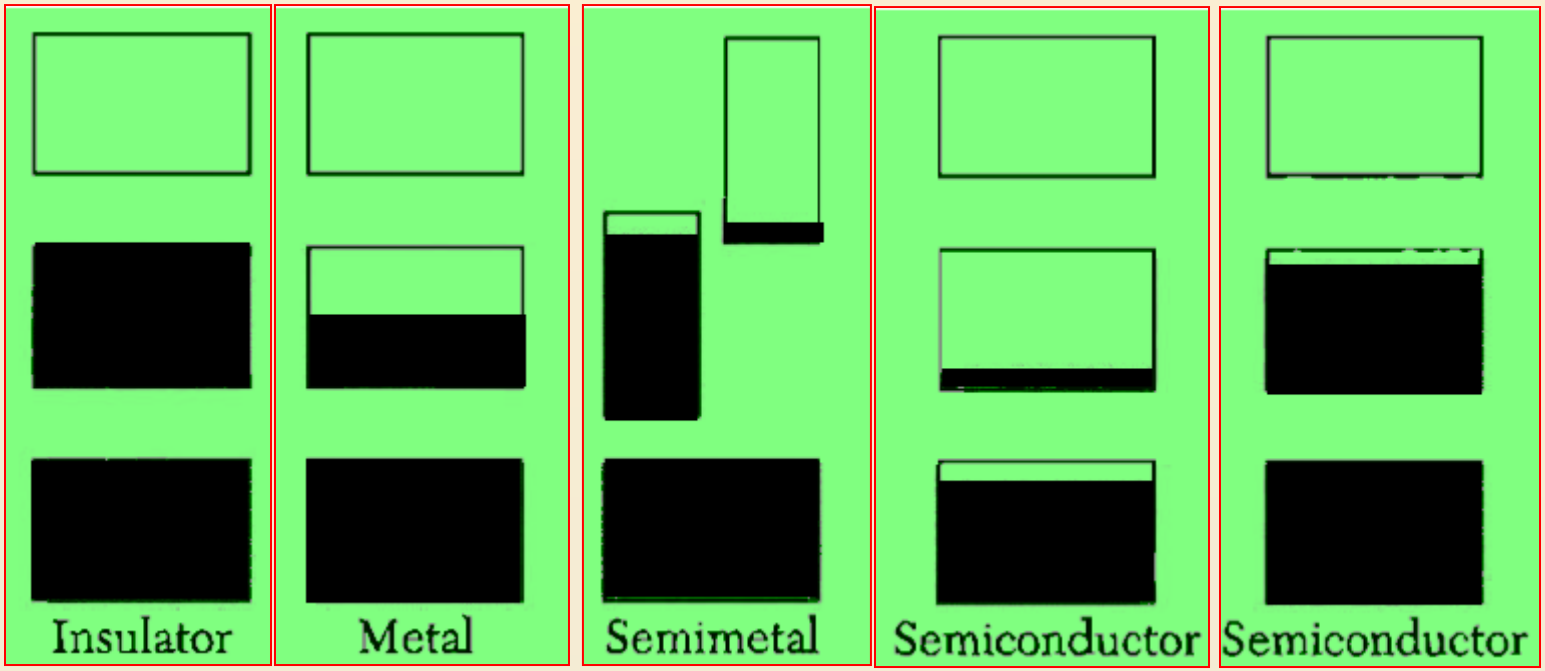
$$\psi_{\vec{k}}(\bar{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\bar{k}}(\bar{r}) \quad \} \sim\sim (6)$$

where $u_{\bar{k}}(\bar{r}+\bar{R}) = u_{\bar{k}}(\bar{r})$

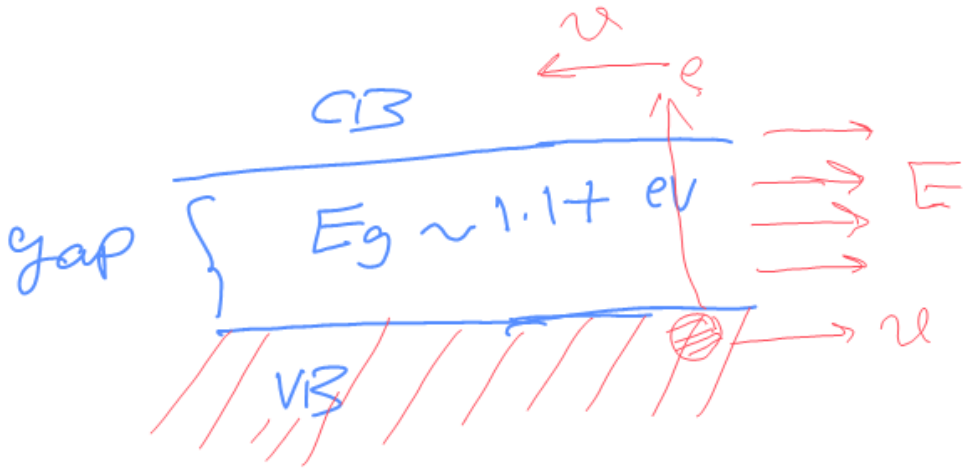
Chapter 7: Energy Bands

Insulators, Metals and Semiconductors

- **Insulator**: if the allowed energy bands are either filled or empty, for then no electrons can move in an electric field.
- **Metal**: if one or more bands are partly filled.
- **Semiconductor or a semimetal**: if one or two bands are slightly filled or slightly empty.



Semiconductors:

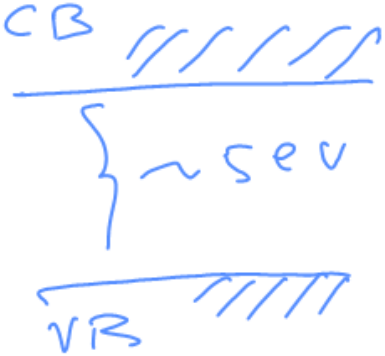


Thermal Energy ~ $K_B T$
~ 25 meV

it is not enough for ↑ statistically only very small No. of e can make it.

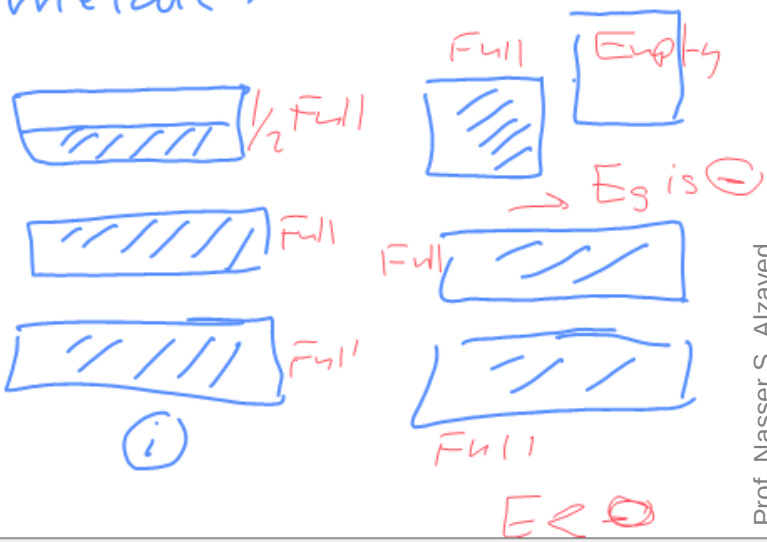
A lot of e
A lot of Empty states

Insulators:



no Temp } Can elevate elec ↑
nor E }

metals:



For the semi metal
$E_g \sim 0$ but the

(1) In Insulators: all electrons are strongly held to their parent atom.

(2) In semiconductors: Some electrons at the T0 orbitals can have some energy to participate in Conductance

(3) in metals: lots of electrons move Between atoms (They are not bound to their parent atoms)

Chapter 7: Energy Bands

Modifications needed for Free Electron Model

- To modify the Free Electron Model; we will assume that electron is not totally free. It must respect the periodicity of the crystal.
- This will directly lead to the important result: **band gap**.
- Also; we introduce the concept of effective mass of electron *m* which may be larger or* smaller than the free electron mass, or may even be negative.
- Negative and Positive effective mass can directly explain for +tive Hall coefficient.

$$R_H = -\frac{eB\tau E_x / mc}{ne^2\tau E_x / m} = -\frac{1}{nec}$$

- This model answers almost all the qualitative questions about the behavior of electrons in metals.

Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL (1-D)

- On the free electron model the allowed energy values are distributed essentially continuously from zero to infinity

$$\varepsilon_k = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \qquad (1)$$

From boundary conditions over a cube of side L :

$$k_x, k_y, k_z = 0; \pm\frac{2\pi}{L}; \pm\frac{4\pi}{L}; \ldots\ldots \qquad (2)$$

wavefunctions are of the form : $\psi_k(\mathrm{r}) = e^{i\mathrm{k}.\mathrm{r}}$ (3)

- The band structure of a crystal can often be explained by the nearly free electron model for which the band electrons are treated as perturbed only weakly by the periodic potential of the ion cores. This model answers almost all the qualitative questions about the behavior of electrons in metals.

Chapter 7: Energy Bands

Bragg Reflections

- Bragg reflection of electron waves in crystals is the cause of energy gaps. *At Bragg reflection wavelike solutions of the Schrodinger equation do not exist, as in Fig. 2 (Forbidden Region)*

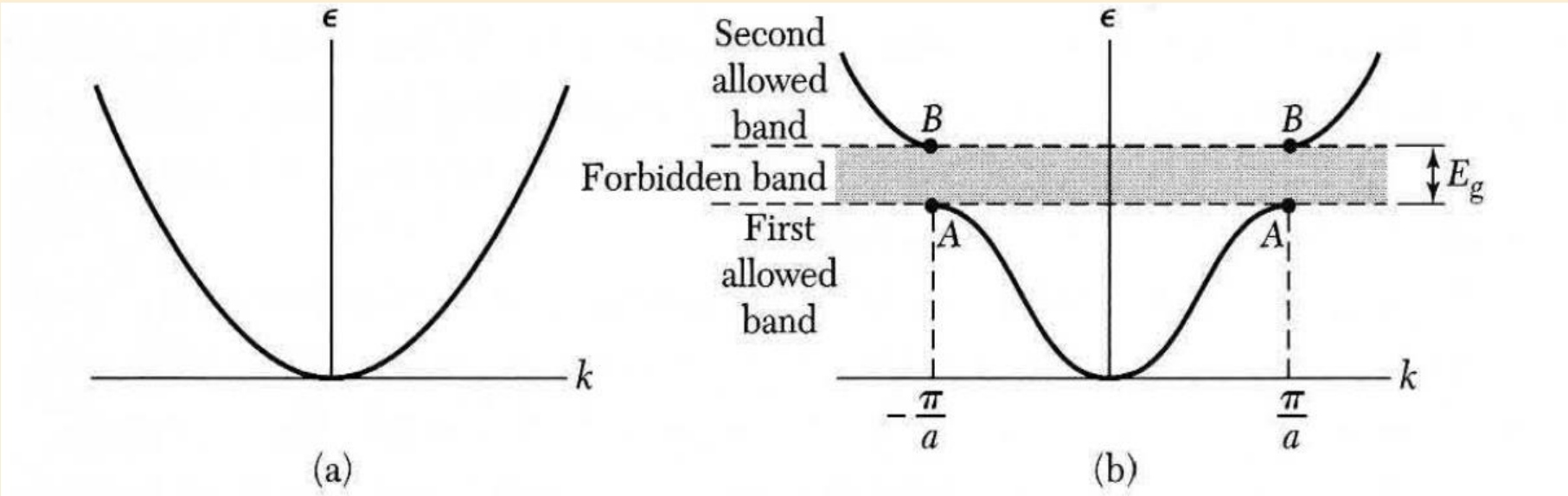


Figure 2 (a) Plot of energy ϵ versus wavevector k for a free electron. (b) Plot of energy versus wavevector for an electron in a monatomic linear lattice of lattice constant a. The energy gap E_g shown is associated with the first Bragg reflection at $k = \pm\pi/a$; other gaps are found at higher energies at $\pm n\pi/a$, for integral values of n.

Chapter 7: Energy Bands

Bragg Reflections

(a) for Free electron:

$$\epsilon(k) = \frac{\hbar^2 k^2}{2m}$$ exponential

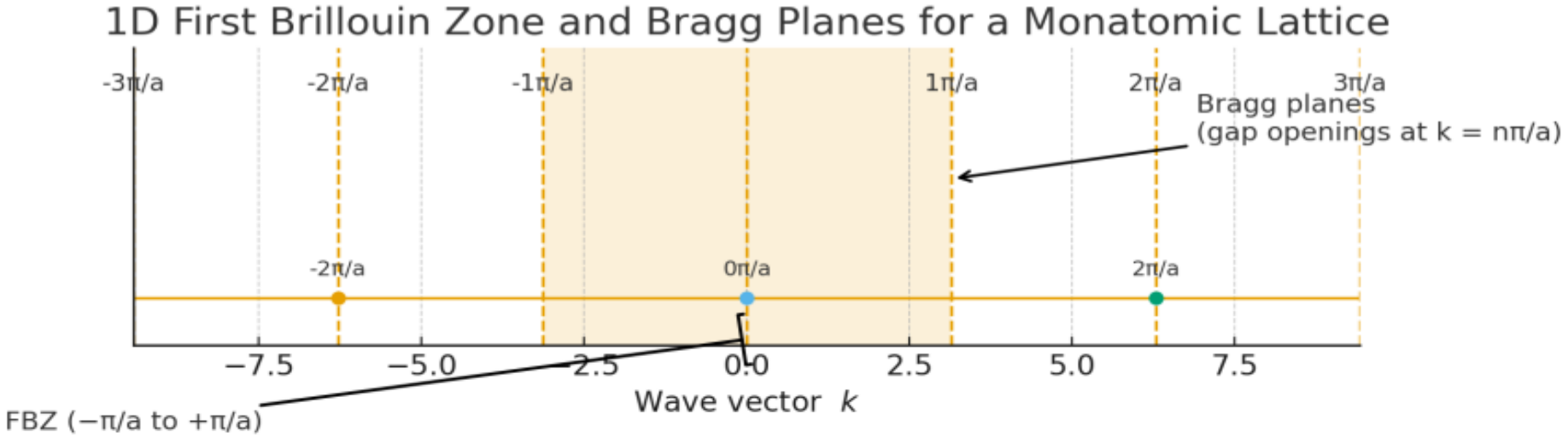
* Lattic effect: absent

$\Rightarrow$ no gaps

(b): for electrons in weak potential (Periodic)

(i) First Brillouin Zone $-\frac{\pi}{a} \rightarrow +\frac{\pi}{a}$ full of e's.

note: crystal is periodic $\rightarrow$ E(k) " " } Period $= \frac{2\pi}{a}$



Bragg Condition: $|k\rangle$ states of the electron

and $|k-G\rangle$ " " " "

are degenerate at $k = \pm \frac{n\pi}{a}$

Bragg Planes

→ " Reflections

→ split of Energy:

Chapter 7: Energy Bands

Bragg Reflections

$$E_{\pm}(k) = E_0\left(\frac{G}{2}\right) \pm \sqrt{\left(\frac{\hbar^2 G}{2m}g\right)^2 + |U_G|^2}$$

from 674.

$$\rightarrow E_g = 2|U_G|.$$

Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL

- Fig. 2, in (a) for entirely free electrons and in (b) for electrons that are nearly free, but with an energy gap at $k = \pm\pi/a$. *The Bragg* condition $(\mathbf{k} + \mathbf{G})^2 = \mathbf{k}^2$ for diffraction of a wave of wavevector **k** becomes in one dimension:

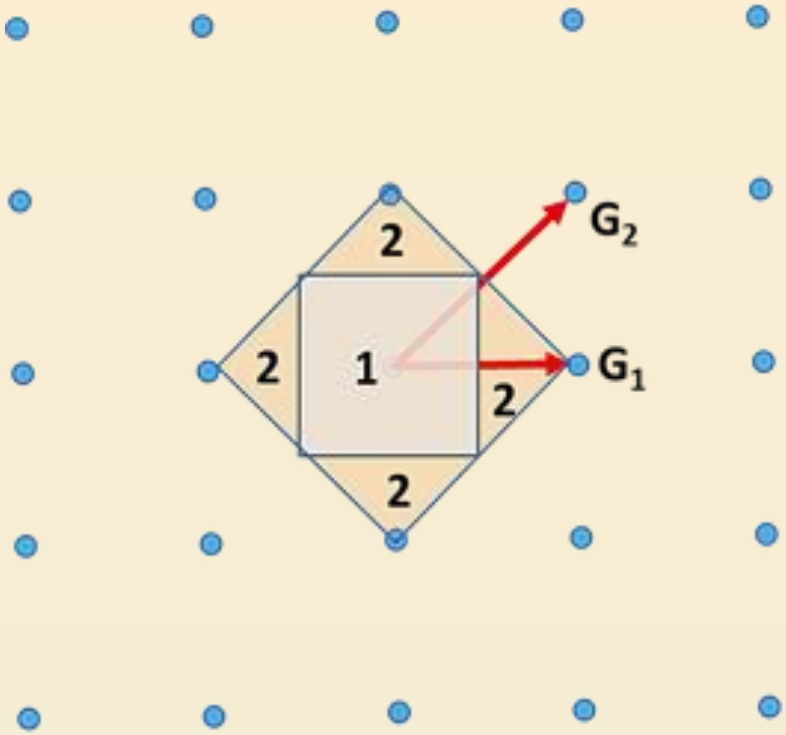
$$k = \pm\frac{1}{2}G = \pm\frac{n\pi}{a} \quad \text{(in 1-D)} \qquad (4)$$

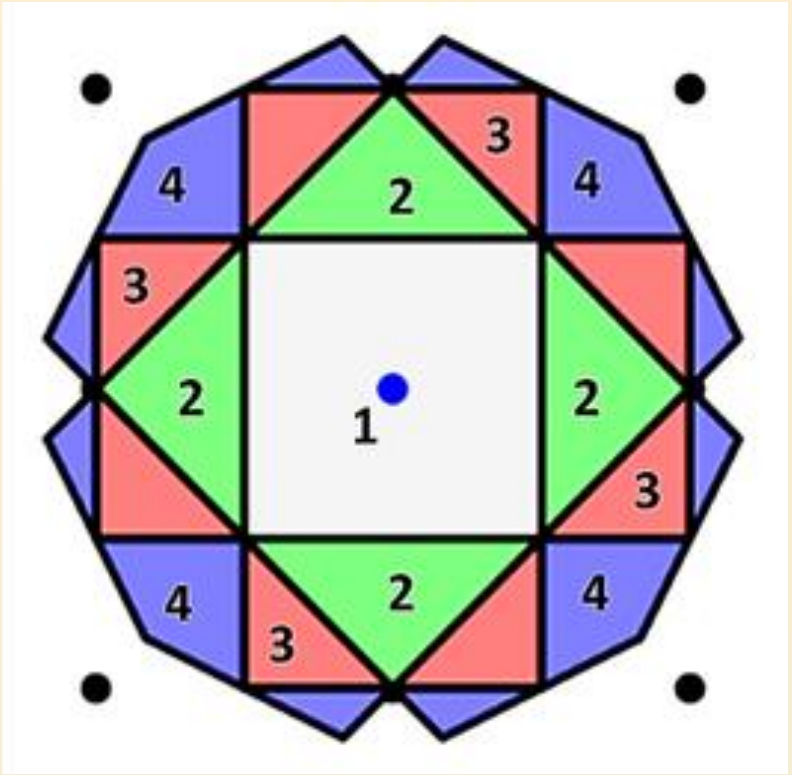
- where $G = 2\pi n/a$ is a reciprocal lattice vector and n is an integer. The first reflections and the first energy gap occur at $k = \pm\pi/a$. The region in k space between $-\pi/a$ and π/a is the first **Brillouin zone of this lattice.** Other energy gaps occur for other values of the integer n.
- 2nd **Brillouin zone** is located between: $\pm 2\pi/a$ *and so on.*

Chapter 7: Energy Bands

Bragg Reflections lead to Band Gap

- ❑ Electron waves will move only inside the B.Z.
- ❑ All waves stop and Reflect at the borders of the B.Z. (From forbidden regions).





Chapter 7: Energy Bands

Bragg Reflections lead to Band Gap

- we will have 3 different types of Waves:
  - Moving to the Right → (will be reflected to the left from *π/a)*
  - Moving to the Left ← (will be reflected to the right from *-π/a)*
  - Standing waves (time independent. Do not move).
- Consequently: Standing waves can be used to describe the case.
- We can form two different standing waves from the two traveling waves:

$$e^{+i\pi x/a} = \cos(\pi x/a) + i\sin(\pi x/a) \rightarrow$$

$$e^{-i\pi x/a} = \cos(\pi x/a) - i\sin(\pi x/a) \leftarrow$$

or:

$$e^{\pm i\pi x/a} = \cos(\pi x/a) \pm i\sin(\pi x/a)$$

Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL

- Hence; we have 2 standing waves: Even (+) and odd (-):

$$\left.\begin{aligned}\psi(+) &= e^{+i\pi x/a} + e^{-i\pi x/a} = 2\cos(\pi x/a)\\ \psi(-) &= e^{+i\pi x/a} - e^{-i\pi x/a} = 2i\sin(\pi x/a)\end{aligned}\right\} \quad (5)$$

- In one dimension; solution to the Schrödinger equation at the boundaries of Brillouin Zone are standing waves.

Origin of the Energy Gap

- The two standing waves Ψ(+) and Ψ(-) pile up electrons at different regions, and therefore the two waves have different values of the potential energy in the field of the ions of the lattice. *This is the origin of the energy gap*.
- Waves traveling in different directions have different energies, leading to energy gap.

Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL

- Let us consider the probability density ρ for both + and – (even and odd) functions.
- ρ is expressed as: $\rho=\psi^*\psi=|\psi|^2$
- For pure travelling wave: $\psi = e^{ikx}$ ➔ $\rho=\psi^*\psi=|\psi|^2 = e^{-ikx}\, e^{ikx} =1$
- This mean that probability of finding electron = 100% (ρ = const.)
- But in our case (Nearly Free Electron), ρ is not Const.

$$\rho(+) = |\psi(+)|^2 \, \alpha \cos^2(\frac{\pi x}{a})$$

$$\rho(-) = |\psi(-)|^2 \, \alpha \sin^2(\frac{\pi x}{a})$$

- Accordingly; for even functions (+): ρ = 1 only at specific values of x; namely at: x =0, a, 2a, ….
- For odd functions (-): ρ = 1 only at: x = 1/2 a, 3/2 a, 5/2 a ….

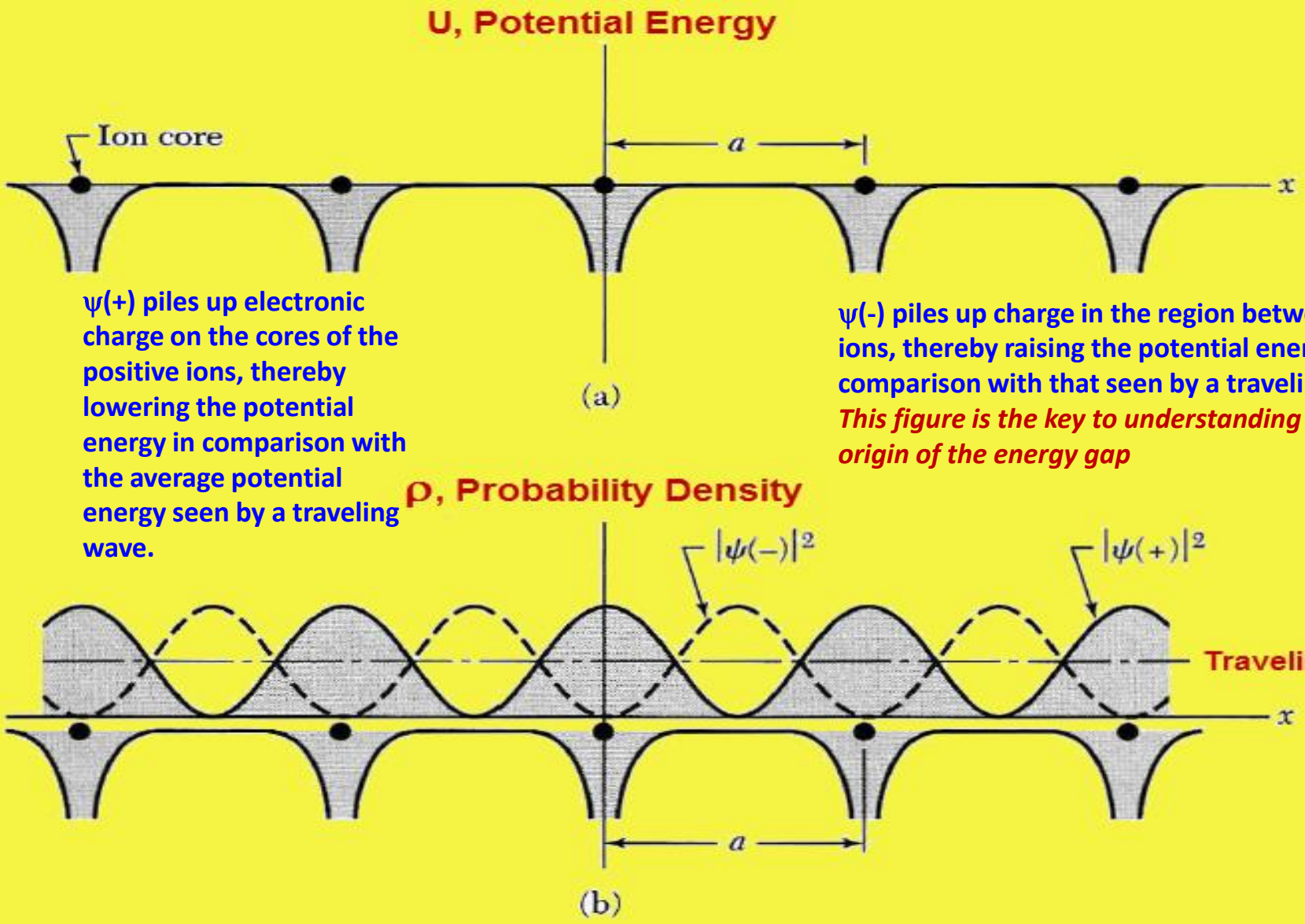
Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL

- Hence; even function probability has its values max (=1) when the Pot. Energy is at lowest values (just at the Ions).
- On the other hand; odd function probability has its values max (=1) in the middle locations between the Ions.
- In other words: (+) function piles up electrons near the Ions while the (-) function piles up electrons in places mid-distance from two ions.
- This leads to an energy gap between the two pools of electrons.
- If we calculate the expectation values (average energy) in these three cases: + , -, and Free electron (travelling wave): we have:
- that of $\rho(+)$ is lower than that of Free Electron
- that of $\rho(-)$ is above that of Free Electron.
- Result is: $\mathbf{E_g}$ difference in energy between the $\rho(+)$ and $\rho(-)$
- *This is the origin of the Band Gap*.

Chapter 7: Energy Bands

NEARLY FREE ELECTRON MODEL



ψ(+) piles up electronic charge on the cores of the positive ions, thereby lowering the potential energy in comparison with the average potential energy seen by a traveling wave.

ψ(-) piles up charge in the region between the ions, thereby raising the potential energy in comparison with that seen by a traveling wave. *This figure is the key to understanding the origin of the energy gap*

Chapter 7: Energy Bands

Magnitude of the Energy Gap

- Let us suppose that the potential energy of an electron in the crystal at point *x is:*

$$U(x) = U\cos\left(\frac{2\pi}{a}x\right) \tag{6}$$

The first-order energy difference between the two standing wave states is :

$$E_g = \int_0^1 U(x)\left[|\psi(+)|^2 - |\psi(-)|^2\right]dx$$

$$= \int U\cos\left(\frac{2\pi}{a}x\right)\left[\cos^2\frac{\pi x}{a} - \sin^2\frac{\pi x}{a}\right]dx$$

$$= U \tag{7}$$

- We see that the gap is equal to the Fourier component of the crystal potential.

eq. ⑥ : we have a weak periodic potential $U(x)$:

$U(x)$ at first reciprocal vector $\bar{G} = \frac{2\pi}{a}$

i.e.:

$$U(x) = U\cos Gx$$

$$= U\cos\left(\frac{2\pi}{a}x\right) \quad \cdots\cdots ①$$

at the FBZ Boundary $k = \pm\frac{G}{2} = \pm\frac{\pi}{a}$:

we have two standing waves:

$$\psi_+(x) \propto \cos\left(\frac{\pi}{a}x\right) \qquad \psi_-(x) \propto \sin\left(\frac{\pi}{a}x\right) \quad ②$$

Using first-order Perturbation Theory

$$\Rightarrow \delta E_{\pm} = \langle \psi_{\pm} | U | \psi_{\pm} \rangle \quad - - - \quad (3)$$

$\therefore$ the gap is

$$E_g = \delta E_+ - \delta E_-$$

$$= \int U(x) \left[|\psi_+|^2 - |\psi_-|^2 \right] dx \qquad (4)$$

$$|\psi_+|^2 - |\psi_-|^2 = \cos^2\theta - \sin^2\theta \cos 2\theta$$

$$= \cos 2Gx$$

$$\therefore E_g = U \int \cos Gx \cdot \cos Gx \, dx$$

$$= U \int_{cell} \cos^2 Gx \, dx$$

$$\therefore E_g = U \int_0^a \cos^2 Gx \, dx \quad \text{---} \quad (5)$$

let $\cos^2 Gx = \frac{1}{2}(1 + \cos 2Gx)$

$$\rightarrow \int_0^a \cos^2 Gx \, dx = \frac{a}{2} \quad \text{----} \quad (6)$$

But wave functions need to normalized.

$$\psi_{\pm}(x) = \sqrt{\frac{2}{a}} \begin{cases} \cos \frac{Gx}{2} \\ \sin \frac{Gx}{2} \end{cases} \quad \text{----} \quad (7)$$

$$\Rightarrow |\psi_+|^2 - |\psi_-|^2 = \frac{2}{a} \cos Gx \quad \text{---} \quad (8)$$

$\therefore$ (11) becomes:

$$E_g = U \int_0^a \cos Gx \cdot \frac{2}{a} \cos Gx \, dx$$

$$= \frac{2U}{a} \int_0^a \cos^2 Gx \, dx = \frac{2U}{a} \cdot \frac{a}{2} = U$$

$$\therefore \boxed{E_g = U} \quad \# \quad \text{----} \quad (9)$$

Please note: $U(x)$ is the gap = amplitude of Fourier component

But in Fourier notation: $U(x) = \sum_G U_G e^{iGx}$ (10)

$\therefore U(x) = U \cos Gx \rightarrow U_G = \frac{1}{2} U$ ---- (11)

How?

$\therefore \cos Gx = \frac{1}{2}\left[e^{iGx} + e^{-iGx}\right]$

$$\therefore E_S = U = 2|U_G| \quad \# \quad -- \quad (12)$$

this Result is same we have in 674

//

;; The Band Gap at the Bragg plane is set by the magnetude of the Fourier Componeat of the Crystal potential at that Reciprocal vector //

Chapter 7: Energy Bands

BLOCH FUNCTIONS

- F. Bloch proved the important theorem that the solutions of the Schrodinger equation for a periodic potential must be of a special form:

$$\psi_k(r) = u_k(r) e^{ik.r} \qquad (8)$$

- $u_k(r)$ *has same periodicity of the crystal with* $u_k(r) = u_k(r + T)$
- T is the translation vector of the lattice in normal space.
- Eq. (8) means that:

*The eigenfunctions of the wave equation for a periodic potential are the product of a plane wave exp(i**k.r**) times a function $u_k(r)$ with the periodicity of the crystal lattice.*

- Bloch functions can he assembled into wave packets to represent electrons that propagate freely through the potential field of the ion cores.

Because of Periodicity:

$$\psi(x+a) = \psi(x) = c\psi(x) \quad (1)$$

with condition: $|c| = 1$

$$\rightarrow \psi(x+2a) = c^2\psi(x) \quad (2)$$

- - - - - - - -

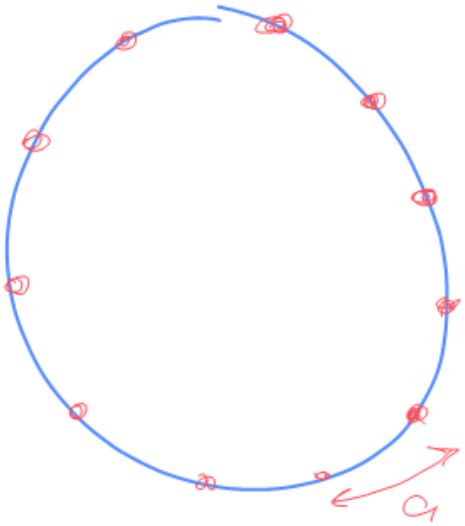
$$\rightarrow \psi(x+Na) = c^N\psi(x) = \psi(x) \quad (3)$$

one full cycle takes us back to the Beginning.

with $c^N = 1 \equiv \sqrt[N]{1}$

N is Integer

total Length of Circle = Na



We can select $C = e^{2i\pi \frac{S}{N}}$ $\quad S = 0, 1, 2, 3 \cdots$

$$\Rightarrow \psi(x+a) = e^{2i\pi \frac{S}{N}} \psi(x)$$

$\Rightarrow$ the validity of eq (B) B.T:

$$\psi_{\bar{k}}(\bar{r}) = u_{\bar{k}}(\bar{r})\, e^{i\bar{k}\cdot\bar{r}}$$

Chapter 7: Energy Bands

BLOCH FUNCTIONS

- We consider *N identical lattice points on a ring of length Na. The potential energy is* periodic in *a, with U(x) = U(x + sa), where s is an integer.*
- symmetry of the ring leads to:

$$\psi(x+a) = C\psi(x) \tag{8}$$

where C is a constant. Then, on going once around the ring:

$$\psi(x+Na) = \psi(x) = C^N \psi(x)$$

bccause $\psi(x)$ must be single-valued.

It follows that C is one of the N roots of unity, or:

$$C = e^{i2\pi s/N} \qquad s = 0, 1, 2, \ldots, N-1 \tag{9}$$

satisfies (8), provided that $U_k(x)$ has the periodicity a, so that $U_k(x) = U_k(x+a)$.

This is the Bloch result (7).

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 04

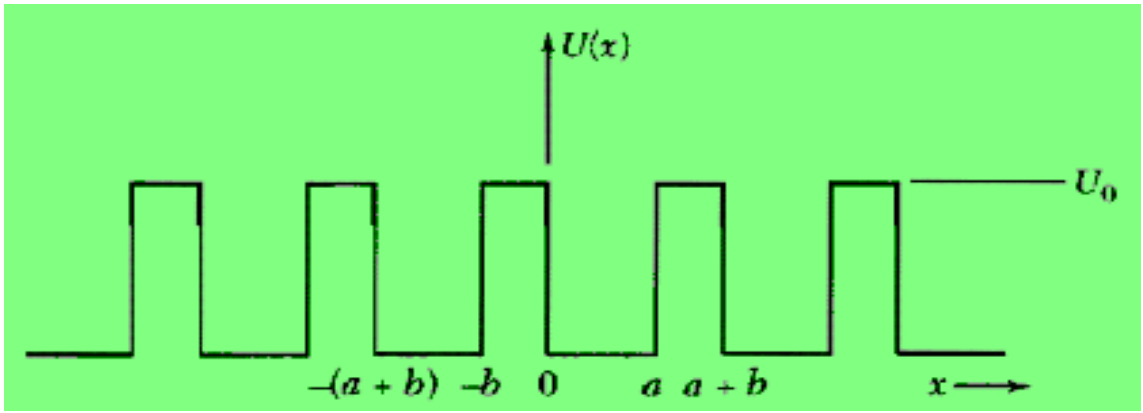
Review of free electron theory

Prof. Nasser S. Alzayed

Chapter 7: Energy Bands

Kronig-Penney Model

- This model solves for periodic potential in a form of a square-well array:



- Schrodinger wave equation for this potential can take the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=\varepsilon\psi \qquad (11)$$

where *U(x)* is the potential energy and ε is the energy eigenvalue.
We have 2 regions: $0 < x < a$ $(U = 0)$ *and* $-b < x < 0$ $(U \neq 0)$

in our Nearly free Electron model NFM we mentioned that $V \neq 0$ in lattice But did not define V.

① Kroig-Penney Model 

② Dirac Comb (δ-function) Model 

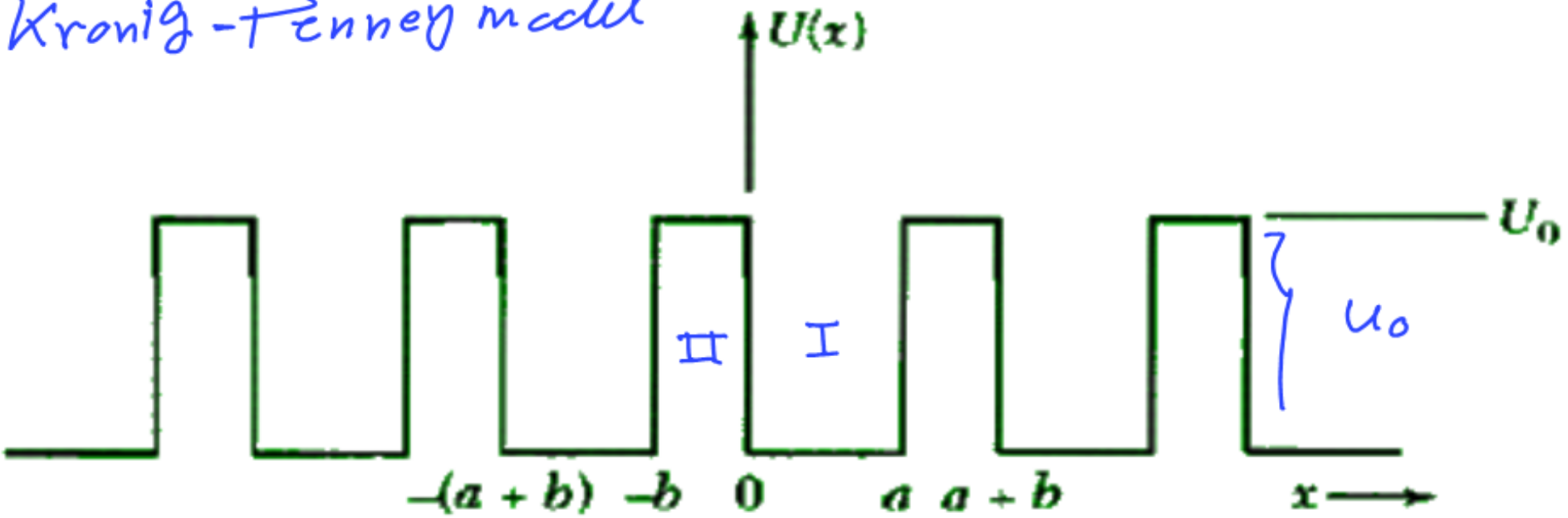
③ Pseudo potential : average Potential

④ Muffin-Tin Potential: potential is spherically symmetric inside non-overlapping spheres and constant in Between

⑤ Plane wave expansion / Fourier Series Potential $V(\vec{r}) \rightarrow$ Fourier sum of Reciprocal Lattice vector.

⑥ Augmented Plane Wave (APW) method.

Kronig-Penney model



we will use Schrödinger Wave Equation in 1-D :

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\,\psi = \epsilon\psi \qquad \text{-----(1)}$$

we have 2 Regions :

$$\left.\begin{array}{lll} \text{I} & 0 < x < a & U = 0 \\ \text{II} & -b < x < 0 & U \neq 0 \end{array}\right\} \text{-----(2)}$$

for Region I:

$$\textcircled{1} \rightarrow -\frac{\hbar^2}{2m}\psi'' + 0 = E\psi \quad \text{-----} \quad \textcircled{3}$$

$$\Rightarrow \psi'' + \frac{2mE}{\hbar^2}\psi = 0 \quad \text{----} \quad \textcircled{3}$$

$$\rightarrow \psi'' - k^2\psi = 0 \quad \text{----} \quad \textcircled{4}$$

$$\text{with } k^2 = \frac{2mE}{\hbar^2} \quad \text{-----} \quad \textcircled{5}$$

with solution of a free electron wave traveling $\rightarrow$ or $\leftarrow$

$$\psi = Ae^{ikx} + Be^{-ikx} \quad \text{-----} \quad \textcircled{6}$$

note that (6) is a combination of two waves one is traveling to $\rightarrow$ and " " $\rightarrow$ " $\leftarrow$

note that (5) $\Rightarrow$ $E = \frac{\hbar^2 k^2}{2m}$ ---- (7)

---

for Region II: $U \neq 0 \Rightarrow$ damping effect.

in this case (1): $\rightarrow$

$$-\frac{\hbar^2}{2m}\psi'' + U_0\psi = E\psi \quad \text{---------} \quad (8)$$

$$\rightarrow \quad \psi'' - \frac{2m(U_0 - E)}{\hbar^2}\psi = 0 \quad \text{-----} \quad (9)$$

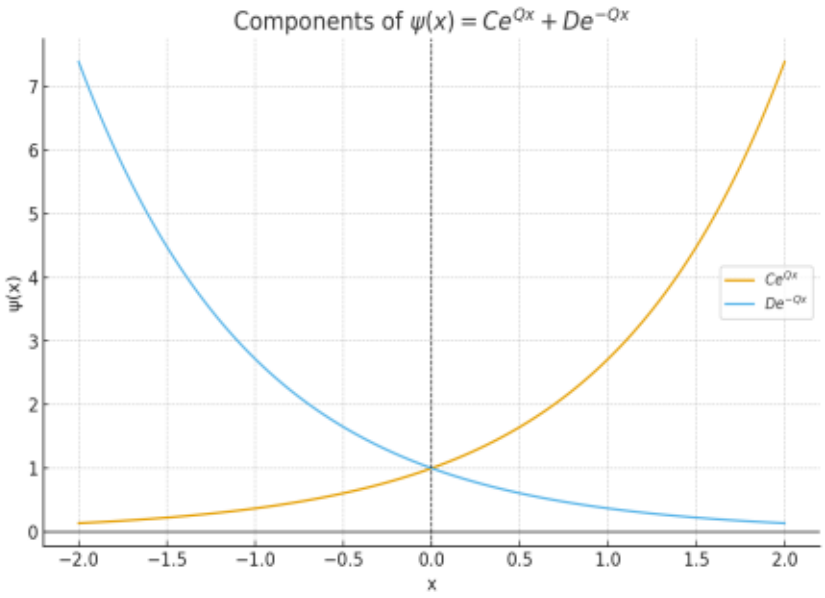
$$\text{OR} \quad \psi'' + Q^2\psi = 0 \quad \text{---} \quad (10)$$

solution of (10) is of the form:

$$\psi = C e^{Qx} + D e^{-Qx} \quad \text{---} \quad (11)$$

(a) $\rightarrow$: $Q^2 = \dfrac{2m(U_0 - E)}{\hbar^2}$

$\rightarrow E = U_0 - \dfrac{\hbar^2 Q^2}{2m}$ -- (12)



we now turn to Bloch's Theorem to find Energy.

We have:

$$\psi = \begin{cases} A e^{ikx} + B e^{-ikx} & (6)\ \text{I} \\ C e^{Qx} + D e^{-Qx} & (11)\ \text{II} \end{cases} \quad \left.\begin{matrix} \psi_I \\ \cdots (12) \\ \psi_{II} \end{matrix}\right\}$$

Now: applying Boundary condition for ψ and ψ' and using eq (6) and (11)..

at $x = 0$

$(6) \rightarrow A + B$

$(11) \rightarrow C + D$

$\therefore \quad A + B = C + D \qquad \cdots\cdots (13)$

from Continuity

ψ' at 0 :

$(6) \rightarrow iK(A - B)$

$(11) \rightarrow Q(C - D)$

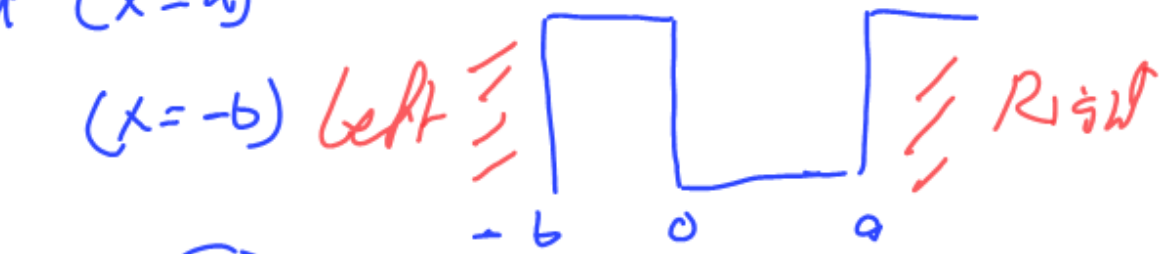
$\therefore \quad iK(A-B) = Q(C-D) \quad ---(14)$

from continuity

Now: Bloch Theorem says:

values at the Right $(x=a)$

$=$ " " " Left $(x=-b)$



$\times$ the phase $e^{i(a+b)}$ (15)

small k

$\therefore \psi(a) = e^{ik(a+b)}\,\psi(-b) \quad ---(16)$

$\psi'(a) = e^{ik(a+b)}\,\psi'(-b) \quad ---(17)$

apply (16) and (17) to (6) and (11) of 6

$$\psi(a) = Ae^{ika} + Be^{-ika}$$

$$\psi'(a) = ik\left[e^{ika} - Be^{-ika}\right] \quad \Big\} \text{---} (18)$$

and $$\psi(-b) = Ce^{-Qb} + De^{Qb}$$

$$\psi'(-b) = Q\left[Ce^{-Qb} - De^{Qb}\right] \quad \Big\} \text{----} (19)$$

Now: apply the Bloch conditions

for ψ: $$Ae^{ika} + Be^{-ika} = e^{ik(a+b)}\left[Ce^{-Qb} + De^{Qb}\right] \text{--} (20)$$

for ψ': $$ik\left(Ae^{ika} - Be^{-ika}\right) = e^{ik(a+b)}\, Q\left[Ce^{-Qb} - De^{Qb}\right] \text{--} (21)$$

small

We need to solve eq. (13), (14), (20) and (21) by putting coefficients A, B, C and D in determinant.

4 unknowns

But solving is very difficult

The final Equation is of the form:

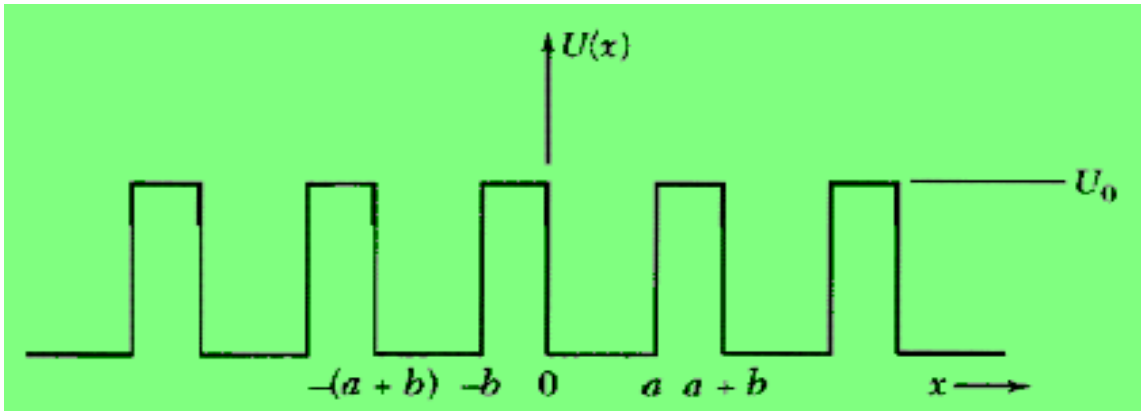
$$\left[\frac{Q^2 - K^2}{2QK}\right] \sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos K(a+b)$$

go to Eq. (21a) :

Chapter 7: Energy Bands

Kronig-Penney Model

- This model solves for periodic potential in a form of a square-well array:



- Schrodinger wave equation for this potential can take the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+U(x)\psi=\varepsilon\psi \qquad (11)$$

where *U(x)* is the potential energy and ε is the energy eigenvalue.
We have 2 regions: $0 < x < a$ $(U = 0)$ *and* $-b < x < 0$ $(U \neq 0)$

- For the first region ($0 < x < a$ *(U = 0)*) we have the wave function:

$$\psi = A e^{iKx} + B e^{-iKx} \tag{12}$$

This is a combination of plane waves traveling to the right and to the left, with energy:

$$\varepsilon = \frac{\hbar^2 K^2}{2m} \tag{13}$$

- In the 2nd region, [$-b < x < 0$*(U ≠ 0)*] wave function takes the form:

$$\psi = C e^{Qx} + D e^{-Qx} \tag{14}$$

with energy:

$$\varepsilon = U_o - \frac{\hbar^2 Q^2}{2m} \tag{15}$$

- Solution of this equation shall be on the Bloch form (7) because it is a periodic potential.
- Thus the solution in the region *a<x<a+b* must be related to the solution (14) in the region -b<x<0 by the Bloch theorem:

$$\psi_k(r) = u_k(r) e^{ik.r} \tag{7}$$

$$\psi(a < x < a+b) = \psi(-b < x < 0) e^{ik(a+b)} \tag{16}$$

- The constants A, B, C, D are chosen so that Ψ and Ψ' are continuous at x=0 and x=a. same as in square potential wells.
- At x = 0 we have (for both conditions): (12) + (14):

$$A + B = C + D \tag{17}$$

Derivatives of (12) and (14) at x = 0 provides:

$$iK(A - B) = Q(C - D) \tag{18}$$

- for the case of x = a; and applying continuity of Ψ and Ψ' we will get:

$$Ae^{iKa} + Be^{-iKa} = (Ce^{-Qb} + De^{Qb})e^{ik(a+b)} \quad (19)$$

$$iK(Ae^{iKa} - Be^{-iKa}) = Q(Ce^{-Qb} - De^{Qb})e^{ik(a+b)} \quad (20)$$

- Solving equations from (17) to (20) can be done by putting all coefficients of A, B, C, D in a determinant. However, such solution is very difficult. We will only write down the final equation:

$$\left[\frac{Q^2 - K^2}{2QK}\right]\sinh Qb \sin Ka + \cosh Qb \cos Ka = \cos k(a+b) \quad (21a)$$

- to simplify the solution; we represent the periodic potential by a periodic Delta Function. Let: b → 0 and $U_o \rightarrow \infty$

❑ We do some approximation:

$Q \gg K \qquad \text{Qb} \ll 1$

$\sinh Qb \to Qb$

$\cosh Qb \to 1$

$\cos k\,(a+b) \to \cos ka$

notice that: $Q^2 \gg K^2$, hence: (21a) $\Rightarrow$

$$\frac{Q^2}{2QK} Qb \sin Ka + \cos Ka = \cos ka$$

$$\left[\frac{P}{Ka}\right] \sin Ka + \cos Ka = \cos ka \qquad (21b)$$

$$with \;\; P = \frac{Q^2 ba}{2}$$

Chapter 7: Energy Bands

Kronig-Penney Model

- The ranges of K for which this equation has solutions are plotted in Fig. 5, for the case P = 3π/2. The corresponding values of the energy are plotted in Fig. 6. Note the ***energy gaps*** at the zone boundaries.

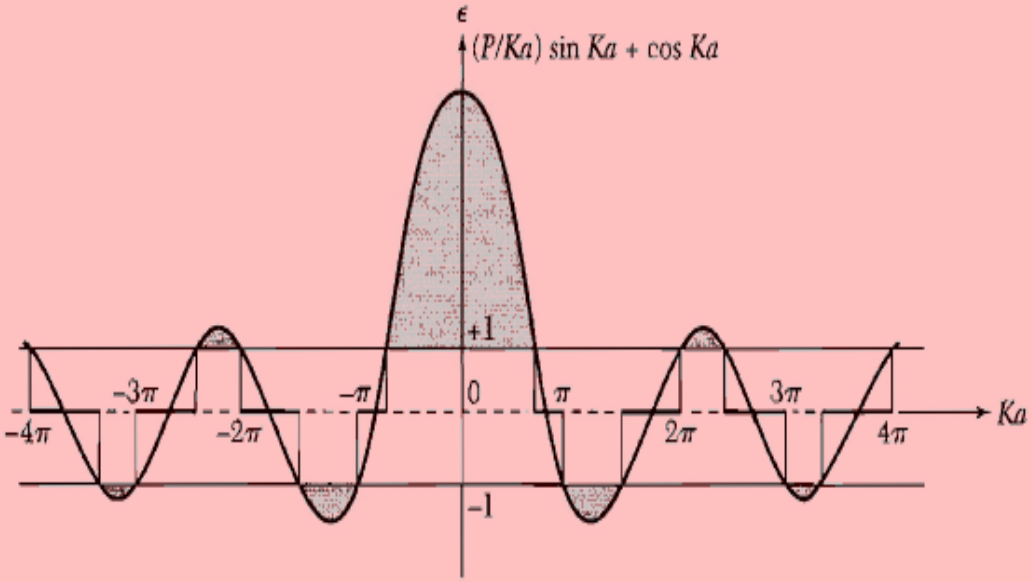
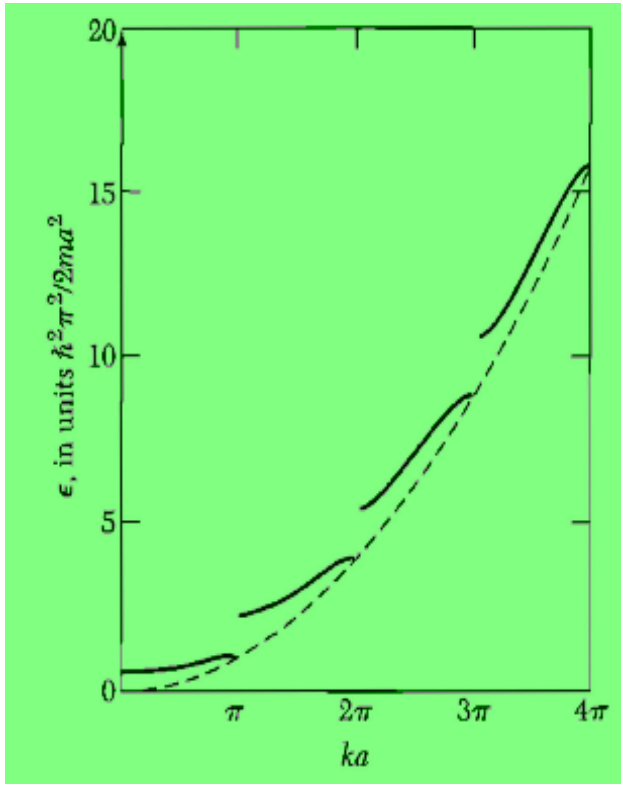
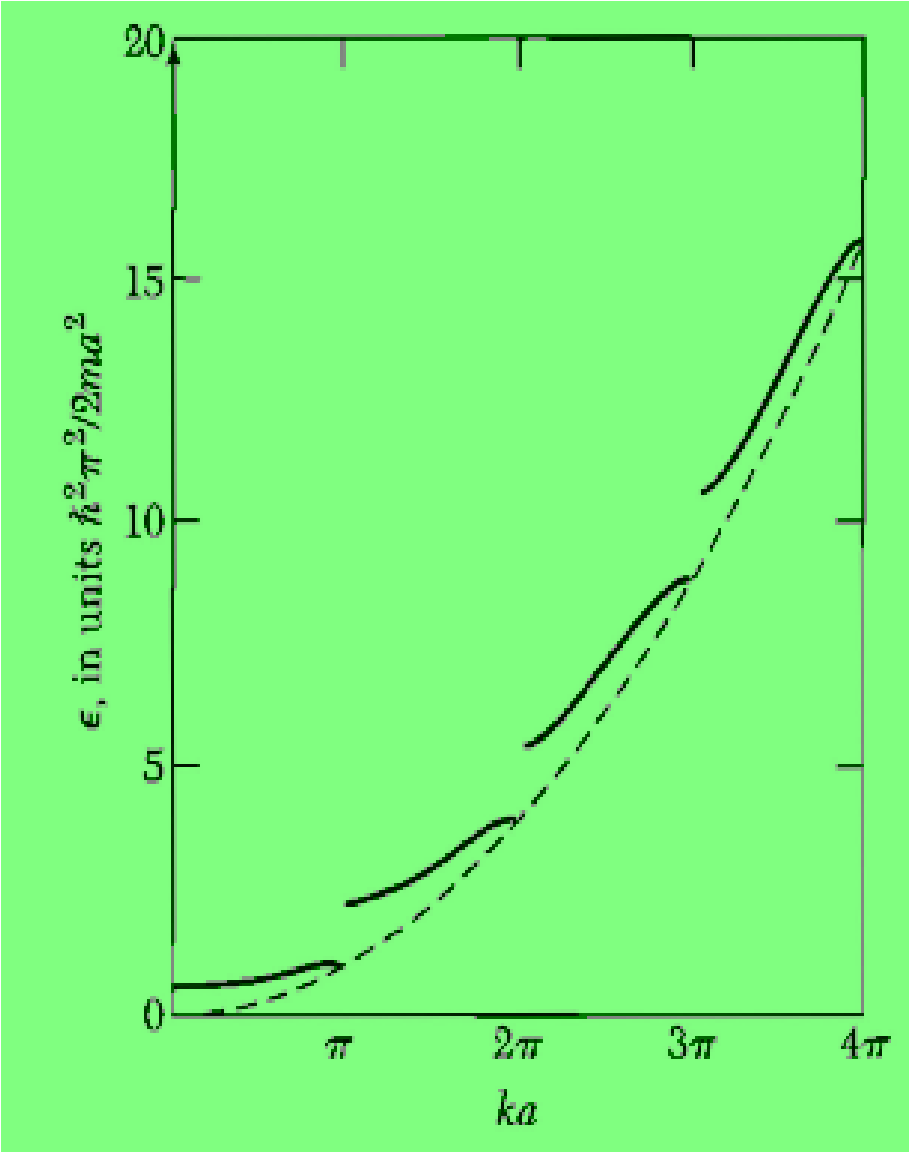


Figure 5 Plot of the function $(P/Ka)\sin Ka + \cos Ka$, for $P = 3\pi/2$. The allowed values of the energy e are given by those ranges of $Ka = (2m\epsilon/\hbar^2)^{1/2}a$ for which the function lies between ± 1. For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.



Chapter 7: Energy Bands

Kronig-Penney Model



- Plot of energy vs. wavenumber for the Kronig-Penney potential, with $P = 3\pi/2$. Notice the energy gaps at $ka = \pi, 2\pi, 3\pi \ldots$

notes:

The NFM could use:

only in 1-D

1. Bloch waves
2. Band formation
3. Energy Gap
4. shows that gap of Fourier component V_G

The model in Reality only give hints that the gaps are at BZ edges.

But Real life is that metals are 3-D not 1-D so it is not practical alone to.

1. it work only for 1-D systems (not Real)
2. Real life is 3-D
3. square wells/steps for V don't describe the Reality.

Chapter 7: Energy Bands

Kronig-Penney Model

(4) it counts for 1-e only
But many metals have significant p/d electron configurations.

∴ KPM is useful in teaching students and learning the simple source of Bands

---

Scientists prefer to use: "Pseudopotential"
"its The effective Potential Between Ions and valence electrons only"
→ core electrons are Ignored

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- We considered in Fig. 3 the approximate form we expect for the solution of the Schrödinger equation if the wave vector is at a zone boundary, as at k = ±π/a.
- Here, we treat in detail the wave equation for a general potential, at general values of k.
- Let *U(x)* denote the potential energy of an electron in a linear lattice of lattice constant *a.* Potential energy is invariant under the lattice translation. Hence: *U(x) = U(x + a).*
- A function invariant under a crystal lattice translation may be expanded as a Fourier series in the reciprocal lattice vectors G.
- As a rule: There is periodicity : There is Fourier Transform
- We write the Fourier series for the potential energy as:

$$U(x) = \sum_G U_G e^{iGx} \qquad (22)$$

Chapter 7: Energy Bands

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

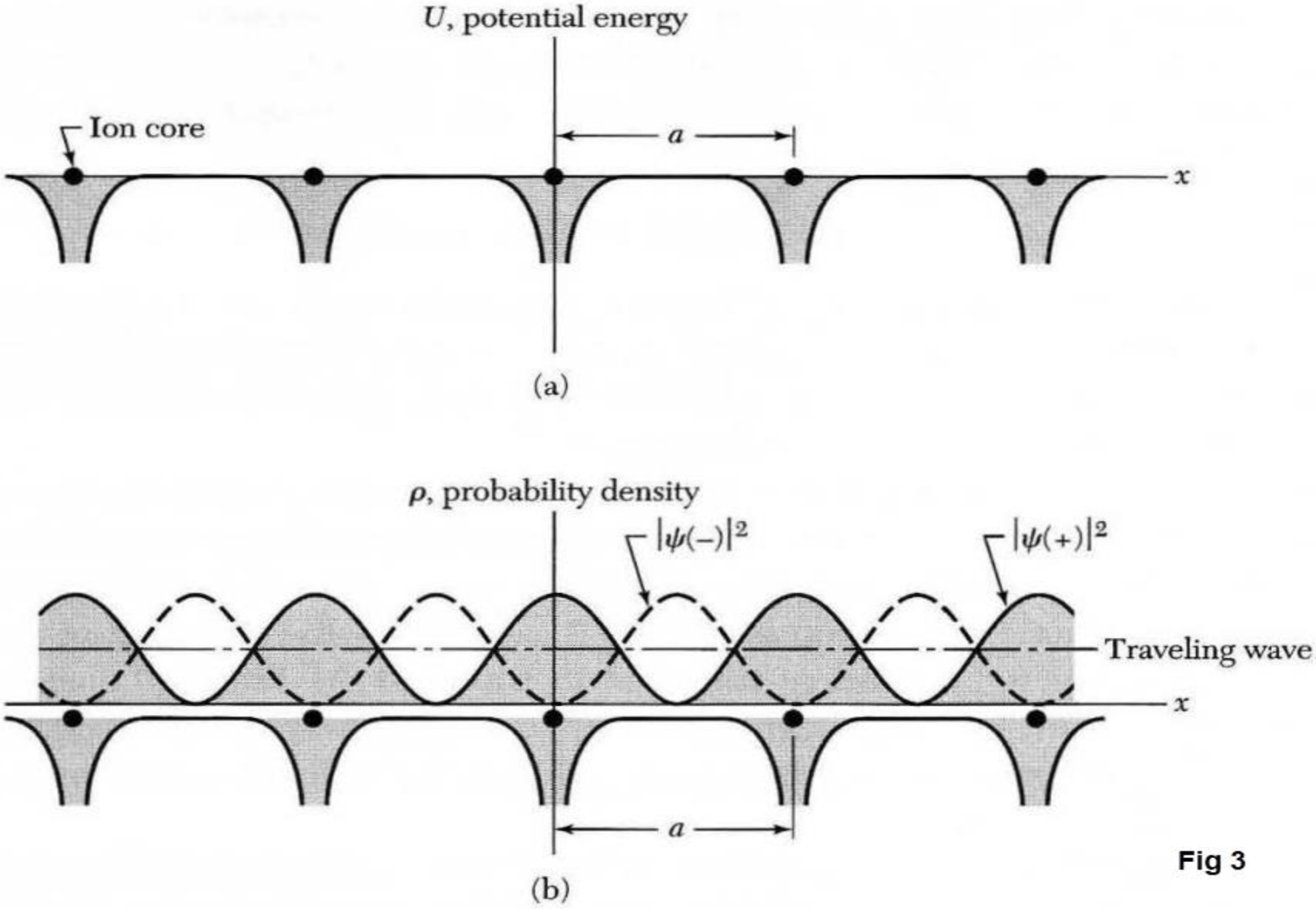


Fig 3

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- Please review Fourier Analysis.
- For actual crystal potentials; the values of the coefficients U_G tend to decrease rapidly with increasing magnitude of G. For a coulomb potential: U_G decreases as $1/G^2$
- In equation (22), we did not specify the x-values. We want to use only **real** values. Accordingly: (22) can be rewritten as:

$$U(x) = \sum_{G>0} U_G (e^{iGx} + e^{-iGx}) = 2\sum_{G>0} U_G \cos Gx \qquad (23)$$

- The wave equation of an electron in the crystal is $H\psi = \varepsilon\psi$ where H is the Hamiltonian and ε is the energy eigenvalue.
- The full equation is then:

$$\left[\frac{p^2}{2m} + U(x)\right]\psi(x) = \left[\frac{p^2}{2m} + \sum_G U(x) e^{iGx}\right]\psi(x) = \varepsilon\psi(x) \qquad (24)$$

WAVE EQUATION OF ELECTRON IN A PERIODIC POTENTIAL

- Equation (24) is written in the one-electron approximation in which the orbital $\psi(x)$ describes the motion of one electron in the potential of the ion cores and in the average potential of the other conduction electrons.
- The wavefunction *$\psi(x)$ may be expressed* as a Fourier series summed over all values of the wavevector permitted by the boundary conditions, so that:

$$\psi = \sum_k C(k) e^{ikx} \qquad (25)$$

- The set of values of *k has the form $2\pi n/L$.*
- To solve the wave equation, substitute (25) in (24) to obtain a set of linear algebraic equations for the Fourier coefficients.
- ***We will take the solution as term by term:***

The kinetic energy term is:

$$\frac{p^2}{2m}\psi(x)=\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2\psi(x)=\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2}=\frac{\hbar^2}{2m}\sum_k k^2C(k)e^{ikx} \qquad (i)$$

and the potential energy term is:

$$U(x)\psi(x)=\left(\sum_G U_G e^{iGx}\right)\psi(x)=\sum_G\sum_k U_G e^{iGx}C(k)e^{ikx} \qquad (ii)$$

The full Schrodinger Eq. becomes:

$$\frac{\hbar^2}{2m}\sum_k k^2C(k)e^{ikx}+\sum_G\sum_k U_G C(k)e^{i(k+G)x}=\varepsilon\sum_k C(k)e^{ikx} \qquad (26)$$

$k' = k + G$
Then $k' \rightarrow k$ dummy index

For 1 K value, this equation becomes:

$$\frac{\hbar^2k^2}{2m}C(k)e^{ikx}+\sum_G U_G C(k-G)e^{ikx}=\varepsilon C(k)e^{ikx} \qquad (27)$$

Solution of the Central Equation

- Each Fourier component must have the same coefficient on both sides of the equation. Thus we have the **central equation:**

$$(\lambda_k - \varepsilon)C(k) + \sum_G U_G C(k-G) = 0 \qquad (27)$$

$$(\lambda_k - \varepsilon)C_k + \sum_G U_G C_{k-G} = 0 \qquad (27)$$

$$with: \lambda_k = \hbar^2 k^2 / 2m \qquad (28)$$

- Eq. (27) is the Algebraic form of the well know Schrodinger equation in a periodic potential (24).
- It is not easy to solve it, but usually one can use only few terms.
- No. of solutions of this equation = no. of equations it has = No. of Fourier coefficients C(K – G).

- *Eq. (27)* represents a set of simultaneous linear equations that connect the coefficients *C(k - G) for all reciprocal lattice vectors G. It is a set because there are as* many equations as there are coefficients C.
- To solve it, the determinant of the coefficients must vanish.
- As an application: for the case when G = g (Shortest values of G):

$$\begin{bmatrix} \lambda_{k-2g}-\varepsilon & U_g & 0 & 0 & 0 \\ U_g & \lambda_{k-g}-\varepsilon & U_g & 0 & 0 \\ 0 & U_g & \lambda_k-\varepsilon & U_g & 0 \\ 0 & 0 & U_g & \lambda_{k+g}-\varepsilon & U_g \\ 0 & 0 & 0 & U_g & \lambda_{k+2g}-\varepsilon \end{bmatrix} \begin{bmatrix} C_{k-2g} \\ C_{k-g} \\ C_k \\ C_{k+g} \\ C_{k+2g} \end{bmatrix} = 0 \qquad (32)$$

- The solution of the determinant (32) gives a set of energy eigenvalues ε_{nk} .

Chapter 7: Energy Bands

Solution of the Central Equation

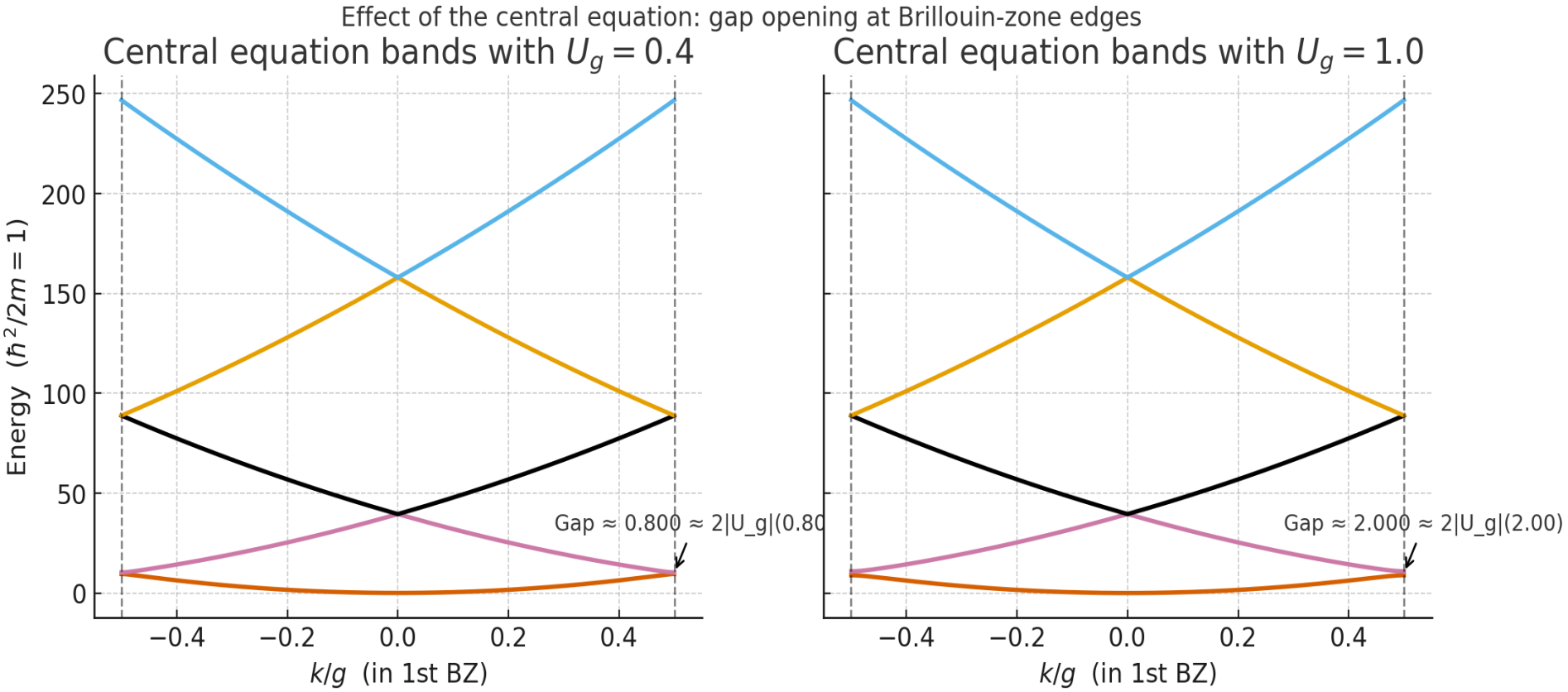
- Band structures are usually plotted as energy versus wavevector in the first Brillouin zone. When wavevectors are outside this zone, they are carried back into the first zone by translation.
- We look for a G such that a k' in the first zone satisfies: $k' + G = k$
- where k is the free electron wavevector in the empty lattice.
- We can drop the ' from k since G can be - or + :

$$\varepsilon(k_x, k_y, k_z) = \frac{\hbar^2}{2m}(k + G)^2 = \frac{\hbar^2}{2m}\left[(k_x + G_x)^2 + (k_y + G_y)^2 + (k_z + G_z)^2\right]$$

- We consider as an example free electron bands of a simple cubic lattice. Suppose we want to exhibit the energy as a function of k in the [100] direction. Let $\hbar^2 / 2m = 1$. *We show* several bands in this empty lattice approximation with their energies $\varepsilon(000)$ at k = 0 and $\varepsilon(k_x 00)$ *along the* k_x *axis in the first zone:*

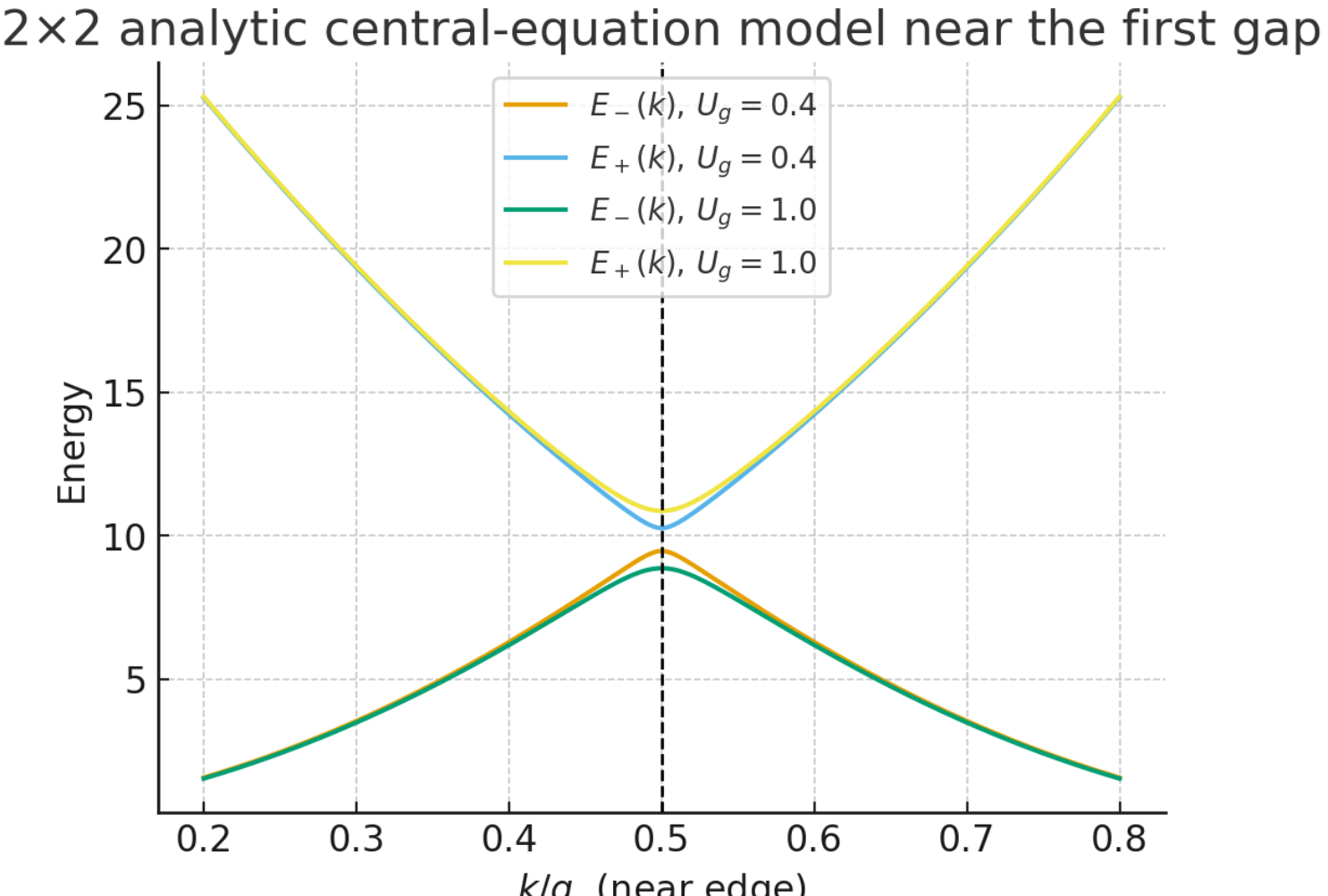
Chapter 7: Energy Bands

Solution of the Central Equation



Chapter 7: Energy Bands

Solution of the Central Equation



Chapter 7: Energy Bands

Empty Lattice Approximation

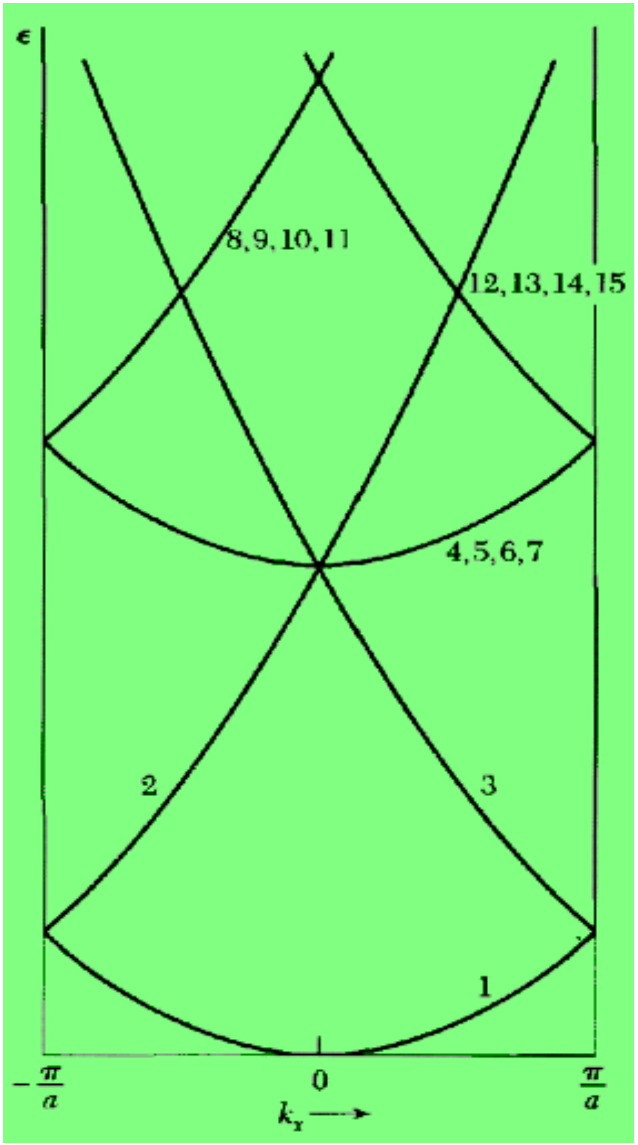


Figure 8 Low-lying free electron energy bands of the empty *sc* lattice, as transformed to the first Brillouin zone and plotted vs. $(k_x 00)$. The free electron energy is $\hbar^2(\mathbf{k}+\mathbf{G})^2/2m$, where the **G**'s are given in the second column of the table. The bold curves are in the first Brillouin zone, with $-\pi/a \leq k_x \leq \pi/a$. Energy bands drawn in this way are said to be in the reduced zone scheme.

We consider as an example the low-lying free electron bands of a simple cubic lattice. Suppose we want to exhibit the energy as a function of **k** in the [100] direction. For convenience, choose units such that $\hbar^2/2m = 1$ .We show several low-lying bands in this empty lattice approximation with their energies $\epsilon(000)$ at $\mathbf{k} = 0$ and ϵ(k,00) along the k_x axis in the first zone:

Band	$Ga/2\pi$	$\epsilon(000)$	$\epsilon(k_x00)$
1	000	0	k_x^2
2,3	100,$\bar{1}$00	$(2\pi/a)^2$	$(k_x \pm 2\pi/a)^2$
4,5,6,7	010,0$\bar{1}$0,001,00$\bar{1}$	$(2\pi/a)^2$	$k_x^2 + (2\pi/a)^2$
8,9,10,11	110,101,1$\bar{1}$0,10$\bar{1}$	$2(2\pi/a)^2$	$(k_x + 2\pi/a)^2 + (2\pi/a)^2$
12,13,14,15	$\bar{1}$10,$\bar{1}$01,$\bar{1}\bar{1}$0,$\bar{1}$0$\bar{1}$	$2(2\pi/a)^2$	$(k_x - 2\pi/a)^2 + (2\pi/a)^2$
16,17,18,19	011,0$\bar{1}$1,01$\bar{1}$,0$\bar{1}\bar{1}$	$2(2\pi/a)^2$	$k_x^2 + 2(2\pi/a)^2$

Chapter 7: Energy Bands

Empty Lattice Approximation

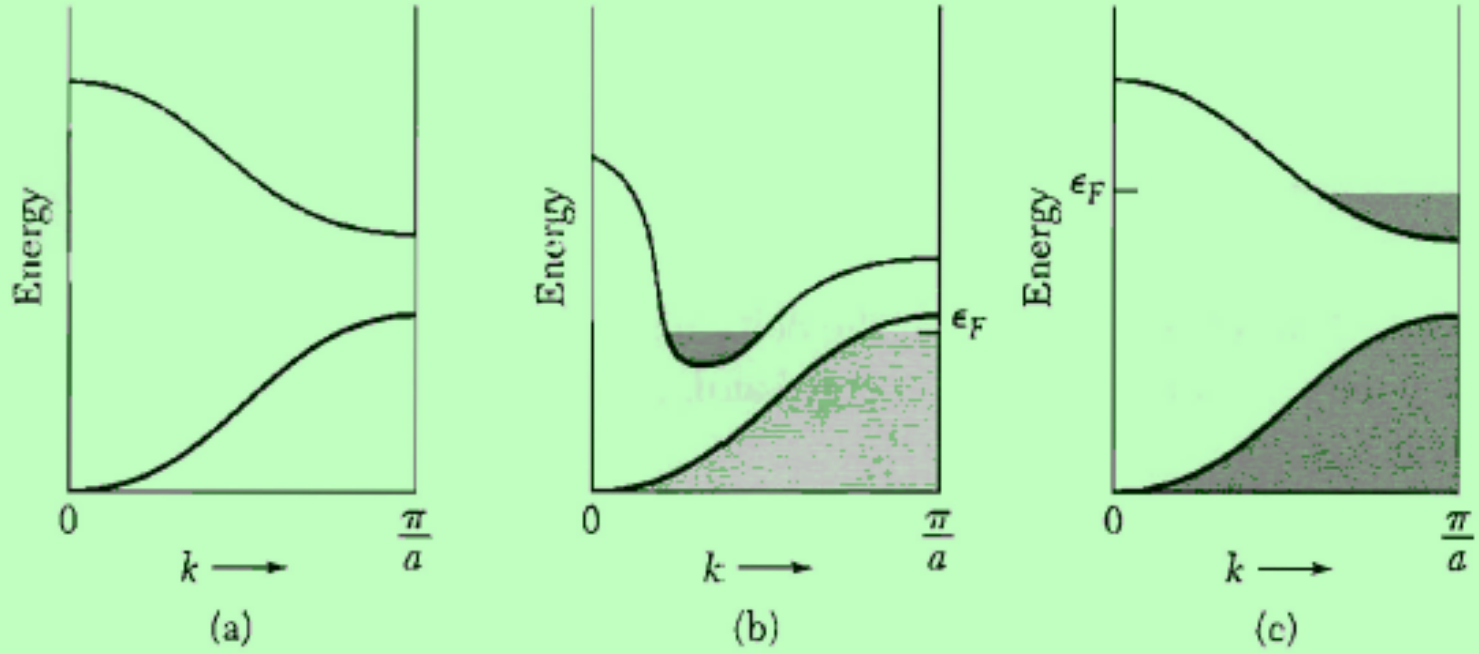


Figure 11 Occupied states and band structures giving (a) an insulator, (b) a metal or a semimetal because of band overlap, and (c) a metal because of electron concentration. In (b) the overlap need not occur along the same directions in the Brillouin zone. If the overlap is small, with relatively few states involved, we speak of a semimetal.

Crystal	Gap	E_g, eV	
		0 K	300 K
Diamond	*i*	5.4	
Si	*i*	1.17	1.11
Ge	*i*	0.744	0.66
αSn	*d*	0.00	0.00
InSb	*d*	0.23	0.17
InAs	*d*	0.43	0.36
InP	*d*	1.42	1.27
GaP	*i*	2.32	2.25
GaAs	*d*	1.52	1.43
GaSb	*d*	0.81	0.68
AlSb	*i*	1.65	1.6
SiC(hex)	*i*	3.0	-
Te	*d*	0.33	-
ZnSb		0.56	0.56

Crystal	Gap	E_g, eV	
		0 K	300 K
HgTe[a]	*d*	-0.30	
PbS	*d*	0.286	0.34-0.37
PbSe	*i*	0.165	0.27
PbTe	*i*	0.190	0.29
CdS	*d*	2.582	2.42
CdSe	*d*	1.840	1.74
CdTe	*d*	1.607	1.44
ZnO		3.436	3.2
ZnS		3.91	3.6
SnTe	*d*	0.3	0.18
AgCl		-	3.2
AgI		-	2.8
Cu_2O	*d*	2.172	-
TiO_2		3.03	-

Chapter 7: Energy Bands

Observations

1. **Larger atoms $\rightarrow$ smaller bandgaps.** Why?

- Larger atoms have more electron shells and the ionic charge is screened from the free flying electron. Consequently electrons will be experiencing lower effective potential in lattices of large atoms.
- We have seen that the bandgap is proportional to the amplitude of the potential.
- While in real crystals the relationship between the potential and the bandgap is more complex, the same logic applies:
  larger atoms $\rightarrow$ smaller potential $\rightarrow$ smaller bandgap.

2. Energy gaps span 0.08-5.4 eV.
3. The wider the gap the heavier the electron.

Chapter 7: Energy Bands

Observations

- For some materials it turns out that the valence band maximum does not coincide with the conduction band minimum
- This means that in order for an optical transition to happen, the electron needs to also obtain extra crystal momentum.
- Electron can get extra momentum from crystal phonons.
- this means that for absorption to happen the photon, the electron and the phonon need to all meet at the same place and time
- Hence, there is a low probability occurrence and hence the absorption is poor for the indirect bandgap materials

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Week No. 05

DIAMAGNETISM AND PARAMAGNETISM 1

Prof. Nasser S. Alzayed

Types of magnetic materials:

1. Diamagnetic → develop a magnetization opposite of app. mag. F
2. Paramagnetic → magnetize in presence of mag. Field magnetic moments in direction of B
3. Ferromagnetic → Create mag. Field by their own spontaneous mag. mom.
4. Antiferromagnetic

These classes Cannot be explained using Classical Theories of electron in solids such as Drude Model. only Quantum Mechanics Can do that

Introduction

- Magnetism in solids is fundamentally a **quantum-mechanical phenomenon**
- This chapter explores two weak (linear) magnetic responses in materials:

  Diamagnetism: induced magnetic moments oppose an applied field: → negative χ.

  Paramagnetism: materials with permanent (or easily induced) magnetic moments align with an applied field → positive χ; often temperature-dependent (e.g., Curie law).
- **Bound electron** diamagnetism (Langevin model) and its quantum treatment
- **Conduction-electron** magnetism in metals: e.g., Pauli paramagnetism & Landau diamagnetism

Introduction

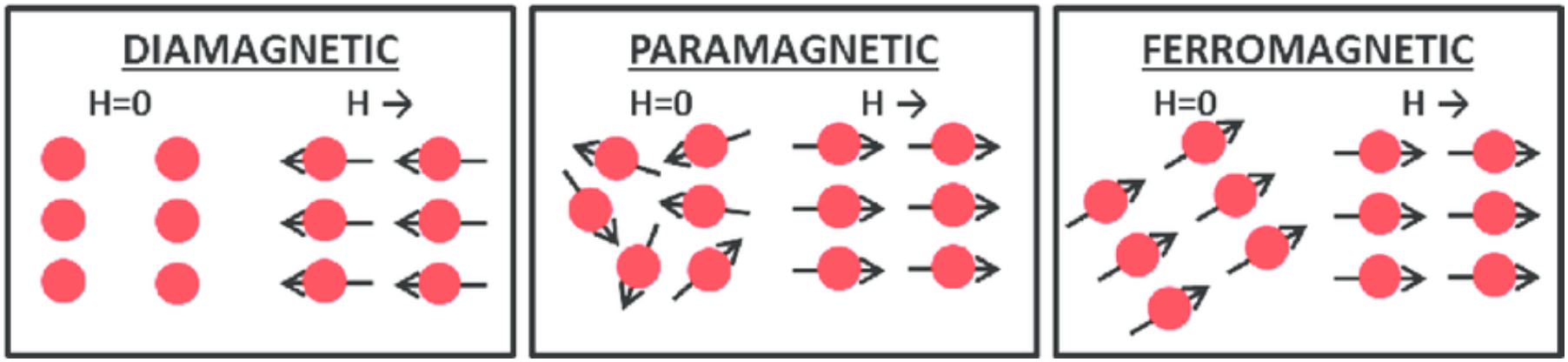
- The magnetic moment of a free atom has three principal sources:
  1. the spin with which electrons are endowed
  2. their orbital angular momentum about the nucleus
  3. the change in the orbital moment induced by an applied magnetic field
- 1 and 2 give ***paramagnetic*** contributions to the magnetization
- 3 gives a ***diamagnetic*** contribution
- Atoms with ***all filled electron shells*** have zero spin and zero orbital moment
- Magnetization M is defined as:

$$\boldsymbol{M} = \frac{1}{\mu_o}\chi \boldsymbol{B} \qquad (1)$$

- χ is magnetic susceptibility, **B**: Magnetic Field Intensity

Introduction

- Substances with a ***negative*** magnetic susceptibility are called **diamagnetic.**
- Substances with a ***positive*** susceptibility are called **paramagnetic**



Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

LANGEVIN DIAMAGNETISM EQUATION

Classical, Bound electrons

- ***Diamagnetism*** is associated with the tendency of electrical charges partially to shield the interior of a body from an applied magnetic field.
- According to *Lenz's law*: when the flux through an electrical circuit is changed, an induced (*diamagnetic*) current is set up in such a direction as to oppose the flux change.
- In a *superconductor*, the induced *current persists* as long as the field is present. The magnetic field of the induced current is opposite to the applied field, and the magnetic moment associated with the current is a diamagnetic moment.
- **Larmor theorem**: *In a magnetic field the motion of the electrons around a central nucleus is, to the first order in B, the same as a possible motion in the absence of B except for the superposition of a precession of the electrons with angular frequency*.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

Larmor precession of Z electrons

- when substance is under external mag. field, electrons will rotate giving *Larmor frequency:*

$$\omega = \frac{eB}{2m} \qquad (2)$$

- If the average electron current around the nucleus is zero initially, the application of the magnetic field will cause a finite current around the nucleus. *The current is equivalent to a magnetic moment opposite to the applied field*.
- This condition is not satisfied in free carrier cyclotron resonance, and the cyclotron frequency of the carriers is twice as in (2)

$$I = \text{charge} \times f = (-Ze)\left(\frac{\omega}{2\pi}\right) = (-Ze)\left(\frac{1}{2\pi}.\frac{eB}{2m}\right) \qquad (3)$$

- This current is called: Larmor precession of Z electrons.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

LANGEVIN DIAMAGNETISM EQUATION

- The magnetic moment μ of a current loop is given by: (current) X (area of the loop):

$$\mu = I \times \text{Area} = I \times \pi\rho^2 = (-Ze)\left(\frac{1}{2\pi}.\frac{eB}{2m}\right)\times \pi\rho^2$$

$$= -\frac{Ze^2B}{4m}\langle\rho^2\rangle \qquad (4)$$

$$\text{with}: \langle\rho^2\rangle = \langle x^2\rangle + \langle y^2\rangle \text{ is the mean square of the radius}$$

- the diamagnetic susceptibility per unit volume is:

$$\chi = \frac{\mu_o N\mu}{B} = -\frac{\mu_o NZe^2}{6m}\langle r^2\rangle \qquad (5)$$

$$\langle r^2\rangle = \frac{3}{2}\langle\rho^2\rangle$$

- Where N = No. of atoms/m³.
- (5) is called: Langevin diamagnetism equation

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

LANGEVIN DIAMAGNETISM EQUATION

- The problem of calculating the diamagnetic susceptibility of an isolated atom is reduced to the calculation of $\langle r^2 \rangle$ for the electron distribution within the atom.
- Typical experimental values of the molar susceptibilities are the following:

	He	Ne	Ar	Kr	Xe
χ_M in CGS in 10^{-6} cm^3/mole:	−1.9	−7.2	−19.4	−28.0	−43.0

- More Examples of Diamagnetic materials:

bismuth	-1.7×10^{-8}
copper	-0.107×10^{-8}
germanium	-0.15×10^{-8}
gold	-0.19×10^{-8}
hydrogen	-2.49×10^{-8}

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

LANGEVIN DIAMAGNETISM EQUATION

- Meaning of Equation (5):
  - The atom as a whole does not possess a permanent magnetic dipole moment.
  - The magnetization is produced by the influence of the external magnetic field on the electron orbits and particularly by the precessional motion.
  - The diamagnetic susceptibility χ is small and negative, because $\langle r^2 \rangle$ is small.
  - Negative susceptibility means that diamagnetism opposes applied magnetic field. (prefix: dia - in opposite or different directions).
  - Note that measurements of χ were once used to get estimates of atomic size through the values of $\langle r^2 \rangle$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

LANGEVIN DIAMAGNETISM EQUATION

- Units of susceptibility:
  - When **M** and **H (B)** both have the (same) units of Amp/meter, then susceptibility (χ) is called the ***volume magnetic susceptibility*** and is dimensionless.
  - There are however two other (SI) measures of susceptibility:
    - mass magnetic susceptibility (χ_{mass}), measured in m^3/kg
    - molar magnetic susceptibility (χ_{mol}) measured in m^3/mol
  - We can convert between these using the density (ρ) in kg m^{-3} and *M* (molar mass) kg/mol.

$$\chi_{mass} = \frac{\chi}{\rho}$$

$$\chi_{mol} = M\,\chi_{mass} = M\,\frac{\chi}{\rho}$$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF DIAMAGNETISM

Quantum Theory of diamagnetism:

(1) The external magnetic field (B) affects the electrons's orbital motion

(2) Hamiltonian when $B = 0$:

$$H_0 = \frac{p^2}{2m_e} + U(\bar{r}) \qquad ----(1)$$

(3) Hamiltonian when $B \neq 0$:

$$H = \frac{1}{2m_e}\left(\vec{p} - \frac{e}{c}A\right)^2 + U(r) \qquad ---(2)$$

(4) Perturbation:

$$H' = -\frac{e}{m_e c}\bar{A}\cdot\bar{p} + \frac{e^2}{2m_e c^2}A^2 \qquad --(3)$$

(5) Energy shift due to $\bar{B}$:

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF DIAMAGNETISM

In first order non-degenerate perturbation theory, the shift ΔE due to $\vec{B}$ is:

$$\Delta E = \langle \psi | H' | \psi \rangle \quad \text{---} \quad (4)$$

$$\Rightarrow \Delta E = -\frac{e}{m_e c} \langle \psi | \vec{A} \cdot \vec{p} | \psi \rangle + \frac{e^2}{2 m_e c^2} \langle \psi | \vec{A}^2 | \psi \rangle \quad (5)$$

$= 0$ due to symmetry considerations

$\neq 0$

$$\therefore \Delta E \approx \frac{e^2}{2 m_e c^2} \langle \psi | \vec{A}^2 | \psi \rangle \quad \text{---} \quad (6)$$

using Coulomb gauge: $\vec{A} = \frac{1}{2} \vec{r} \times \vec{B}$ --- (7)

(7) in (6) !

$$\Delta G = \frac{e^2}{2m_e c^2} \cdot \frac{1}{4} \cdot B^2 \langle r^2 \rangle \quad ----- (8)$$

We did not specify $\vec{B}$ direction for z only : $\vec{B} = B_z \hat{z}$; $\langle r^2 \rangle = \frac{2}{3} \langle r^2 \rangle$

$$\Rightarrow \Delta E = \frac{e^2 B^2}{12 m_e c^2} \langle r^2 \rangle \quad ----- (9)$$

$\Rightarrow$ Associated mag. moment:

$$M = -\frac{\partial \Delta E}{\partial B} = -\frac{e^2 B}{6 m_e c^2} \langle r^2 \rangle \quad ----- (10)$$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF DIAMAGNETISM

(10) $\Rightarrow$ $$M = -\frac{e^2 B}{6mc^2}\langle r^2\rangle \quad \ldots (12)$$

$$\therefore \chi = \frac{\mu_0 N M}{B}$$

$$= -\frac{\mu_0 \cdot N \cdot \frac{e^2 B}{6mc^2}}{B}\langle r^2\rangle$$

$$\therefore \chi = -\frac{\mu_0 N e^2}{6mc^2}\langle r^2\rangle \quad \ldots (11)$$

this is the same as eq (5)

$\rightarrow$ Langevin diamagnetism is in agreement with Q.M.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF DIAMAGNETISM

- Diamagnetism can be considered from Quantum Mechanics also:
- Hamiltonian due to magnetic field can be expressed as:

$$\mathrm{H} = \frac{ie\hbar}{2mc}\left(\nabla A + A.\nabla\right) + \frac{e^2}{2mc^2}A^2 \qquad (6)$$

↳ 2 for symmetry

- If the magnetic field is uniform and in the *z* direction:

$$\left.\begin{aligned} A_x &= -\frac{1}{2}yB \\ A_y &= \frac{1}{2}xB \\ A_z &= 0 \end{aligned}\right\} \qquad (7)$$

$\Rightarrow \nabla \cdot A = 0$ $\quad \frac{\partial}{\partial x}A_x = 0$ / $\frac{\partial}{\partial y}A_y = 0$, $\frac{\partial}{\partial z}A_z = 0$

$$\Rightarrow \mathrm{H} = \frac{ie\hbar B}{2mc}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) + \frac{e^2B^2}{8mc^2}\left(x^2 + y^2\right) \qquad (8)$$

Paramagnetism

- The first term on the right is proportional to the orbital angular momentum component L_2 if r is measured from the nucleus.
- In mononuclear systems this term gives rise only to paramagnetism
- 2nd term gives for a *spherically symmetric* system a contribution:

$$E' = \frac{e^2 B^2}{12mc^2}\langle r^2 \rangle \qquad (9)$$

- The associated *magnetic moment* is diamagnetic:

$$\mu = \frac{\partial E'}{\partial B} = -\frac{e^2 B}{6mc^2}\langle r^2 \rangle \qquad (10)$$

$$\Rightarrow \chi = \frac{\mu_o N \mu}{B} = -\frac{\mu_o N}{\cancel{B}}\frac{e^2 \cancel{B}}{6mc^2}\langle r^2 \rangle = -\frac{\mu_o N e^2}{6mc^2}\langle r^2 \rangle \qquad (10a)$$

- This result is the same as in (5) after we use Z=1 for mononuclear system and give c = 1. Hence, Quantum mechanics and Classical mechanics provide same result for diamagnetism.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

PARAMAGNETISM (Introduction)

What We Seek to Understand in Paramagnetism

- Why some materials develop a **weak positive magnetization** in an external magnetic field.
- How this magnetization depends on **temperature** and **field strength**.
- Why the effect **disappears when the field is removed**, unlike in ferromagnetism.

Remember:

- **Magnetic Moment (μ):** arises from **orbital** and **spin** angular momenta of electrons.
- **Magnetization (M):** the average alignment of all atomic moments per unit volume.
- **Thermal Agitation:** tends to randomize moment directions — competition between **thermal energy (kT)** and **magnetic energy (μ·B)**.
- **Statistical Concept:** overall magnetization is a **statistical average** of microscopic orientations.
- **Classical vs. Quantum View:**
  - Classical: moments vary continuously in direction.
  - Quantum: orientations are **quantized** into discrete states (mJ levels).

Our Goal in Next Steps

- Derive expressions for M and $\chi = \frac{M}{B}$ using:
  - **Langevin's classical model**, and
  - **Quantum Brillouin function**.
- Compare how quantization modifies the simple thermal averaging picture.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

Langevin (classical) theory of Paramagnetism

- The paramagnet consists of an array of permanent magnetic dipoles: μ
- In a uniform field *B* they have:

Potential Energy $U = -\boldsymbol{\mu} \cdot \boldsymbol{B}$ (C1)

- A dipole ***parallel*** to the field has the lowest energy
- For the dipole to lower its energy (and become parallel to the field) we need a second mechanism. This is provided by the thermal vibrations
- The magnetic field "would like" the dipoles aligned to lower their energy
- The thermal vibrations "would like" to randomize and disorder the magnetic dipoles
- We can therefore expect a statistical theory, based on a "competition" between these two mechanisms

❑ Hence:

$$K_B T \approx -\boldsymbol{\mu} \cdot \boldsymbol{B} \qquad \text{(C2)}$$

❑ We can use Boltzmann statistics to obtain the number *dn* of dipoles with energy between *U* and *U + dU*

$$dn = c\, e^{-U/K_B T}\, dU \qquad (C3)$$

$$(\text{C1}) \rightarrow U = -\mu \text{B} \cos\theta \qquad (C4)$$

$$\therefore dU = \mu \text{B} \sin\theta\, d\theta \qquad (C5)$$

$$\text{total magnetization:}$$

$$M = N \langle \mu \rangle \qquad (C6)$$

$$\text{But Also :}$$

$$M = \int_0^{\infty} \mu \cos\theta\, dn \qquad (C7)$$

Langevin (classical) theory of Paramagnetism

$$(\mathrm{C}\,6) \rightarrow \frac{M}{\langle \mu \rangle} = N \qquad (C\,8)$$

$$(C\,7) \rightarrow \frac{M}{\mu} = \int_0^{\infty} \cos\theta \, dn \qquad (C\,9)$$

$$\therefore (\mathrm{C}\,9) \div (\mathrm{C}\,8):$$

$$\frac{\langle \mu \rangle}{\mu} = \frac{\int_0^{\infty} \cos\theta \, dn}{N} = \frac{\int_0^{N} \cos\theta \, dn}{\int_0^{N} dn}$$

Now $(\mathrm{C3})$ for dn and $(\mathrm{C5})$ for dU and $(\mathrm{C4})$ for U:

$$\therefore \frac{\langle \mu \rangle}{\mu} = \frac{\int_0^{\pi} \cos\theta . c\, e^{-U/K_B T} \, dU}{\int_0^{N} c\, e^{-U/K_B T} \, dU}$$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

Langevin (classical) theory of Paramagnetism

$$\frac{\langle \mu \rangle}{\mu} = \frac{\int_0^{\pi} \cos\theta . c\, e^{\mu \mathrm{B}\cos\theta / K_B T} \left(\mu \mathrm{B} \sin\theta d\theta\right)}{\int_0^{\pi} c\, e^{\mu \mathrm{B}\cos\theta / K_B T} \left(\mu \mathrm{B} \sin\theta d\theta\right)} \qquad (C10)$$

$$\text{let: } x = \frac{\mu \mathrm{B}\cos\theta}{K_B T} = a\cos\theta \qquad (C11)$$

$$\rightarrow dx = -a\sin\theta d\theta$$

$$\therefore (C10) \rightarrow : \frac{\langle \mu \rangle}{\mu} = \frac{1}{a} \frac{\int_{-a}^{+a} x\, e^x dx}{\int_{-a}^{+a} e^x dx} \qquad (C12)$$

$$\rightarrow \frac{\langle \mu \rangle}{\mu} = \frac{1}{a} \frac{(\mathrm{x}-1)e^x \Big|_{-a}^{+a}}{e^x \Big|_{-a}^{+a}} = \frac{1}{a} \frac{a\left[e^a + e^{-a}\right] - \left[e^a - e^{-a}\right]}{\left[e^a - e^{-a}\right]}$$

$$\Rightarrow \frac{\langle M \rangle}{M} = \frac{\int_0^{\pi} \cos\theta\, e^{a\cos\theta} \sin\theta\, d\theta}{\int_0^{\pi} e^{a\cos\theta} \sin\theta\, d\theta} \quad \cdots (1) \qquad a = \frac{MB}{K_B T}$$

Now: $x = a\cos\theta \Rightarrow dx = -a\sin\theta\, d\theta$

$$\rightarrow \sin\theta\, d\theta = -\frac{dx}{a} \quad \text{and} \quad \cos\theta = \frac{x}{a}$$

and $\theta = 0 \Rightarrow x = a$, $\theta = \pi \Rightarrow x = -a$

$$\therefore \int_0^{\pi} \cos\theta\, e^{a\cos\theta} \sin\theta\, d\theta = \int_a^{-a} \frac{x}{a}\left(-\frac{dx}{a}\right) e^{x} = \frac{1}{a^2}\int_{-a}^{a} x e^{x} dx \quad \cdots (2)$$

and denominator: $\int_0^{\pi} e^{a\cos\theta} \sin\theta\, d\theta = \int_a^{-a} e^{x}\left(-\frac{dx}{a}\right) = \frac{1}{a}\int_{-a}^{a} e^{x} dx$ (3)

$$\therefore \frac{\langle M \rangle}{M} = \frac{\frac{1}{a^2}\int_{-a}^{a} x e^{x} dx}{\frac{1}{a}\int_{-a}^{a} e^{x} dx} = \frac{1}{a}\,\frac{\int_{-a}^{+a} x e^{x} dx}{\int_{-a}^{a} e^{x} dx}$$

Langevin (classical) theory of Paramagnetism

$$\rightarrow \frac{\langle \mu \rangle}{\mu} = \frac{\left[e^{a} + e^{-a} \right]}{\left[e^{a} - e^{-a} \right]} - \frac{1}{a} \qquad (C13)$$

$$\text{the quantity: } \frac{\left[e^{a} + e^{-a} \right]}{\left[e^{a} - e^{-a} \right]} - \frac{1}{a} = L(a) \qquad (C14)$$

$$\text{is called Langevin function } L(a)$$

$$\therefore \langle \mu \rangle = \mu L(a) \qquad (C15)$$

$$\therefore L\left(\frac{\mu \mathrm{B}}{K_B T} \right) = \frac{\left[e^{\frac{\mu \mathrm{B}}{K_B T}} + e^{-\frac{\mu \mathrm{B}}{K_B T}} \right]}{\left[e^{\frac{\mu \mathrm{B}}{K_B T}} - e^{-\frac{\mu \mathrm{B}}{K_B T}} \right]} - \frac{K_B T}{\mu \mathrm{B}} \qquad (C16)$$

- We can use equations (C6) and (C15) with (C16) to calculate for the magnetization M.

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

Langevin (classical) theory of Paramagnetism

$$(C\,6)\,\&\,(\mathrm{C}15):$$

$$\because M = N\langle\mu\rangle = N.\mu.L\left(\frac{\mu \mathrm{B}}{K_B T}\right)$$

$$when: \frac{\mu \mathrm{B}}{K_B T} \ll 1 \quad (\text{small B and high T})$$

$$L\left(\frac{\mu \mathrm{B}}{K_B T}\right) \approx \frac{1}{3}.\frac{\mu \mathrm{B}}{K_B T}$$

$$\therefore M = N\langle\mu\rangle = N.\mu.\frac{1}{3}.\frac{\mu \mathrm{B}}{K_B T} = \frac{N\mu^2 B}{3K_B T} \qquad (C17)$$

$$\therefore \chi = \frac{M}{B} = \frac{N\mu^2}{3K_B T} = \frac{C}{T} \qquad (C18)$$

- This is the same as (22) for Q.P. except for: the effective No. of Bohr magnetons (due to quantization)

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

PARAMAGNETISM

- Paramagnetism: susceptibility is +
  - aluminium 0.82×10^{-6}
  - calcium 1.40×10^{-6}
  - magnesium 0.69×10^{-6}
  - platinum 1.65×10^{-6}
  - tantalum 1.10×10^{-6}

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Week No. 06

DIAMAGNETISM AND PARAMAGNETISM 2

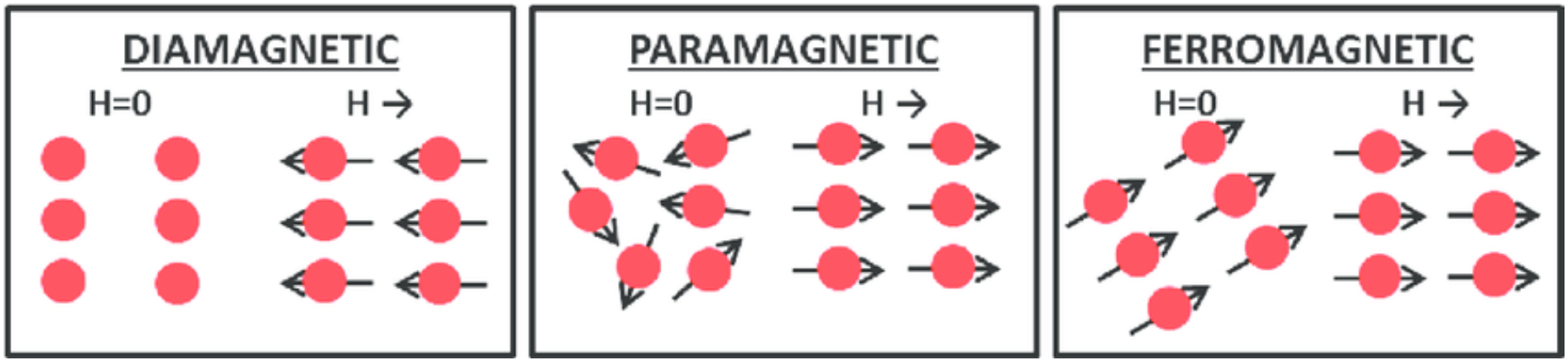
Prof. Nasser S. Alzayed

Types of magnetic materials:

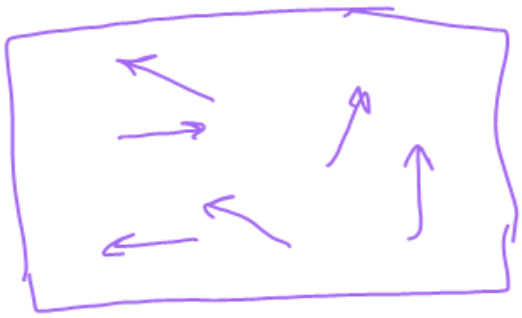
1. Diamagnetic → develop a magnetization opposite of app. mag. F
2. Paramagnetic → magnetize in presence of mag. Field magnetic moments in direction of B
3. Ferromagnetic → Create mag. Field by their own spontaneous mag. mom.
4. Antiferromagnetic

These classes Cannot be explained using Classical Theories of electron in solids such as Drude Model. only Quantum Mechanics Can do that

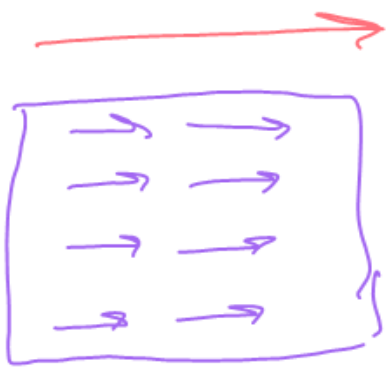
Chapter 11: DIAMAGNETISM AND PARAMAGNETISM



Paramagnetism



$B = 0$



$\Rightarrow \vec{m}$

$\equiv$ mag. moment

$B \neq 0$

Magnetization $\vec{M} = \frac{\vec{m}}{V} = \chi_m \frac{\vec{B}}{\mu_0}$

$\vec{m}$: magnetic moment

M : magnetization

V : volume

χ_m : magnetic susceptibility

μ_0 : vacu. permeability.

"Paramagnetism"

normal material + $B^{ext.} \Rightarrow$ Paramagnetic

due to $\uparrow$ spin $\Rightarrow \mu$ (mag. moment)

$$\mu = -g \mu_B S$$

↳ Bohr magneton

$$\mu_B = \frac{e\hbar}{2m_e}$$

Energy of e in a magnetic field $= -\bar{\mu} \cdot \bar{B}$

$$= g \mu_B \bar{B} \cdot \bar{S}$$

Now spin $\vec{S}$ could $\vec{S} \rightrightarrows \vec{B}$ or

antiparallel $\vec{S} \rightleftarrows \vec{B}$

$g = 2$

$\vec{S} = \begin{cases} +\frac{1}{2} & \vec{S} \uparrow\uparrow \vec{B} \\ -\frac{1}{2} & \vec{S} \uparrow\downarrow \vec{B} \end{cases}$

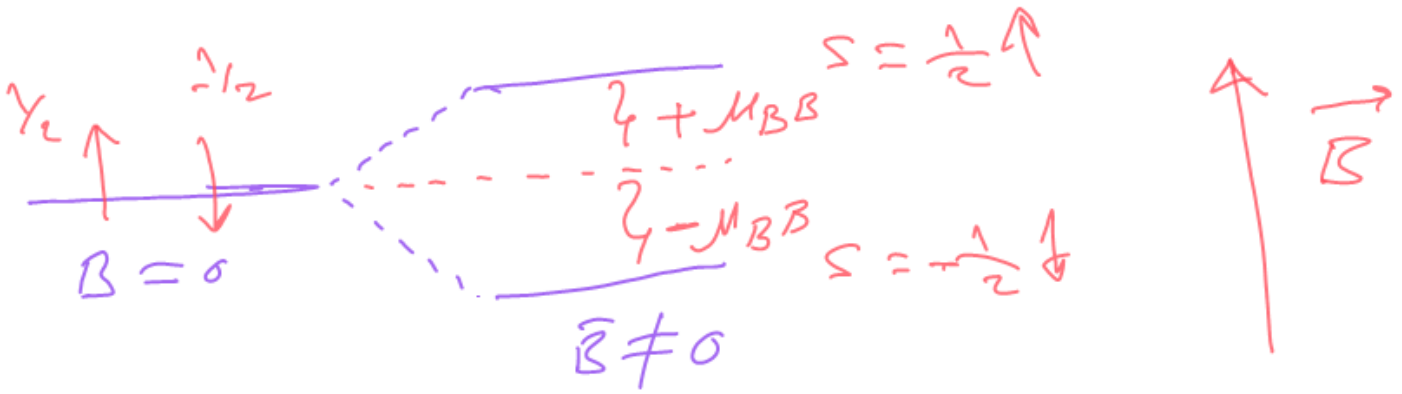
g is called Lande factor or g-factor

$\therefore \varepsilon = 2 \times \mu_B B \cdot \frac{1}{2} \cos(0)$

$= \mu_B B$

$= -\mu_B B$

$\uparrow\downarrow$ $\cos 180 = -1$

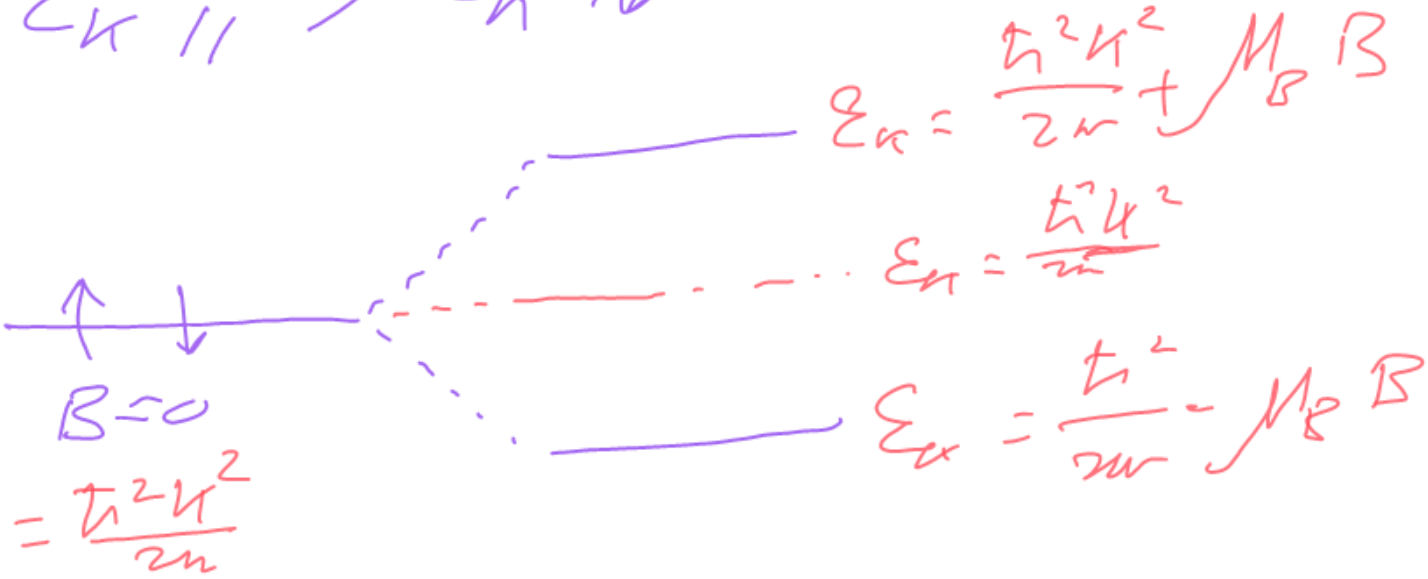


The Total Energy of electron:

$$\varepsilon_k \begin{cases} = \dfrac{\hbar^2 k^2}{2m} + \mu_B B & s \uparrow \\ = \dfrac{\hbar^2 k^2}{2m} - \mu_B B & s \downarrow \end{cases}$$

B

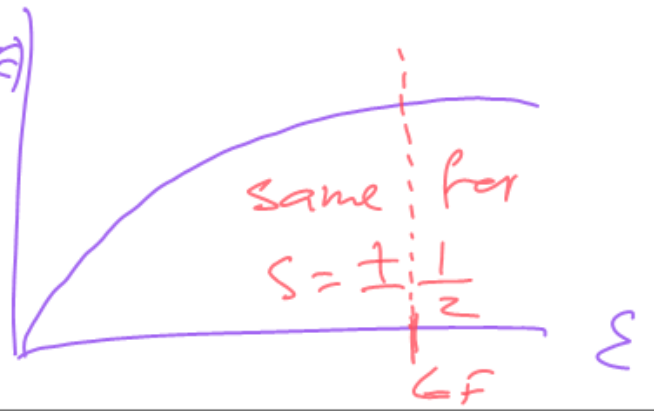
$\Rightarrow \varepsilon_{k\uparrow} > \varepsilon_{k\downarrow}$



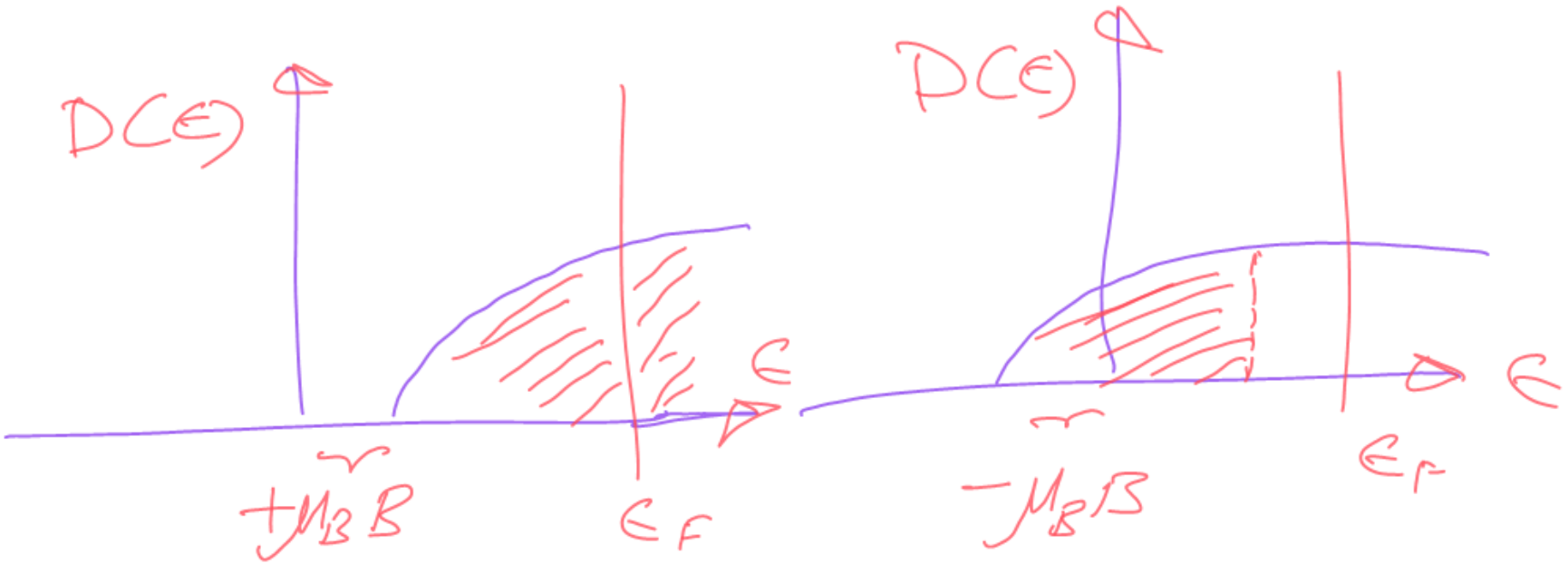
According to Sommerfeld:
only electrons that are near Fermi Surface will Participate in magnitization

What about the density of states?

when $B = 0$ $D(\epsilon) \propto \epsilon^{1/2}$



When $B \neq 0$



$s = +\frac{1}{2}$

some electrons are pushed above Fermi surface ϵ_F

$s = -\frac{1}{2}$

some electrons are pulled down the Fermi surface ϵ_F

Steps:

① $B = 0 \Rightarrow$ All electrons are Below OR Just at ϵ_F

② $B \neq 0 \Rightarrow$ $+\frac{1}{2} \Rightarrow$ above ϵ_F

$-\frac{1}{2} \Rightarrow$ Below ϵ_F

③ $\Rightarrow$ vacant states Below ϵ_F

$\Rightarrow s = +\frac{1}{2} \Rightarrow$ Fill in these states

Remember: No. of electrons = Constant

④ $\Rightarrow$ Increase in net magnetization inside the solid.

(5) → No. of electrons with $+\mu$:

$$N_+ = \underbrace{\frac{1}{2}\int_0^{\epsilon_F} D(\epsilon)\,d\epsilon}_{B=0 \text{ part}} + \underbrace{\frac{1}{2}D(\epsilon_F)\mu_B B}_{\text{due to } B\neq 0} \qquad (1)$$

$\frac{1}{2}$ to count only the $+\frac{1}{2}$ electrons

and: No. of electrons with $-\mu$:

$$N_- = \underbrace{\frac{1}{2}\int_0^{\epsilon_F} D(\epsilon)\,d\epsilon}_{B=0 \text{ part}} - \underbrace{\frac{1}{2}D(\epsilon_F)\mu_B B}_{\frac{1}{2} \text{ of electrons only}} \qquad (2)$$

(6) total magnetization M:

$$M = (N_+ - N_-)\mu_B$$

$$= (① - ②)\mu_B$$

$$\therefore \boxed{M = D(\epsilon_F)\mu_B^2 B} \quad \not\quad (3)$$

↳ Pauli Paramagnetization of metals

note: M is Independent of T.

(7) $$\chi = \frac{dM}{dH} = \mu_0 \frac{dM}{dB} = D(\epsilon_F)\mu_B^2$$

$$\therefore \boxed{\chi = D(\epsilon_F)\mu_0\mu_B^2} \quad \not\quad (4)$$

Chapter 11: Magnetic Moment of an Atom

What is ($\vec{\mathrm{m}}$) for an Atom?
The magnetic moment ($\vec{\mu}$) for an atom comes from two main sources:
1. Orbital Angular Momentum $\vec{L}$
2. Spin $\vec{\mathrm{S}}$

(1) Orbital Contribution

$$\vec{\mu} = -\mu_B \vec{L} \quad (g = 1)$$

(2) Spin Contribution

$$\vec{\mu} = -2\mu_B \vec{S} \quad (g = 2)$$

For an Atom with Many Electrons, If an atom has multiple electrons with angular momenta $\vec{l_1}$, $\vec{l_2}$, $\vec{l_3}$, then:

$$\vec{L} = \vec{l_1} + \vec{l_2} + \vec{l_3} + \cdots$$

Similarly, the total spin is:

$$\vec{\mathrm{S}} = \vec{s_1} + \vec{s_2} + \vec{s_3} + \cdots$$

Chapter 11: Total Magnetic Moment and Landé g-Factor

Total Angular Momentum

$$\vec{J} = \vec{L} + \vec{S}$$

Total Magnetic Moment

$$\vec{\mu}_{\text{tot}} = -g\mu_B \vec{J}$$

Expanding for individual contributions:

$$\vec{\mu}_{\text{tot}} = -\mu_B \vec{L} - 2\mu_B \vec{S}$$

Definition of Landé g-Factor

$$g\vec{J} = \vec{L} + 2\vec{S}$$

where:

* (g = 1) for orbital magnetic moment
* (g = 2) for spin magnetic moment

Taking the Dot Product with $\vec{J}$)

$$g\vec{J} \cdot \vec{J} = \vec{L} \cdot \vec{J} + 2\vec{S} \cdot \vec{J}$$

Expanding further:

$$gJ^2 = \vec{L} \cdot \left(\vec{L} + \vec{S}\right) + 2\vec{S} \cdot \left(\vec{L} + \vec{S}\right)$$

Simplifying:

$$gJ^2 = L^2 + \vec{L} \cdot \vec{S} + 2\vec{S} \cdot \vec{L} + 2S^2$$

Combining terms:

$$gJ^2 = L^2 + 2S^2 + 3\vec{L} \cdot \vec{S}$$

How to find expectation value in Q.M.

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle \quad \cdots (1)$$

For $gJ^2 = L^2 + 2S^2 + 3\bar{L}\cdot\bar{S}$ $\cdots (2)$

(1) $\langle J^2 \rangle = J(J+1)\hbar^2$

(2) $\langle L^2 \rangle = L(L+1)\hbar^2$

(3) $\langle S^2 \rangle = S(S+1)\hbar^2$

(4) $\langle \bar{L}\cdot\bar{S} \rangle = \frac{1}{2}[J(J+1) - L(L+1) - S(S+1)]\hbar^2$

(2) $\rightarrow$ $gJ(J+1) = L(L+1) + 2S(S+1) + 3\bar{L}\cdot\bar{S}$ $\cdots (3)$

$\because J^2 = L^2 + S^2 + 2\bar{L}\cdot\bar{S}$ $\cdots (4)$

Chapter 11: Total Magnetic Moment and Landé g-Factor

$$\rightarrow \quad \bar{L}\cdot\bar{S} = \frac{J^2 - L^2 - S^2}{2} \quad \text{---} \quad (5)$$

$$\therefore \langle \bar{L}\cdot\bar{S} \rangle = \frac{J(J+1) - L(L+1) - S(S+1)}{2} \quad \text{---} \quad (6)$$

(6) in (2) $\Rightarrow$ eq. (2) in notes

Chapter 11: Expectation Values and Landé g-Factor Derivation

Writing the Expectation Values:

$$gJ(J+1) = L(L+1) + 2S(S+1) + 3\vec{L}\cdot\vec{S} \quad (1)$$

We know that:

$$J^2 = L^2 + S^2 + 2\vec{L}\cdot\vec{S}$$

Therefore,

$$\vec{L}\cdot\vec{S} = \frac{J^2 - L^2 - S^2}{2}$$

Taking expectation values:

$$\vec{L}\cdot\vec{S} = \frac{J(J+1) - L(L+1) - S(S+1)}{2} \quad (2)$$

Substituting (2) into (1)

$$gJ(J+1) = L(L+1) + 2S(S+1) + \frac{3}{2}J(J+1) - \frac{3}{2}L(L+1) - \frac{3}{2}S(S+1)$$

$$= L(L+1) + 2S(S+1) + 3\left[\frac{J(J+1) - L(L+1) - S(S+1)}{2}\right] \quad (3)$$

$$\rightarrow gJ(J+1) = \frac{3}{2}J(J+1) + \frac{3}{2}S(S+1) - \frac{1}{2}L(L+1) \quad (3)$$

$$\rightarrow \mathrm{g} = \left[\frac{3J(J+1)+S(S+1)-L(L+1)}{2J(J+1)}\right] \quad (4)$$

and

$$\vec{\mu}_{\mathrm{tot}} = -\mathrm{g}\mu_B\vec{\mathrm{J}}$$

Now: we consider magnetization of large no. of atoms.

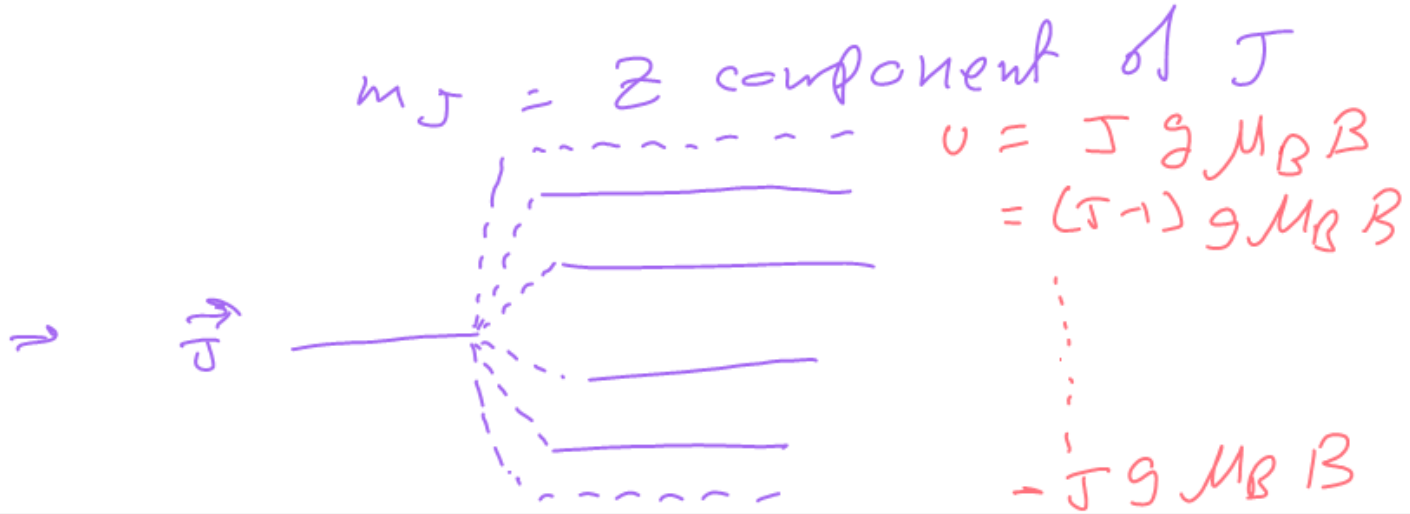
$$\therefore \vec{M}_{tot} = -g\mu_B \vec{J}$$

$$\vec{m} = n\vec{M}_{atom} \quad \text{(mag mom. / unit volume)}$$

if $\vec{B} = B\hat{z}$

$$\Rightarrow U = -\vec{M}\cdot\vec{B} = g\mu_B m_J B$$

m_J = z component of J



*

The normalized probability of occupation of energy levels in * is:

$$P_{m_J} = \frac{e^{-g\mu_B m_J B/k_B T}}{\sum_{m_J=-J}^{+J} e^{-g\mu_B m_J B/k_B T}}$$

magnetic moment in the z-Direction:

$$M_z = -g\mu_B m_J$$

$$\Rightarrow \text{total magnetic moment} = \sum M_{z m_J} P_{m_J}$$

$$\Rightarrow M_J = \frac{\sum_{m_J=-J}^{+J} -g\mu_B m_J \, e^{-g\mu_B m_J B/k_B T}}{\sum_{m_J=-J}^{+J} e^{-g\mu_B m_J B/k_B T}}$$

this M_J is T dependent.

at low T: $\dfrac{\mu_B B}{k_B T} \ll 1$

$$\Rightarrow M_J = \frac{\sum_{m_J=-J}^{+J} -g\mu_B m_J \left(1 - \dfrac{g\mu_B m_J B}{k_B T}\right)}{\sum_{m_J=-J}^{+J} \left(1 - \dfrac{g\mu_B m_J B}{k_B T}\right)}$$

(1) (2) (3)

Now; we have:

$$① \quad \sum_{m_J=-J}^{+J} m_J = 0$$

$$② \quad \sum_{J=1}^{J} m_J^2 = \frac{J(J+1)(2J+1)}{6}$$

$\Rightarrow$ ① above $= 0$

② $\rightarrow$ $\dfrac{g^2 \mu_B^2 B m_J^2}{K_B T}$

③ $\rightarrow$ $2J+1$

$$\therefore M_z = \frac{\sum_{m_J=-J}^{+J} \dfrac{g^2 \mu_B^2 B m_J^2}{K_B T}}{(2J+1)}$$

$$= \frac{g^2 \cdot \mu_B^2 \cdot B}{K_B T} \cdot \frac{\sum_{-J}^{+J} m_J^2}{(2J+1)}$$

$J = -J \rightarrow +J$

$$= \frac{g^2 \cdot \mu_B^2 \cdot B}{K_B T} \cdot \frac{\textcircled{2}\, J(J+1)(2J+1)}{6\,(2J+1)}$$

$\textcircled{3}$

$$\therefore \mu_z(T) = \frac{g^2 \cdot \mu_B^2 \cdot B}{3 K_B T} J(J+1)$$

$$\because \mu = \chi_M \frac{B}{\mu_0}$$

comparing $\Rightarrow$

$$\chi_m = n \frac{\mu_0 \cdot g^2 \cdot \mu_B^2 J(J+1)}{3 k_B T} = \frac{C}{T}$$

n → no. of atoms / m^3

$\therefore \quad \chi_m = \frac{C}{T}$ (Curie's Law)

$$\boxed{C = \frac{n \cdot \mu_0 \cdot g^2 \cdot \mu_B^2 J(J+1)}{3 k_B}}$$

We get: $\frac{\vec{m}}{m^3} = \vec{M} = \frac{C}{T}$

$\therefore$ Paramagnetic susceptibility $\propto \frac{1}{T}$

$= \frac{C}{T}$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

PARAMAGNETISM

- Paramagnetism: susceptibility is +
  - aluminium 0.82×10^{-6}
  - calcium 1.40×10^{-6}
  - magnesium 0.69×10^{-6}
  - platinum 1.65×10^{-6}
  - tantalum 1.10×10^{-6}

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF PARAMAGNETISM

- The *magnetic moment* of an atom or ion in free space is given by:

$$\boldsymbol{\mu} = \gamma \hbar \boldsymbol{J} = -g\mu_B \boldsymbol{J} \qquad (1)$$

Where :

$$\boldsymbol{J} = \boldsymbol{L} + \boldsymbol{S}$$

$$\textbf{Classically: } \boldsymbol{\mu} = \frac{q}{2m}\boldsymbol{L}$$

- μ_B is called Bohr magneton: $\mu_B = e\hbar / emc$ = spin magnetic moment of ***free electron***.
- The quantity γ is call **gyromagnetic ratio:**

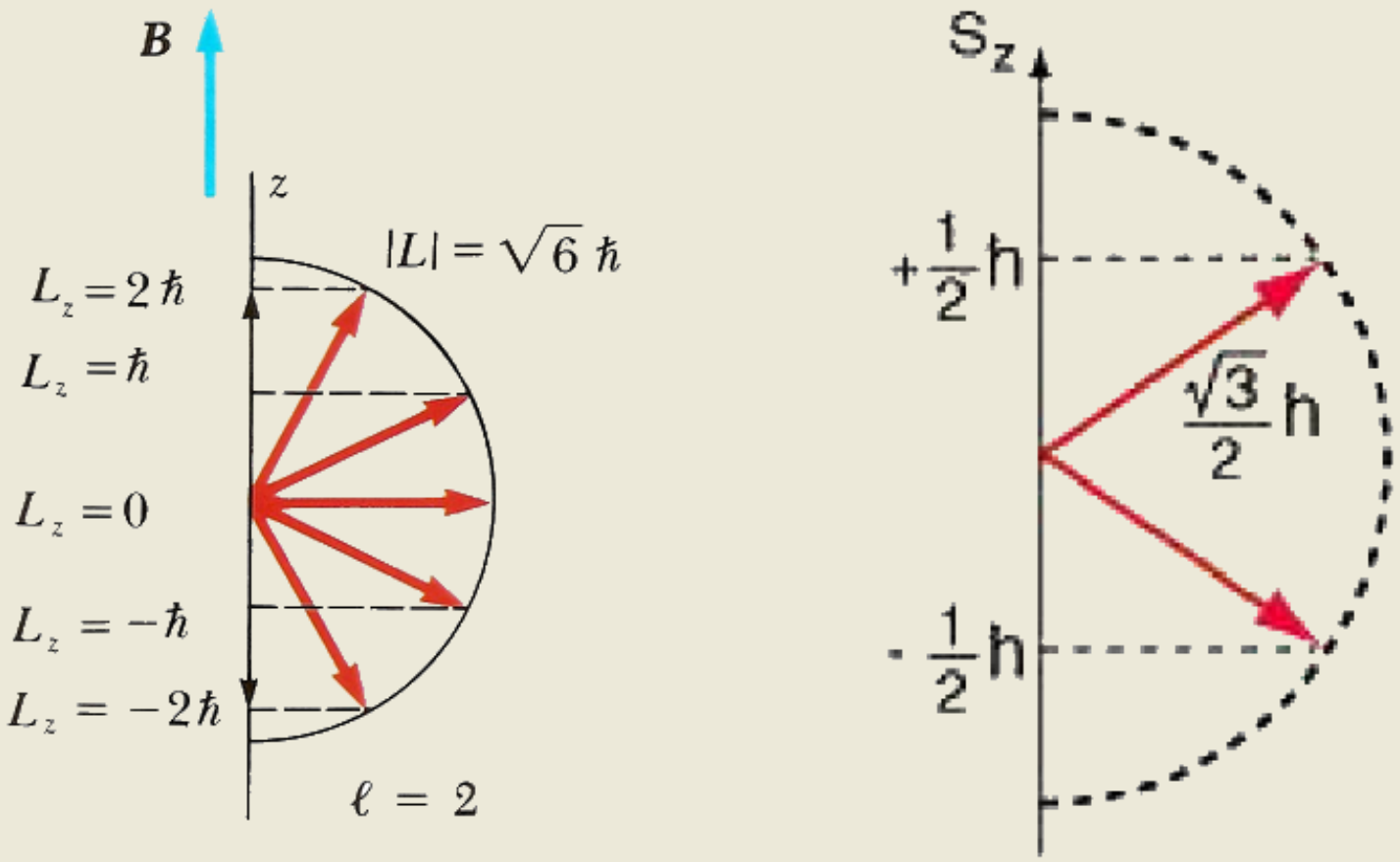
$$\gamma = \frac{\mu}{J}$$

g-factor is defined as:

$$g = -\frac{\gamma}{\mu_B}\hbar \qquad (2)$$

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF PARAMAGNETISM



Quantization of orbital angular momentum (left)

Quantization of Spin angulalr mementum (right)

QUANTUM THEORY OF PARAMAGNETISM

- For an electron spin g = 2.0023, usually taken as 2.00.
- For a free atom the g factor is given by the Lande equation:

$$g = 1 + \frac{J(J+1) + S(S+1) - L(L+1)}{2J(J+1)} \qquad (3)$$

- The energy levels of the system in a magnetic field are:

$$U = -\boldsymbol{\mu} . \boldsymbol{B} = m_J g \mu_B B \qquad (4)$$

- where m_J is the azimuthal quantum number = $J, J - 1, \ldots, -J$
- For a single spin with no orbital moment we have $m_J = \pm ½$ & g =2

$$U = \pm \mu_B B \qquad (5)$$

- This means that we have a splitting in the energy levels into 2 values separated by: 2μB

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

QUANTUM THEORY OF PARAMAGNETISM

- 2 Energy levels show up for a free electron when subjected to external magnetic field.

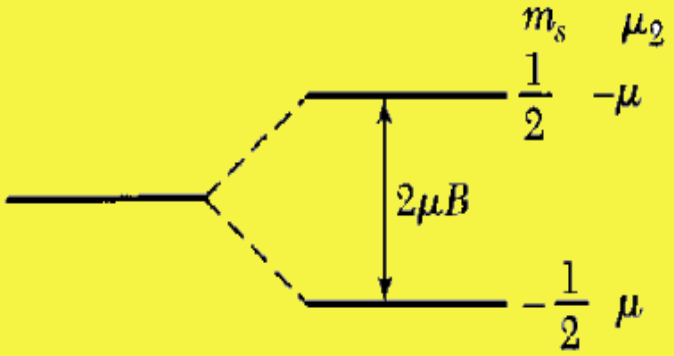


Figure 2 Energy level splitting for one electron in a magnetic field B directed along the positive z axis. For an electron the magnetic moment μ is opposite in sign to the spin S, so that $\mu = -g\mu_B S$. In the low-energy state the magnetic moment is parallel to the magnetic field.

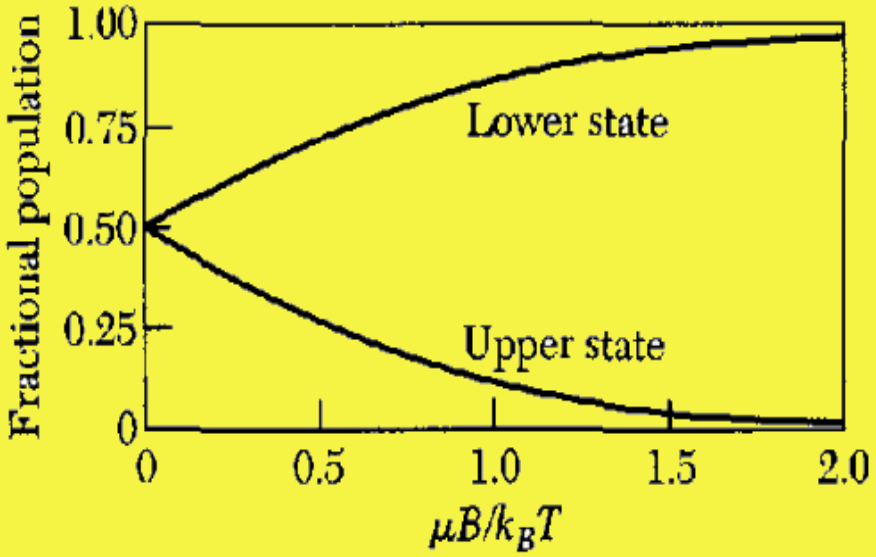


Figure 3 Fractional populations of a two-level system in thermal equilibrium at temperature T in a magnetic field B. The magnetic moment is proportional to the difference between the two curves.

- If we have a system of N atoms per unit volume.
- Magnetization can be calculated as

$$M = N \times (\text{Maxwell Boltzman Statistical Average of all Magnetic moments along B})$$

$$M = N \times \sum_{m_j=-J}^{+J} \frac{-m_j g \mu_B e^{-m_j g \mu_B B / K_B T}}{e^{-m_j g \mu_B B / K_B T}} \qquad (6)$$

$$\text{For the Case: } \frac{m_j g \mu_B B}{K_B T} \ll 1$$

$$\text{We can use the expansion: } e^{-x} = 1 - x + \frac{x^2}{2!} + \ldots$$

- Hence, we can only take first 2 terms of the expansion on both numerator and denominator

❑We get

$$M = Ng\mu_B \frac{\sum_{m_j=-J}^{+J} -m_j \left(1 - \frac{m_j g\mu_B B}{K_B T}\right)}{\sum_{m_j=-J}^{+J} \left(1 - \frac{m_j g\mu_B B}{K_B T}\right)} \qquad (7)$$

$$\rightarrow M = Ng\mu_B \frac{\sum_{m_j=-J}^{+J} -m_j + \sum_{m_j=-J}^{+J} \frac{m_j^2 g\mu_B B}{K_B T}}{\sum_{m_j=-J}^{+J} 1 - \sum_{m_j=-J}^{+J} \frac{m_j g\mu_B B}{K_B T}} = Ng\mu_B \frac{\sum_{m_j=-J}^{+J} -m_j + \frac{g\mu_B B}{K_B T} \sum_{m_j=-J}^{+J} m_j^2}{\sum_{m_j=-J}^{+J} 1 - \frac{g\mu_B B}{K_B T} \sum_{m_j=-J}^{+J} m_j} \qquad (8)$$

We have:

$$\sum_{m_j=-J}^{+J} -m_j = 0 \ , \ \sum_{m_j=-J}^{+J} 1 = (2J+1) \ , \ \sum_{m_j=-J}^{+J} m_j^2 = 2\sum_{m_j=0}^{+J} m_j^2 = \frac{J(J+1)(2J+2)}{3} \qquad (9)$$

❑We get

$$\sum_{m_j=-J}^{+J} -m_j = 0 \ , \ \sum_{m_j=-J}^{+J} 1 = (2J+1) \ , \ \sum_{m_j=-J}^{+J} m_j^2 = 2\sum_{m_j=0}^{+J} m_j^2 = \frac{J(J+1)(2J+2)}{3}$$

$$\therefore M = N\frac{g^2\mu_B^2 B}{K_B T}\left[\frac{\frac{J(J+1)(2J+2)}{3}}{(2J+1)}\right] \qquad (10)$$

$$\therefore M = N\frac{g^2\mu_B^2 B}{3K_B T}J(J+1) \qquad (11)$$

$$\because \chi = \frac{M}{B} = \frac{Ng^2\mu_B^2}{3K_B T}J(J+1) \qquad (12)$$

❑The quantity: $g\sqrt{J(J+1)} = p$ is called: the effective No. of Bohr magnetons:

$$\therefore \chi = \frac{N\mu_B^2 p^2}{3K_B T} = \frac{C}{T} \qquad (13)$$

- (22) is the same as for classical Langvien theory treatment.

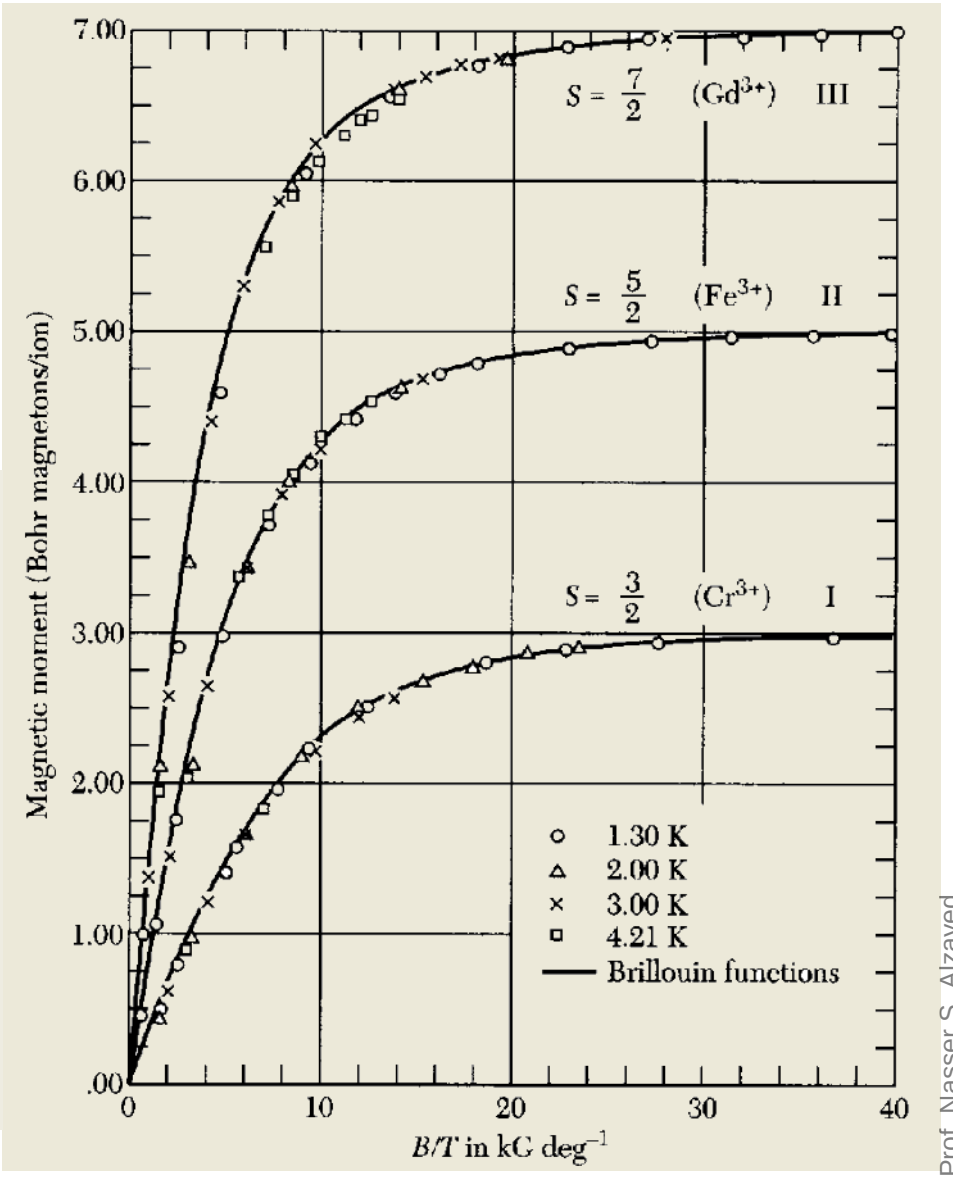


Figure 4
Plot of magnetic moment versus B/T for spherical samples of (I) potassium chromium alum, (II) ferric ammonium alum, and (III) gadolinium sulfate octahydrate. Over 99.5% magnetic saturation is achieved at 1.3 K and about 50,000 gauss (5T).

- The constant C in eq. 13 is called: Curie constant.
- Eq. 13 is called: Curie Law
- Results for the paramagnetic ions in a gadolinium salt are shown in Fig. 5

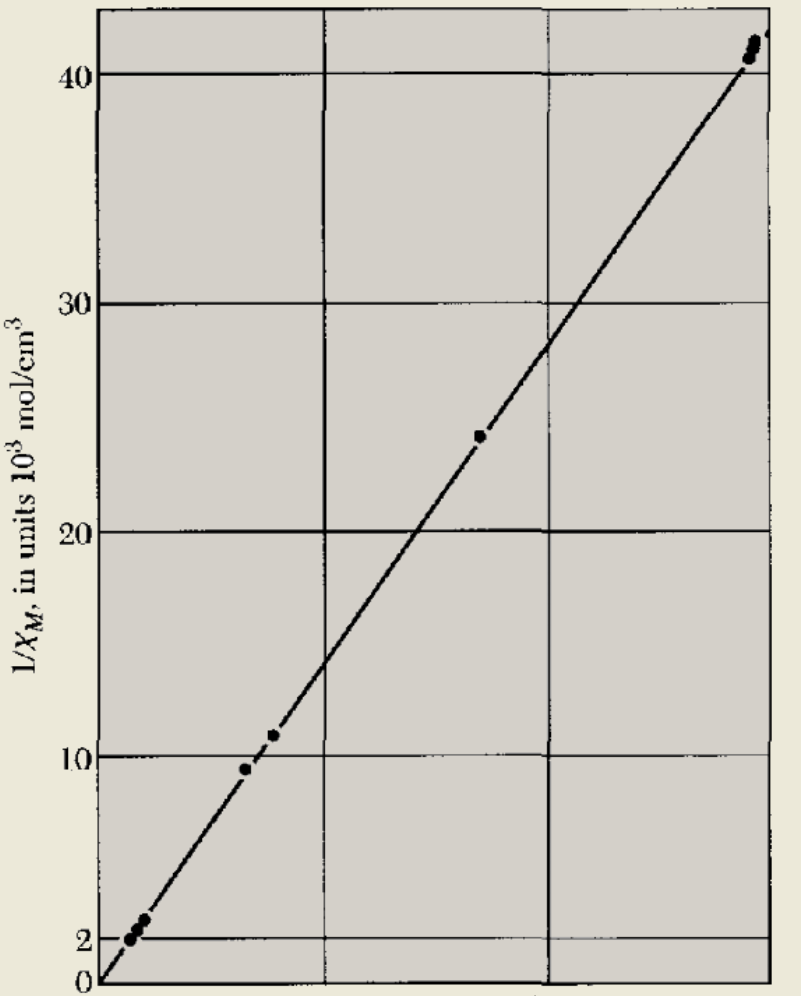


Figure 5
Plot of $1/\chi$ vs T for a gadolinium salt, $Gd(C_2H_3S0_4)_3 - 9H_20$. The straight line is the Curie law

Chapter 11: DIAMAGNETISM AND PARAMAGNETISM

Rare Earth Ions

- What distinguishes the magnetic behavior of one ion species from another is the number of *4f* electrons compacted in the inner shell with a radius of perhaps 0.3 Å
- The calculated magnoton numbers are obtained with g values from the Lande result (3)
- The discrepancy between the experimental magneton numbers and those calculated is quite marked for Eu^{3+} and Sm^{3+} ions.
- For these ions it is necessary to consider the influence of the high states of the *L* - S multiplet, as the intervals between successive states of the multiplet are not large compared to k_BT at room temperature
- A multiplet is the set of levels of different J values arising out of a given *L* and *S*.
- The *levels* of a multiplet are split by the spin-orbit interaction.

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 07

Chapter 12:
Ferromagnetism and Antiferromagnetism

Prof. Nasser S. Alzayed

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

NOTATION: (CGS) $B = H + 4\pi M$; (SI) $B = \mu_0(H + M)$. We call B_a the applied magnetic field in both systems of units: in CGS we have $B_a = H_a$ and in SI we have $B_a = \mu_0 H_a$. The susceptibility is $\chi = M/B_a$ in CGS and $\chi = M/H_a = \mu_0 M/B_a$ in SI. One tesla = 10^4 gauss.

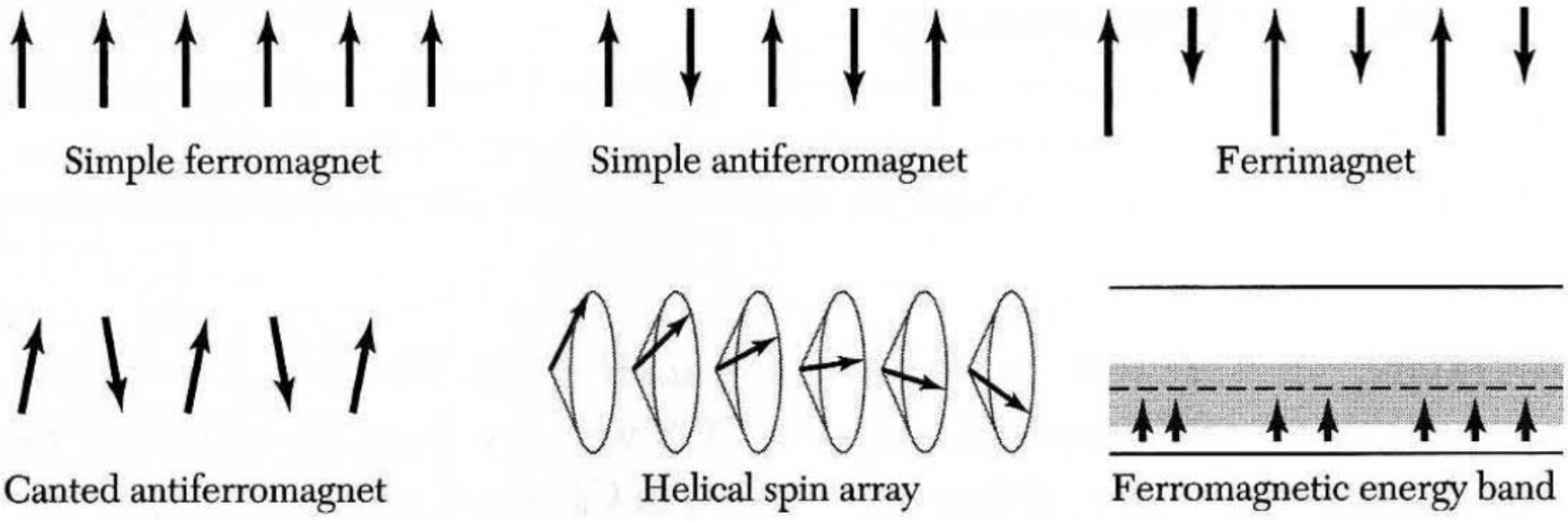


Figure 1 Ordered arrangements of electron spins.

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

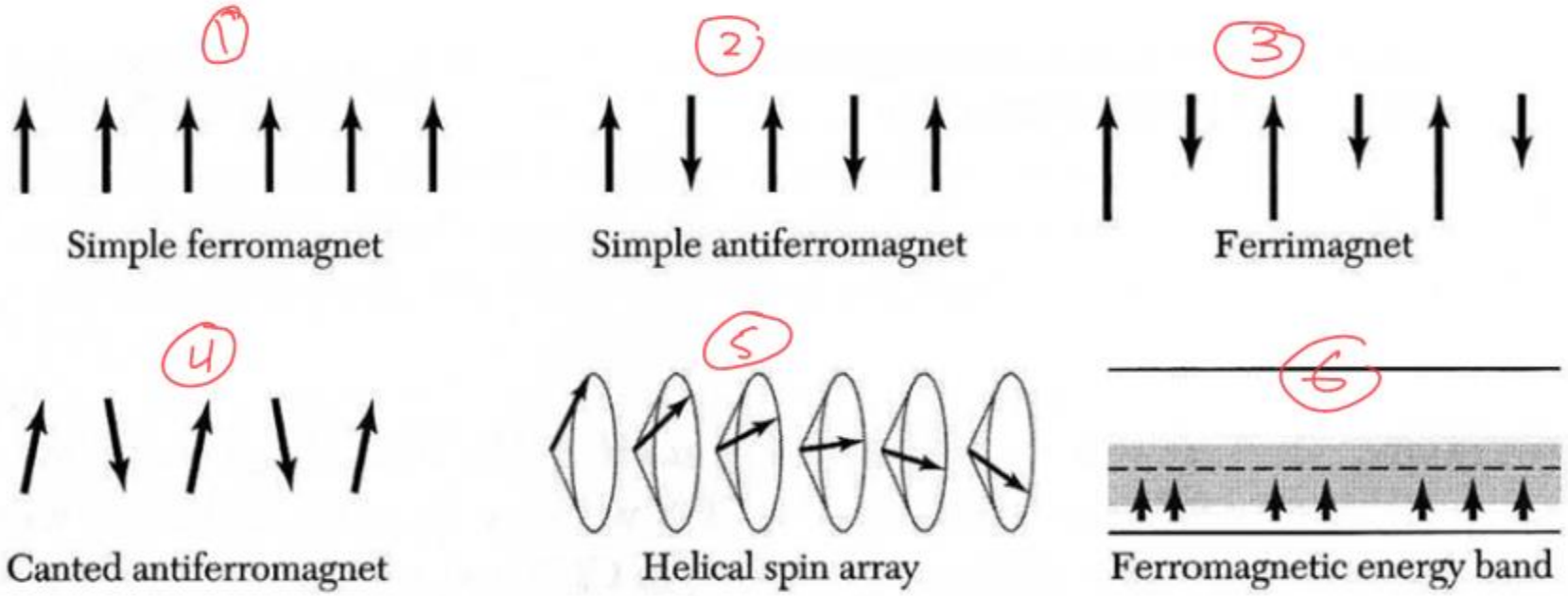


Figure 1 Ordered arrangements of electron spins.

(1) All spins are /// parallel.
→ strong magnetization

(2) adjacent spins are ↑↓ antiparallel
→ Zero magnetization

Fe Iron

MnO Manganese oxi

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

(3) opposite spins unequal in magnitude
→ Partial net magnetization Fe_3O_4 : magnetite

(4) spins mostly antiparallel α-Fe_2O_3 : Hematite
→ weak net magnetic moment.

(5) spins rotate gradually forming a spiral Mn Si manganese silicide
→ Zero or small macroscopic magnetization

(6) we have a split ↑ and ↓ bands Ni : Nickel
→ net spin polarization of electrons.

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

Ferromagnetism:

Ferro: taken from Latin word: Ferrum = Iron

⇒ Ferro: is Iron or Similar material depend.

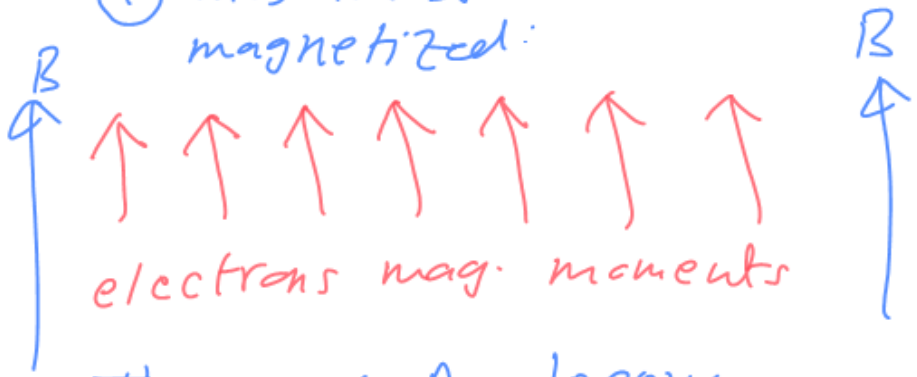
* In Periodic table Iron is Fe (from Ferrum)

Ferromagnetet: strongly pulled by mag.

examples: Fe, Co, Ni ...

Ferromagnetic feature:

① they are spontaneously magnetized:



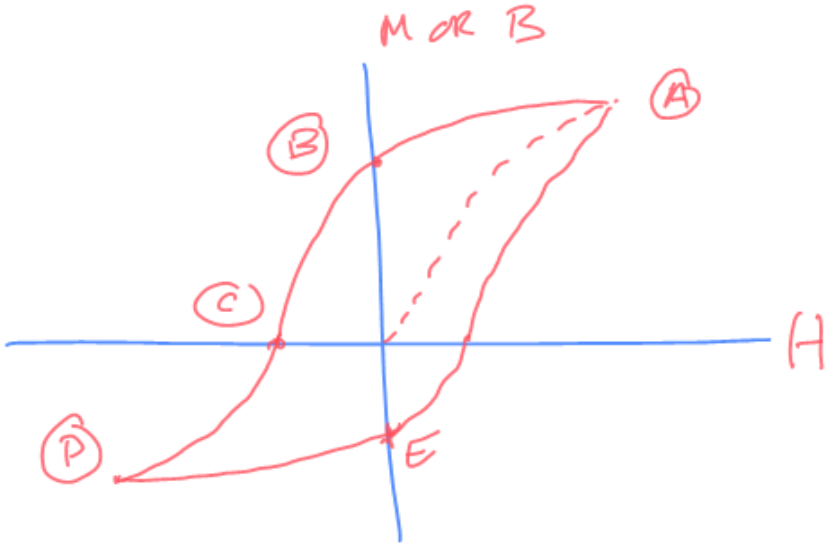
② they are Analogous to Ferroelectrics

Ferromagnetics	Ferroelectric
magnetic field	→ Electric field
magnetization	→ Polarization
magnetic moment	→ Dipole moment

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

③ Magnetization Increase as $\vec{B}_{ext}$ Increase with Hysteresis effect.



Ⓐ : saturation if H increase → B or M : no change

Ⓑ Remanence: the flux density that Remains after H = 0

Ⓒ Coercivity: at this H value M = 0

Ⓓ same as Ⓐ But in -ive H

Ⓔ First point when material is diamagnetized.

Ⓕ End of M-H full Loop.

at Ⓐ all spins are ↑↑↑

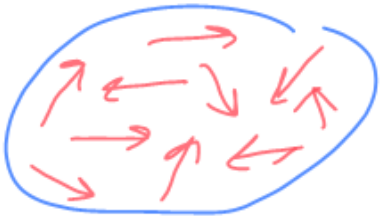
at Ⓓ " " " ↓↓↓

no more electron spins ⇒ Saturation

④ at $T = T_c$ M disappears

⑤ at $T > T_c$:

$$\chi = \frac{C}{T - T_c}$$ Curie-Weiss Law

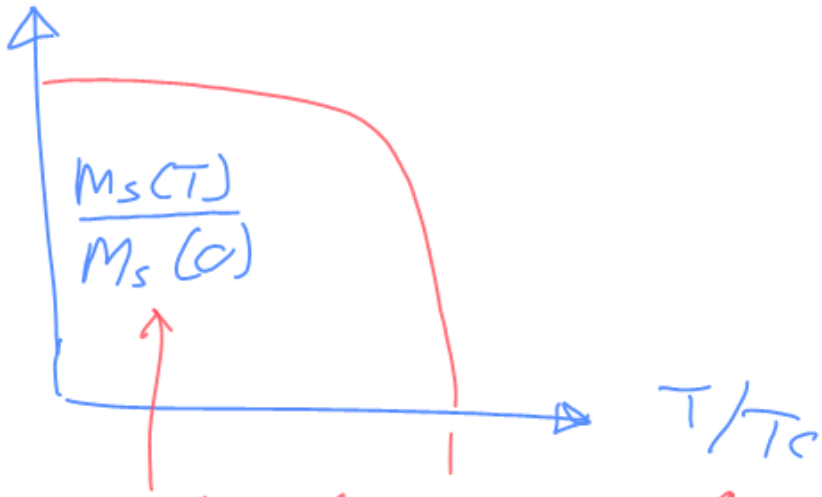


⑥ made of domains

each domain: $10^9 - 10^{15}$ atoms

→ net magnetization = 0

⑦ Saturation magnetization



⑧ Appears in metals + Insulators

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

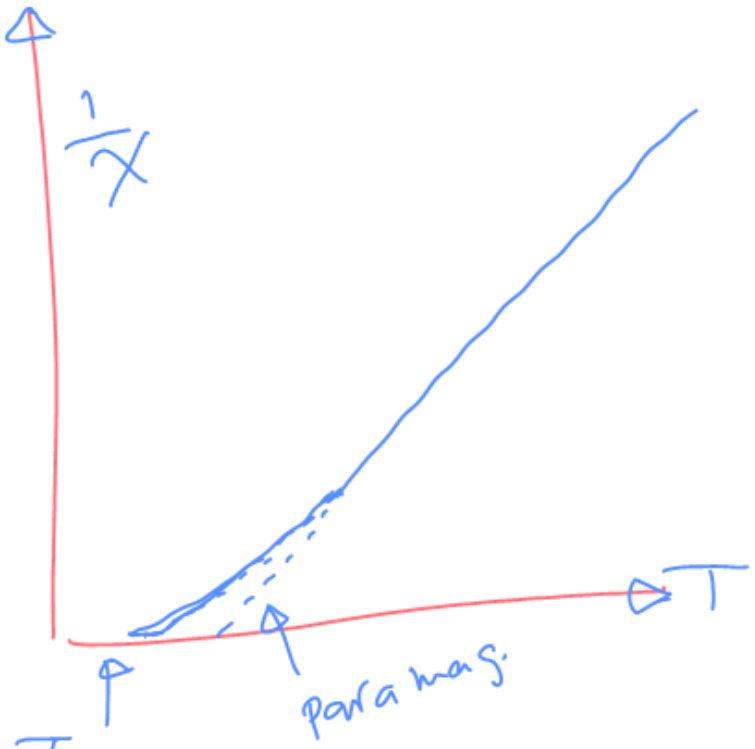
To plot $\chi = \frac{C}{T - T_c}$

we take

$$\frac{1}{\chi} = \frac{T - T_c}{C}$$

as $T \to T_c$

$\chi \to \infty$ (not defined)



$T_c = 358^{\circ}C$ for Nickel

Chapter 12: Ferromagnetism and Antiferromagnetism

FERROMAGNETIC ORDER

- A ferromagnet has a spontaneous magnetic moment. A magnetic moment ***even in zero applied magnetic field***.
- The existence of a spontaneous moment suggests that electron ***spins and magnetic moments are arranged in a regular manner***
- all of the spin arrangements sketched in Fig. 1 except the simple antiferromagnet have a spontaneous magnetic moment, called the saturation moment.

Chapter 12: Ferromagnetism and Antiferromagnetism

Curie Point and Weiss field

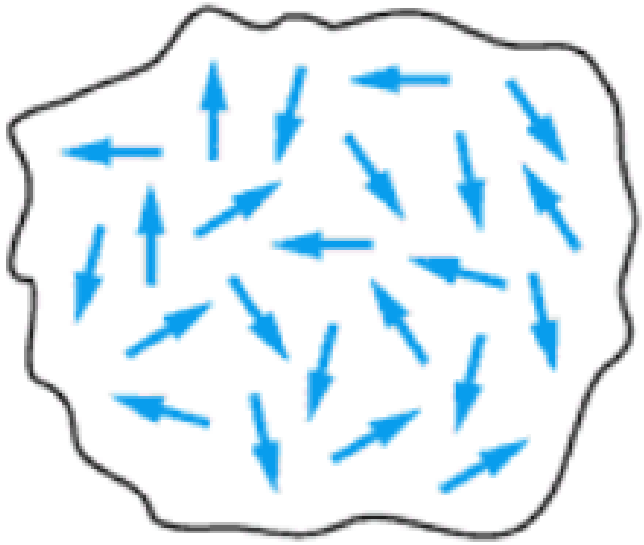
- If we have paramagnet with a concentration of N ions of spin S
- If all magnetic moments parallel to each other ➔ ferromagnet
- The field between all magnetic moments is called: ***Weiss field***
- The spin order is destroyed at some temperature
- We call Weiss field (Exchange field) $\mathbf{B}_E$
- $\mathbf{B}_E$ can be as high as 1000 Tesla. It is α to magnetization

$$\mathbf{B}_E = \lambda \mathbf{M} \qquad (1)$$

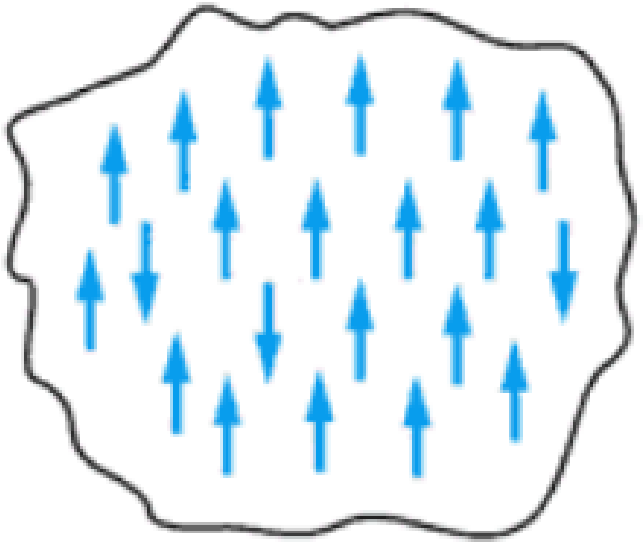
- λ is proportionality constant.
- (1) means that each *one spin* is affected by the average magnetization of all other spins
- We define ***Curie temperature*** (T = T_c) as the temperature above which the spontaneous magnetization vanishes

Curie Point and Weiss field

- We define ***Curie temperature*** (T = T_c)as the temperature above which the spontaneous magnetization vanishes



Above T_c



Below T_c

- Consider the paramagnetic phase:
- If we apply a magnetic field B_a ➔ ***M*** ➔ $\boldsymbol{B}_E$

$$\mathbf{M} = \chi_p (B_a + B_E) \qquad (2)$$

- were χ_p is the paramagnetic susceptibility

$$\because \chi_p = \frac{C}{T} \qquad (11.22)$$

$$\therefore \mathbf{M}T = C(B_a + \lambda M)$$

$$\Rightarrow B_a = \frac{\mathbf{M}T}{C} - \lambda M = \left(\frac{T}{C} - \lambda\right) M$$

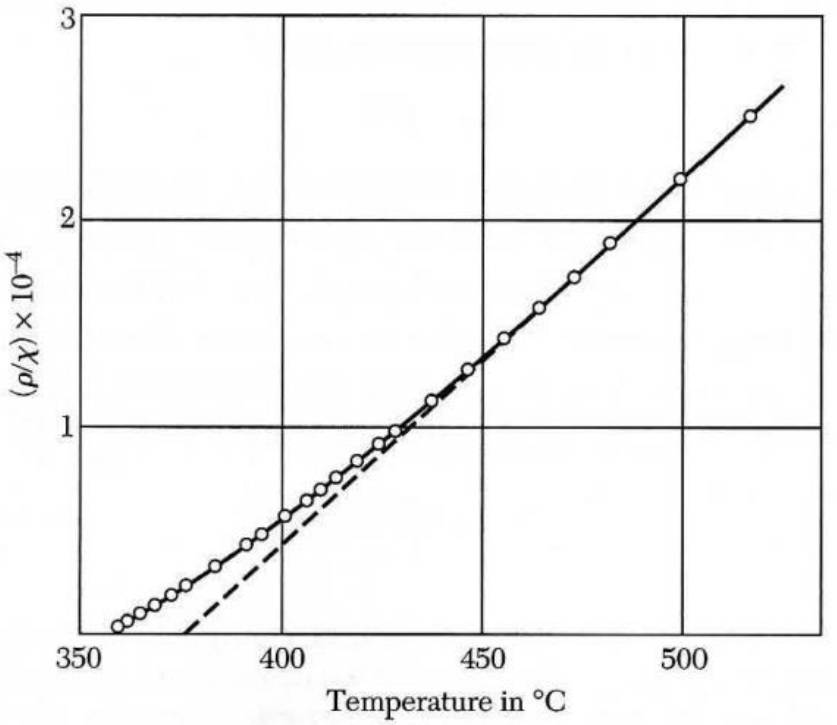
$$\therefore \chi = \frac{M}{B_a} = \frac{M}{\left(\frac{T}{C} - \lambda\right) M} = \frac{C}{T - \lambda C} \qquad (3)$$

- (3) has a singularity at $T = \lambda C$
- For temperatures $\leq$ T , there exists a spontaneous magnetization
- Hence, Curie-Weiss Law is:

$$\therefore \chi = \frac{C}{T - T_C} \qquad (4)$$

Figure 2

Reciprocal of the susceptibility per gram of nickel in the neighborhood of the Curie temperature (358°C). The density is ρ. The dashed line is a linear extrapolation from high temperatures.



- To calculate for λ, we use (4) and (11.22)
- From Chapter 11:

$$M = N\frac{g^2\mu_B^2 B}{3K_B T}J(J+1) \qquad (11.22)$$

- we use spin only here, hence J ➔ S and T ➔ T_C

$$\therefore M = N\frac{g^2\mu_B^2 B}{3K_B T}S(S+1) \qquad (5)$$

$$(1) \Rightarrow \lambda = \frac{B}{M} = \frac{B}{N\frac{g^2\mu_B^2 B}{3K_B T_c}S(S+1)} = \frac{3K_B T_c}{Ng^2 S(S+1)\mu_B^2} \qquad (6)$$

- For iron $T_c \approx 1000$ K, g = 2, and S = 1; (6) ➔ $\lambda = 5000$. With $M \approx$ 1700 we have $B_E = \lambda M \approx (5000)(1700) = 10^7$ G = 10^3 T

- It is possible to use *the mean field approximation* below the Curie temperature to find the magnetization as a function of temperature

$$\because M = N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \qquad (7)$$

$$(1) \rightarrow \mathrm{B} = \lambda \mathrm{M}$$

$$\therefore M = N\mu \tanh\left(\frac{\mu\lambda \mathrm{M}}{k_B T}\right) \qquad (8)$$

- (8) has solutions in the range: $0 < T < T_c$
- to solve (8), we use: reduced magnetization: *m* and reduced temperature: *t*

$$m = \frac{M}{N\mu}, \quad t = \frac{k_B T}{N\mu^2 \lambda} \qquad (9\,\mathrm{a})$$

$$\therefore m = N\,\mu \tanh\left(\frac{m}{t}\right) \qquad (9\,\mathrm{b})$$

- We then plot the right and left sides of this equation separately as functions of m, as in Fig. 3. The intercept of the two curves gives the value of *m* at the temperature of interest

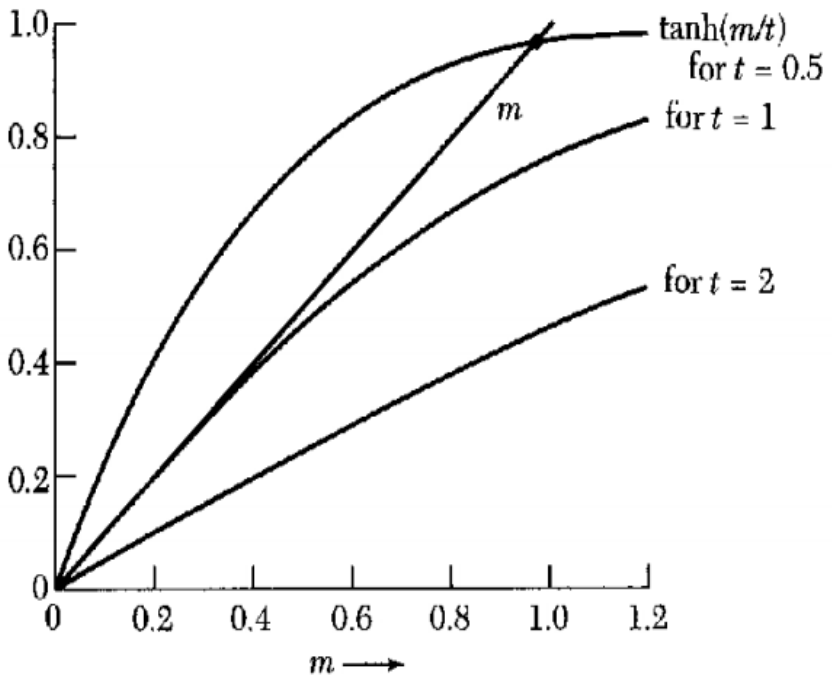
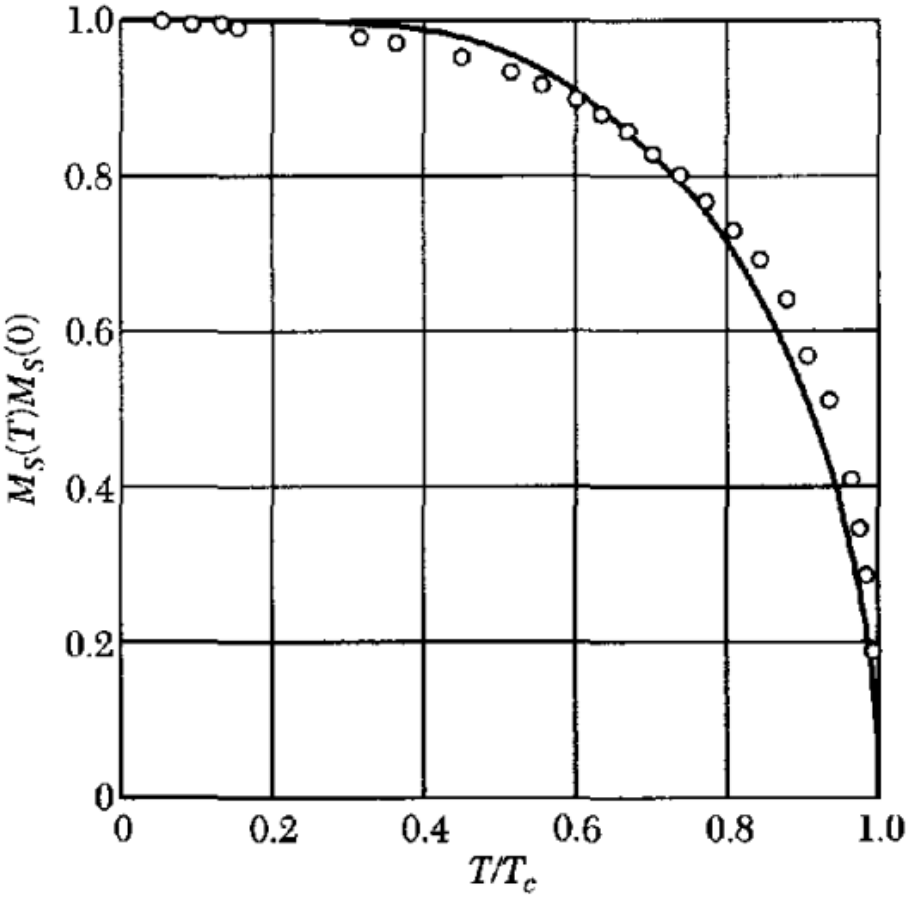


Figure 3 Graphical solution of Eq. (9b) for the reduced magnetization m as a function of temperature. The left-hand side of Eq. (9b) is plotted as a straight-line m with unit slope. The right-hand side is tanh(m/t) and is plotted vs. *m* for three different values of the reduced temperature *t* .The three curves correspond to $2T_c$, T_c and $O.5T_c$

- Experimentally as in Fig. 4 (For nickel)

- as shown in Fig. 4 for nickel. As T increases, the magnetization decreases smoothly to zero at $T = T_c$ This behavior classifies the usual ferromagnetic/paramagnetic transition as a second-order transition.
- In the figure: Solid line is theoretical curve for S = ½ on the mean field theory



Temperature Dependence of the Saturation Magnetization

$$\because M = N\mu \tanh\left(\frac{\mu B}{k_B T}\right) \qquad (11.17)$$

$$(1) \rightarrow \mathrm{B} = \lambda \mathrm{M}$$

$$\therefore M = N\mu \tanh\left(\frac{\mu\lambda \mathrm{M}}{k_B T}\right) \qquad (8)$$

T ≪ Tc :

$$(8) \rightarrow \tanh x \simeq 1 - 2e^{-2x}$$

$$\gamma \rightarrow M(0) = NM \tanh(\infty) = NM$$

$$\gamma \rightarrow M(T) \approx 1 - 2e^{-2\frac{\mu\lambda M}{K_B T}}$$

$$\therefore \Delta M = NM\left[1 - 1 + 2e^{-2\frac{\mu\lambda M}{K_B T}}\right] = 2NM\, e^{-2\frac{\mu\lambda M}{K_B T}} \qquad (10)$$

Temperature Dependence of the Saturation Magnetization

$$\because M = NM$$

$$\therefore \Delta M = 2NM\, e^{-\frac{2NM^2\lambda}{K_B T}}$$

$$\therefore \frac{2NM^2\lambda}{K_B T} = \frac{2}{T}\left(\frac{NM^2\lambda}{K_B}\right) = \frac{2}{T}(\lambda C) = \frac{2T_c}{T}$$

Temperature Dependence of the Saturation Magnetization

❑ For $T \ll T_C$ the argument of tanh in (8) is large, and:

$$\because \tanh x \cong 1 - 2e^{-2x}$$

$$\therefore (8) \text{ for } \Delta M = M(0) - M(T):$$

$$\Rightarrow \Delta M \approx N\mu\left[1 - 1 + 2e^{-\frac{2N\mu^2\lambda}{k_B T}}\right] = 2N\mu e^{-\frac{2N\mu^2\lambda}{k_B T}} \qquad (10)$$

$$\text{Note: } \frac{2N\mu^2\lambda}{k_B T} = \frac{2}{T}\left(\lambda . \frac{N\mu^2}{k_B}\right) = \frac{2}{T}(\lambda . C) = \frac{2T_c}{T}$$

$$\therefore (10) \rightarrow \Delta M \approx 2N\mu e^{-\frac{2T_c}{T}}$$

$$for: T = 0.1T_c:$$

$$\frac{\Delta M}{N\mu} = \frac{\Delta M}{M} \simeq 2 \times e^{-2(0.1)} = 2 \times 10^{-3} \qquad (11)$$

Chapter 12: Ferromagnetism and Antiferromagnetism

Saturation Magnetization at Absolute Zero

Table 1 Ferromagnetic crystals

Substance	Magnetization M_s, in gauss: Room temperature	Magnetization M_s, in gauss: 0 K	n_B(0 K), per formula unit	Curie temperature, in K
Fe	1707	1740	2.22	1043
Co	1400	1446	1.72	1388
Ni	485	510	0.606	627
Gd	—	2060	7.63	292
Dy	—	2920	10.2	88
MnAs	670	870	3.4	318
MnBi	620	680	3.52	630
MnSb	710	—	3.5	587
CrO_2	515	—	2.03	386
$MnOFe_2O_3$	410	—	5.0	573
$FeOFe_2O_3$	480	—	4.1	858
$NiOFe_2O_3$	270	—	2.4	(858)
$CuOFe_2O_3$	135	—	1.3	728
$MgOFe_2O_3$	110	—	1.1	713
EuO	—	1920	6.8	69
$Y_3Fe_5O_{12}$	130	200	5.0	560

Chapter 12: Ferromagnetism and Antiferromagnetism

Saturation Magnetization at Absolute Zero

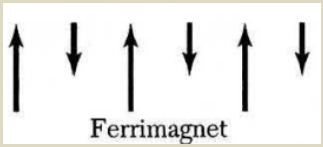
- n_B is the effective magneton no. $M_s(0) = n_B N \mu_B$

Why n_B is nonintegral?

1- Because of the spin-orbit interaction which adds or subtracts some orbital magnetic moment

2- the conduction electron magnetization induced locally about a paramagnetic ion core.

3- if there is one atom of spin projection - S for every two atoms +S, the average spin is ⅓S.



- At ground state (0 K), there are only few materials that show simple ferromagnetic behavior: all ionic spins parallel ↑ ↑ ↑ ↑ ↑
- Examples are: $CrBr_3$, EuO, and EuS.
- sometimes these materials are called: *simple ferromagnetic insulators*

MAGNONS

- *Magnon* = quantized spin wave
- *Photons, Phonons, and Magnons are all quantized*
- The ground state of a simple ferromagnet has all spins parallel.
- Consider *N* spins each of magnitude S on a line or a ring, with nearest-neighbor spins coupled by the *Heisenberg interaction*:

$$U = -2J\sum_{p=1}^{N} S_p . S_{p+1} \qquad (12)$$

- The quantization of spin waves proceeds as for photons and phonons. The energy of a mode of frequency ω_k with n_k magnons is given by:

$$\varepsilon_k = (n_k + \frac{1}{2})\hbar\omega_k \qquad (26)$$

Chapter 12: Ferromagnetism and Antiferromagnetism

MAGNONS

- The excitation of a magnon corresponds to the reversal of one spin =½

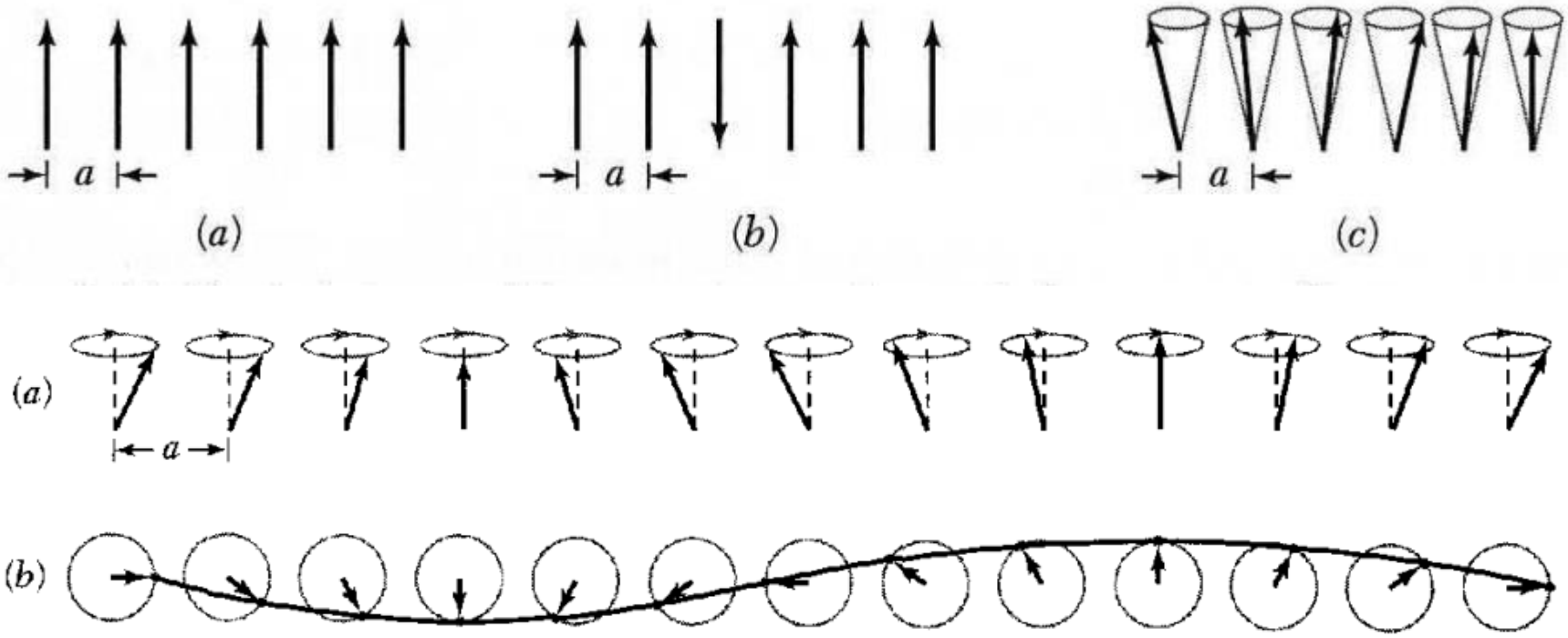


Figure 9 A spin wave on a line of spins. (a) The spins viewed in perspective. (b) Spins viewed from above, showing one wavelength. The wave is drawn through the ends of the spin vectors.

Thermal Excitation of MAGNONS

Thermal excitation of magnons-

* magnons can be created by thermal exitation
* density of states: $\frac{\text{No. of exited magnons}}{\text{total No. of spins}}$

* Each magnon lowers $\downarrow$ the z-component of the total spin by $\underline{1}$ unit

* total No. of magn. in all states exited at Temp. T;

$$\sum_{K} n_K = \int_0^{\infty} d\omega\, z(\omega)\cdot \bar{n}_K \quad ---(1)$$

$z(\omega)$: density of states; $\bar{n}_K$: average No. of magnons.

Thermal Excitation of MAGNONS

* In 3-D: No. of modes / Unit volume $= \left(\frac{1}{2\pi}\right)^3 \left(\frac{4}{3}\pi k^3\right)$ (2)

$$\Rightarrow z(\omega)d\omega = \left(\frac{1}{2\pi}\right)^3 \frac{4\pi}{3} \cdot 3k^2 dk \quad \text{---} \quad (3)$$

$$\rightarrow \quad z(\omega) = \left(\frac{1}{2\pi}\right)^3 4\pi k^2 \frac{dk}{d\omega} \quad \text{---} \quad (4)$$

* from dispersion Relation:

$$\hbar\omega = 2JSa^2k^2 \quad \text{---} \quad (5)$$

$$\Rightarrow \frac{dk}{d\omega} = \frac{\hbar}{4JSa^2k} \quad \text{---} \quad (6)$$

$$(5) \rightarrow k = \left(\frac{\hbar\omega}{2JSa^2}\right)^{1/2} \quad \text{---} \quad (7)$$

(7) in (6) for 4π:

$$\frac{dk}{d\omega} = \frac{\hbar}{4JSa^2}\left(\frac{2JSa^2}{\hbar\omega}\right)^{1/2}$$

$$= \frac{1}{2}\left(\frac{\hbar}{2JSa^2}\right)^{1/2}\frac{1}{\sqrt{\omega}} \quad ---(8)$$

(8) in (4): $Z(\omega) = \left(\frac{1}{2\pi}\right)^3 4\pi\left[\frac{\hbar\omega}{2JSa^2}\right]\cdot\frac{1}{2}\left(\frac{\hbar}{2JSa^2}\right)^{1/2}\frac{1}{\sqrt{\omega}}$

$$\therefore Z(\omega) = \frac{1}{8\pi^3}\cdot\frac{4\pi}{2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\omega^{1/2}$$

$$\therefore Z(\omega) = \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\omega^{1/2} \quad ---(9)$$

↳ density of modes of magnons.

Thermal Excitation of MAGNONS

We can use (9) in (1).

But we need to consider thermal equilibrium conditions:

$\bar{n}_k \longrightarrow$ plank's distribution function:

$$\bar{n}_k = \langle n_k \rangle = \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} \quad \text{---} \quad (10)$$

(9) and (10) in (1) :

$$\Rightarrow \sum_k n_k = \int_0^{\omega_c} \frac{1}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \omega^{1/2} \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1} \, d\omega \quad (11)$$

$$= \frac{1}{4\pi^2} \left(\frac{\hbar}{2JSa^2}\right)^{3/2} \int_0^{\omega_c} \frac{\omega^{1/2}}{e^{\frac{\hbar\omega}{k_B T}} - 1} \, d\omega \quad (12)$$

Thermal Excitation of MAGNONS

Now: let $x = \frac{\hbar\omega}{k_B T} \Rightarrow d\omega = \frac{k_B T}{\hbar} dx$ --- (13)

$$\Rightarrow \sum_k n_k = \frac{1}{4\pi^2}\left(\frac{k_B T}{2JSa^2}\right)^{3/2} \int_0^{\beta} \frac{x^{1/2}}{e^x - 1} dx \quad (14)$$

from tables

$$\sum_k n_k = 0.0587 \left(\frac{k_B T}{2JSa^2}\right)^{3/2} \quad --- (15)$$

this is the No. of mag. excited thermally / unit volume.

$$\Rightarrow \frac{\Delta M}{M(0)} = \frac{0.0587}{SQ} \cdot \left(\frac{k_B T}{2JS}\right)^{3/2}$$

where $\alpha/a^3 \equiv$ No. of atoms per unit volume

$\alpha = 1, 2, 4$ for sc, bcc and fcc lattice

Thermal Excitation of MAGNONS

- In thermal equilibrium the average value of the number of magnons excited in the mode **k** is given by the Planck distribution

$$\langle n_k \rangle = \frac{1}{e^{(\hbar\omega_k / k_B T)} - 1} \qquad (27)$$

- Total No. of magnon excited at T using D(ω) as the number of magnon modes per unit frequency range, is:

$$\sum_k n_k = \int D(\omega) \langle n(\omega) \rangle d\omega \qquad (28)$$

- The integral is taken over all values of k (in the 1st Brillouin zone).
- Magnons have a single polarization for each value of k. In three dimensions the numher of modes of wavevector less than *k* is:

$$(\text{density per unt volume}) \times (\text{total volume in k-space}) = \left(\frac{1}{2\pi}\right)^3 . \left(\frac{4}{3}\pi k^3\right)$$

$$\therefore \frac{d\omega}{dk} = \left(\frac{1}{2\pi}\right)^3 .\left(4\pi k^2\right)$$

$$\text{from}\,(25): \hbar\omega = (2JSa^2)k^2$$

$$\therefore \frac{d\omega}{dk} = \frac{4JSa^2k}{\hbar} = \frac{4JSa^2}{\hbar}\sqrt{\frac{\hbar\omega}{2JSa^2}} = 2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2} \qquad (29)$$

- Hence, density of modes for magnons is:

$$\therefore \frac{d\omega}{dk} = \left(\frac{1}{2\pi}\right)^3 .\left(4\pi k^2\right)$$

$$\text{from}\,(25): \hbar\omega = (2JSa^2)k^2$$

$$\therefore \frac{d\omega}{dk} = \frac{4JSa^2k}{\hbar} = \frac{4JSa^2}{\hbar}\sqrt{\frac{\hbar\omega}{2JSa^2}} = 2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2} \qquad (29)$$

- whence the number of magnons $D(\omega)d\omega$ with frequency in $d\omega$ at ω is: $\left(\frac{1}{2\pi}\right)^3 .\left(4\pi k^2\right)\frac{dk}{d\omega}d\omega$

Thermal Excitation of MAGNONS

$$\because \left(\frac{1}{2\pi}\right)^3 .\left(4\pi k^2\right)\frac{dk}{d\omega}d\omega$$

$$\because \hbar\omega = (2JSa^2)k^2 \rightarrow k^2 = \frac{\hbar\omega}{2JSa^2}$$

$$\because \frac{d\omega}{dk} = 2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2}$$

$$\therefore D(\omega) = \left(\frac{1}{2\pi}\right)^3 .(4\pi)\frac{\hbar\omega}{2JSa^2}\frac{1}{2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2}}$$

$$\therefore D(\omega) = \frac{1}{8\pi^3}.4\pi.\frac{\hbar\omega}{2JSa^2}.\frac{1}{2}\frac{1}{\omega^{1/2}}.\left(\frac{\hbar}{2JSa^2}\right)^{1/2}$$

$$\therefore D(\omega) = \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\omega^{1/2} \qquad (29)$$

$$\therefore (28) \Rightarrow \sum_k n_k = \int D(\omega)\langle n(\omega)\rangle d\omega = \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\int_0^\infty \frac{\omega^{1/2}}{e^{(\hbar\omega_k/k_BT)}-1}d\omega$$

❑ Integral from tables =$(0.0587)(4\pi^2)$

Thermal Excitation of MAGNONS

$$\because \left(\frac{1}{2\pi}\right)^3 .\left(4\pi k^2\right)\frac{dk}{d\omega}d\omega$$

$$\because \hbar\omega = (2JSa^2)k^2 \rightarrow k^2 = \frac{\hbar\omega}{2JSa^2}$$

$$\because \frac{d\omega}{dk} = 2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2}$$

$$\therefore D(\omega) = \left(\frac{1}{2\pi}\right)^3 .(4\pi)\frac{\hbar\omega}{2JSa^2}\frac{1}{2\left(\frac{2JSa^2}{\hbar}\right)^{1/2}\omega^{1/2}}$$

$$\therefore D(\omega) = \frac{1}{8\pi^3}.4\pi.\frac{\hbar\omega}{2JSa^2}.\frac{1}{2}\frac{1}{\omega^{1/2}}.\left(\frac{\hbar}{2JSa^2}\right)^{1/2}$$

$$\therefore D(\omega) = \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\omega^{1/2} \qquad (29)$$

$$\therefore (28) \Rightarrow \sum_k n_k = \int D(\omega)\langle n(\omega)\rangle d\omega = \frac{1}{4\pi^2}\left(\frac{\hbar}{2JSa^2}\right)^{3/2}\int_0^\infty \frac{\omega^{1/2}}{e^{(\hbar\omega_k/k_BT)}-1}d\omega$$

❑ Integral from tables =$(0.0587)(4\pi^2)$

$$\Rightarrow \sum_k n_k = \left(\frac{\hbar}{2JSa^2}\right)^{3/2} (0.0587)$$

- We can arrange terms to get:

$$\frac{\Delta M}{M(0)} = \frac{0.0587}{SQ} \cdot \left(\frac{k_B T}{2JS}\right)^{3/2}$$

- This result is thc **Bloch $T^{3/2}$ law** and has been confirmed experimentally

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025/2022

Lecture No. 08

Chapter 12:
Ferromagnetism and Antiferromagnetism

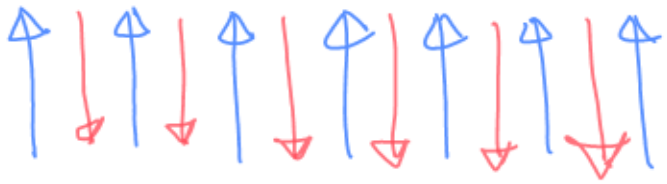
Prof. Nasser S. Alzayed

ANTIFERROMAGNETIC ORDER

Antiferromagnetism Properties:

① spins in so,

They are anti-parallel



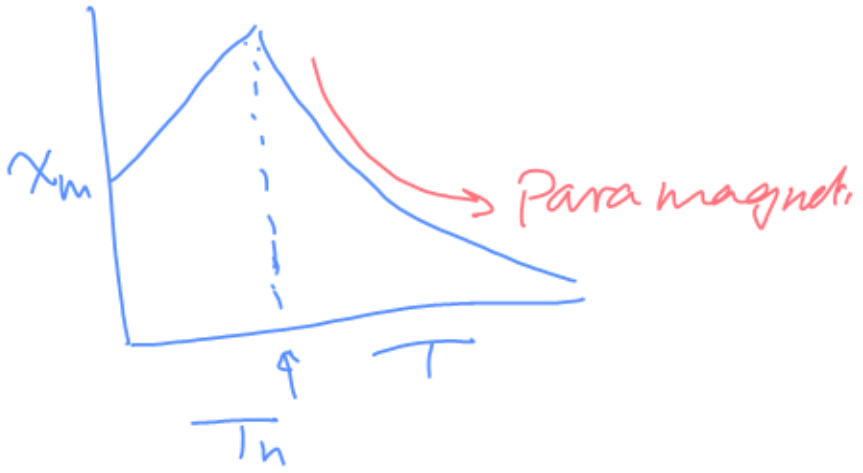
this happens when distances Between atoms are very small

⇒ exchange forces Lead to anti-parallel spin orientation

② it was first observed experim. By Bizette, Squire & Tsai 1938

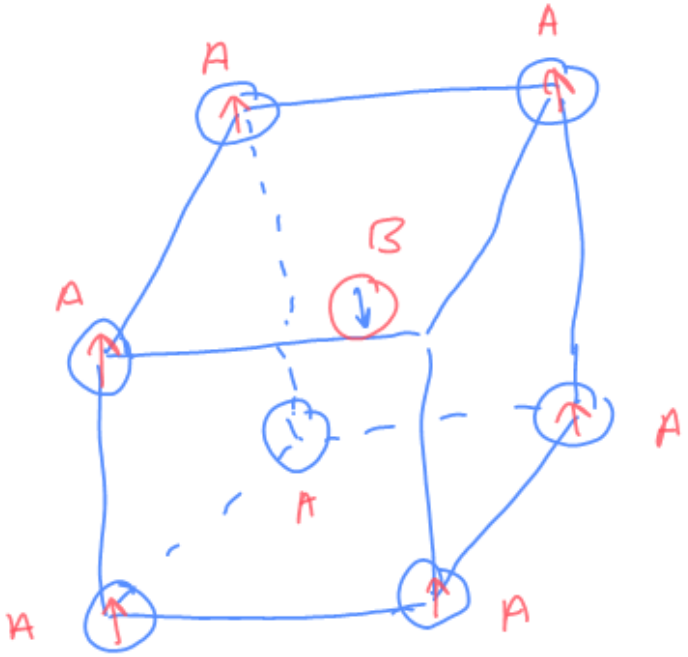
in: MnO

③ χ_m is like:



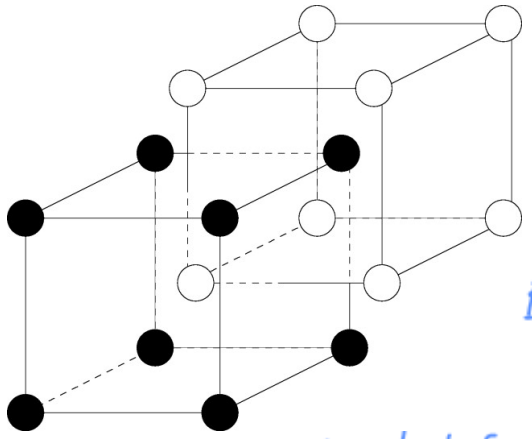
only antiferromagnetic material show max vs. T.

④ It can be explained using Lattices:



2 sublattice model

④ in MnF_2: Also Antif



B atoms

A atoms

two sublattice model

Molecular Field theory of Anti-Ferromagnetism

① At $T=0$: net magnetization $=0$

② As $T \longrightarrow$ up , magnetization increases

③ It keeps increasing up to $T=T_N$

④ N : for Neal (Neal point).

⑤ When $T > T_N \Rightarrow$ Paramagnetic

⑥ Assume that we do have Two Types of Ions
$-\frac{1}{2}$ are (A) $+\frac{1}{2}$ are (B):

⑦ Internal field for (A) Ions : $H_A = H - \lambda M_B$ ①

" " " (B) " : $H_B = H - \lambda M_A$ ②

λ : Internal field Constant

$\equiv$ Weiss constant

(8) we have 2 cases:

Case 1: $T > T_N$: Paramagnetism

from our prev. lectures:

$$M = N g \mu_B \tanh\left(\frac{g\mu_B}{k_B T} B\right)$$

$$\equiv N g \mu_B \tanh\left(\frac{g \mu_B \mu_0}{k_B T} H\right)$$

$$\Rightarrow M_A = N g \mu_B \tanh\left[\frac{g\mu_B \mu_0}{k_B T}(H - \lambda M_B)\right] \quad (3)$$

and $M_B = N g \mu_B \tanh\left[\frac{g\mu_B \mu_0}{k_B T}(H - \lambda M_A)\right]$ (4)

At high T : $\tanh x \approx x$

(3) $\rightarrow$ $$M_A \approx \frac{N g^2 \mu_B^2 \mu_0 (H - \lambda M_B)}{k_B T} \quad \text{---(5)}$$

(4) $\rightarrow$ $$M_B \approx \frac{N g^2 \mu_B^2 \mu_0 (H - \lambda M_A)}{k_B T} \quad \text{---(6)}$$

$\Rightarrow$ Total magnetization $= M = M_A + M_B$

$\Rightarrow$ $$M = \frac{N g^2 \mu_B^2 \mu_0 (2H - \lambda M)}{k_B T} \quad \text{----(7)}$$

(9): for χ : let $M \parallel H$:

$$\chi = \frac{M}{H} = \frac{N g^2 \mu_B^2 \mu_0}{k_B T} \left(\frac{2H - \lambda M}{H}\right) \quad \text{---(8)}$$

$$\Rightarrow \chi = \frac{C}{T}\left(2 - \frac{\lambda M}{H}\right)$$

C: Curie Const (9)

$$\Rightarrow \chi = \frac{C}{T}(2 - \lambda\chi)$$

$$= \frac{2C}{T} - \frac{\lambda C}{T}\chi$$

$$\Rightarrow \chi + \frac{\lambda C}{T}\chi = \frac{2C}{T}$$

$$\Rightarrow \chi\left(1 + \frac{\lambda C}{T}\right) = \frac{2C}{T}$$

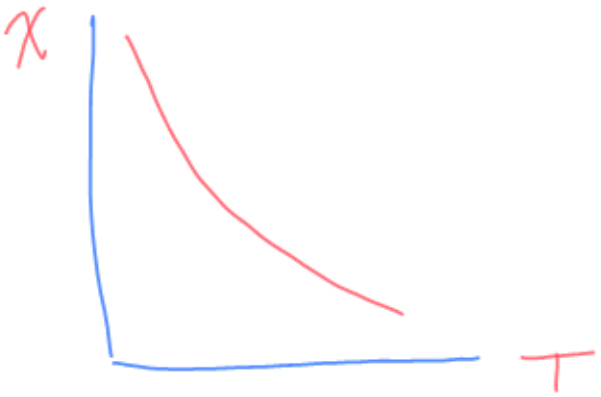
$$\Rightarrow \chi = \frac{2C}{T} \div \frac{T + \lambda C}{T} = \frac{2C}{T} \times \frac{T}{T + \lambda C}$$

$$\therefore \chi = \frac{2C}{T + \lambda C}$$

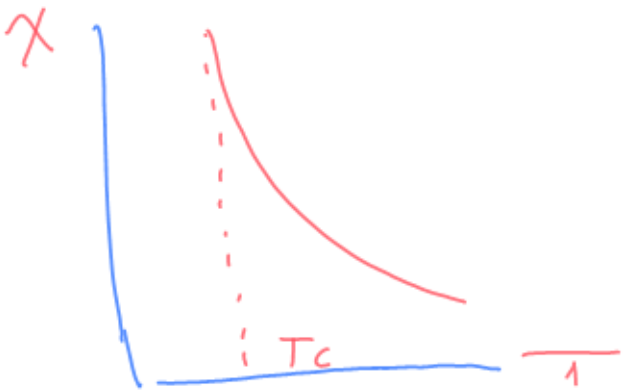
$$\boxed{\therefore \chi = \frac{2C}{T + T_N}} \quad \cdots (10)$$

Remember $\chi_p = \frac{C}{T - T_c}$ (Paramagnetic)

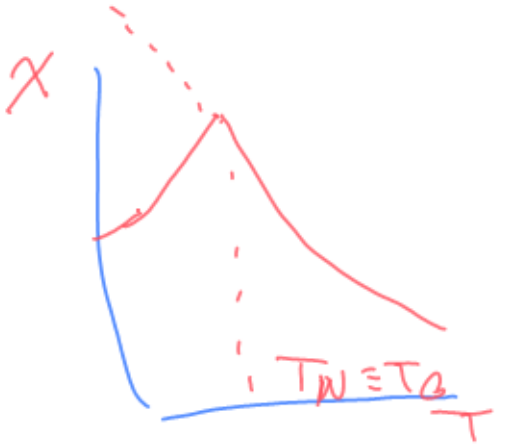
2C's one for (A) (B)



Paramagnetic



Ferromagnetic



antifer.

Spontaneous Magnetization when $T > T_N$:

if $H = 0$; $M_A = \frac{N g^2 \mu_B^2 \mu_0}{K_B T} (H - \lambda M_B)$ $\quad H = 0$

$$= -\lambda \frac{N g^2 \mu_B^2 \mu_0}{K_B T} M_B$$

$$= -\frac{C}{T} \lambda M_B$$

$$\Rightarrow M_A + \frac{C\lambda}{T} M_B = 0 \quad \text{----- (11)}$$

Also $M_B + \frac{C\lambda}{T} M_A = 0 \quad$ ---- (12)

(11) and (12) can have only $M_A = M_B = 0$ solution

$\Rightarrow$ When $T > T_N$ and $H = 0$ No Spontaneous Mag.

2. Antiferromagnet $\xrightarrow{T > T_N}$ Paramagnet

at $T = T_N$: (11) and (12) $\Rightarrow$

$$M_A + \frac{c\lambda}{T_N} M_B = 0 \quad \cdots (13)$$

$$M_B + \frac{c\lambda}{T_N} M_A = 0 \quad \cdots (14)$$

$$\Rightarrow (M_A - M_B) + \frac{c\lambda}{T_N}(M_B - M_A) = 0$$

$$\rightarrow (M_A - M_B) - \frac{c\lambda}{T_N}(M_A - M_B) = 0$$

$$\Rightarrow \frac{c\lambda}{T_N} - 1 = 0 \Rightarrow c\lambda = T_N \quad \text{as expected} \quad (15)$$

Case 2°. $T < T_N$

short: Antiferromagnetics: $T > T_N$ } ⇒ Paramagnetic
Ferromagnetics: $T > T_c$ }

here also:

1. A atoms Interact with B atoms only
2. χ depends on H direction

tow states:

a- H ⊥ spin

b- H // "

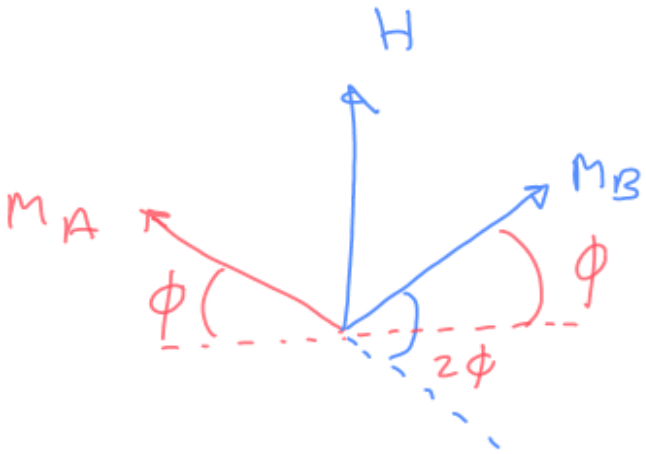
a) If H ⊥ spin of A & B:

⇒ Both M_A & M_B will allign with H if Possible

$\Rightarrow$ they will adjust at angle of 2ϕ (See drawing)

2ϕ is small angle.

from ① and ② with $H=0$ where only Molecular field is Concidered:



M_A component on B: $-\lambda M_A \sin 2\phi \;//\; H$

$\simeq -\lambda M_A (2\phi) \;//\; H$

At equilibrium: $H = 2\phi \lambda M_B$ ---(15)

$\therefore |M_B| = |M_A|$

$\Rightarrow M \simeq 2\phi \frac{M_A}{M_B}$ ---(16)

$$\Rightarrow M = \frac{2\phi \cdot H}{2\phi\lambda} \Rightarrow M = \frac{H}{\lambda} \quad ---(17)$$

$$\Rightarrow \chi_\perp = \frac{M}{H} = \frac{M}{\lambda \cdot M} = \frac{1}{\lambda}$$

$$\therefore \chi_\perp = \frac{1}{\lambda} \quad ----(18)$$

note that the $\chi_\perp$ is not T dep.

b) if H // spin

Since $M_A \uparrow$ and $M_B \downarrow \Rightarrow M = 0$ at $T = 0$ K

$\rightarrow \chi_{//} = 0$ at $T = 0$ K

As $T \rightarrow$ up to T_N

$\Rightarrow \chi_{//}$ increases as well

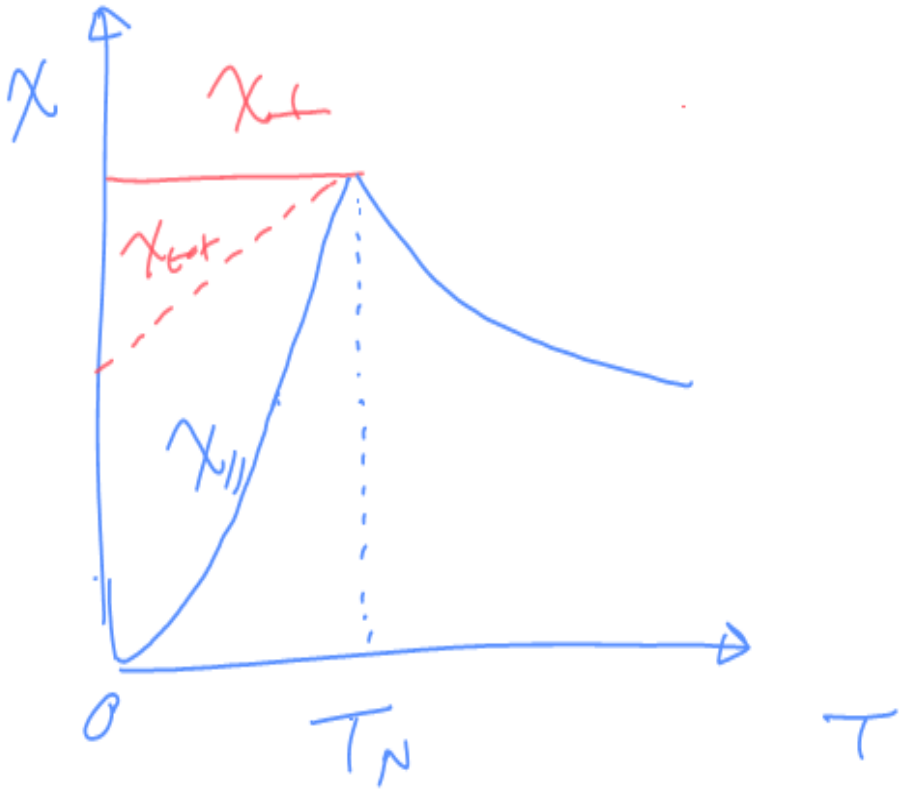
χ_{total} is expressed as $(T = 0)$

$$\chi_{total} = \frac{1}{3}\chi_{//}(0) + \frac{2}{3}\chi_{\perp}(0) = \frac{2}{3}\chi_{\perp}(0)$$

at the max $T = T_N$:

$$\chi_{tot} = \frac{2}{3}\chi_{\perp}(0) = \frac{2}{3}\chi_{\perp}(T_N) = \frac{2}{3}\chi(T_N)$$

ANTIFERROMAGNETIC ORDER



Magnetic Phase Transition ?

Rule:

Whenever order is destroyed

→ paramagnetism (default magnetic state)

When $T \to \infty$ ⇒ destroy of order

⇒ spins are Random

⇒ magnetic field ⇒ new order

① Ferromagnet: $T < T_c$ ordered state

$T > T_c$ none ordered state : Paramagnetism

Analogy: Imagine a classroom of students (magnetic moments). In the ferromagnetic state, a strict teacher (exchange interaction) makes them all face the front. As the room gets hotter (thermal energy), the students get fidgety. At a critical temperature (T_C), they can no longer sit still and start looking in all random directions (paramagnetic state).

② AntiFerromagnetism: $T < T_N$: ordered state

$T > T_N$: none " " : paramanetism

Analogy: Imagine a dance with partners (neighboring moments). In the antiferromagnetic state, the choreography (exchange interaction) dictates that one partner spins left while the other spins right, perfectly balanced. As the room heats up (thermal energy), the dancers get sloppy. Above T_N, they abandon the choreography entirely and just move randomly (paramagnetic state). The group as a whole still has no preferred direction, but now it's due to chaos, not perfect order.

Chapter 12: Ferromagnetism and Antiferromagnetism

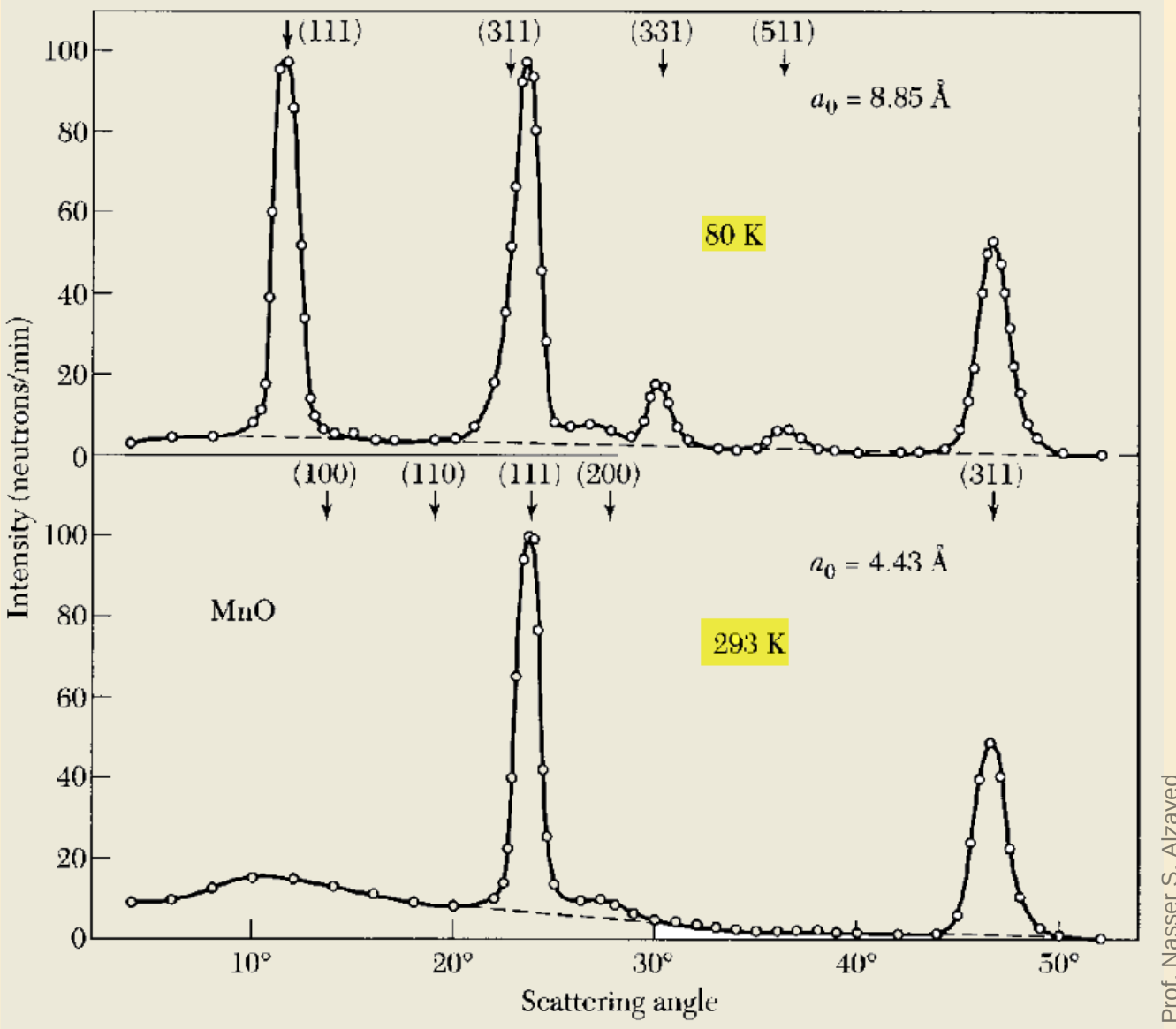
ANTIFERROMAGNETIC ORDER

- Fig. 17 shows a classical example of magnetic structure for MnO, which has the NaCl structure.
- At 80 K there are extra neutron reflections not present at 293 K.
- The reflections at 80 K may be classified in terms of a cubic unit cell of lattice constant 8.85 Å.
- At 293 K the reflections correspond to an fcc unit cell of lattice constant 4.43 Å
- But the lattice constant determined by x-ray reflection is 4.43 Å at both temperatures, 80 K and 293 K. We conclude that the chemical unit cell has the 4.43 Å lattice parameter, but that at 80 K the electronic magnetic moments of the Mn^{2+} ions are ordered in some nonferromagnetic arrangement.

Chapter 12: Ferromagnetism and Antiferromagnetism

ANTIFERROMAGNETIC ORDER

Figure 17 Neutron diffraction patterns for MnO below and above the spin-ordering temperature of 120 K. The reflection indices are based on an 8.85 Å cell at 80 K and on a 4.43 Å cell at 293 K. At the higher temperature the Mn^{2+} ions are still magnetic, but they are no longer ordered.



Chapter 12: Ferromagnetism and Antiferromagnetism

ANTIFERROMAGNETIC ORDER

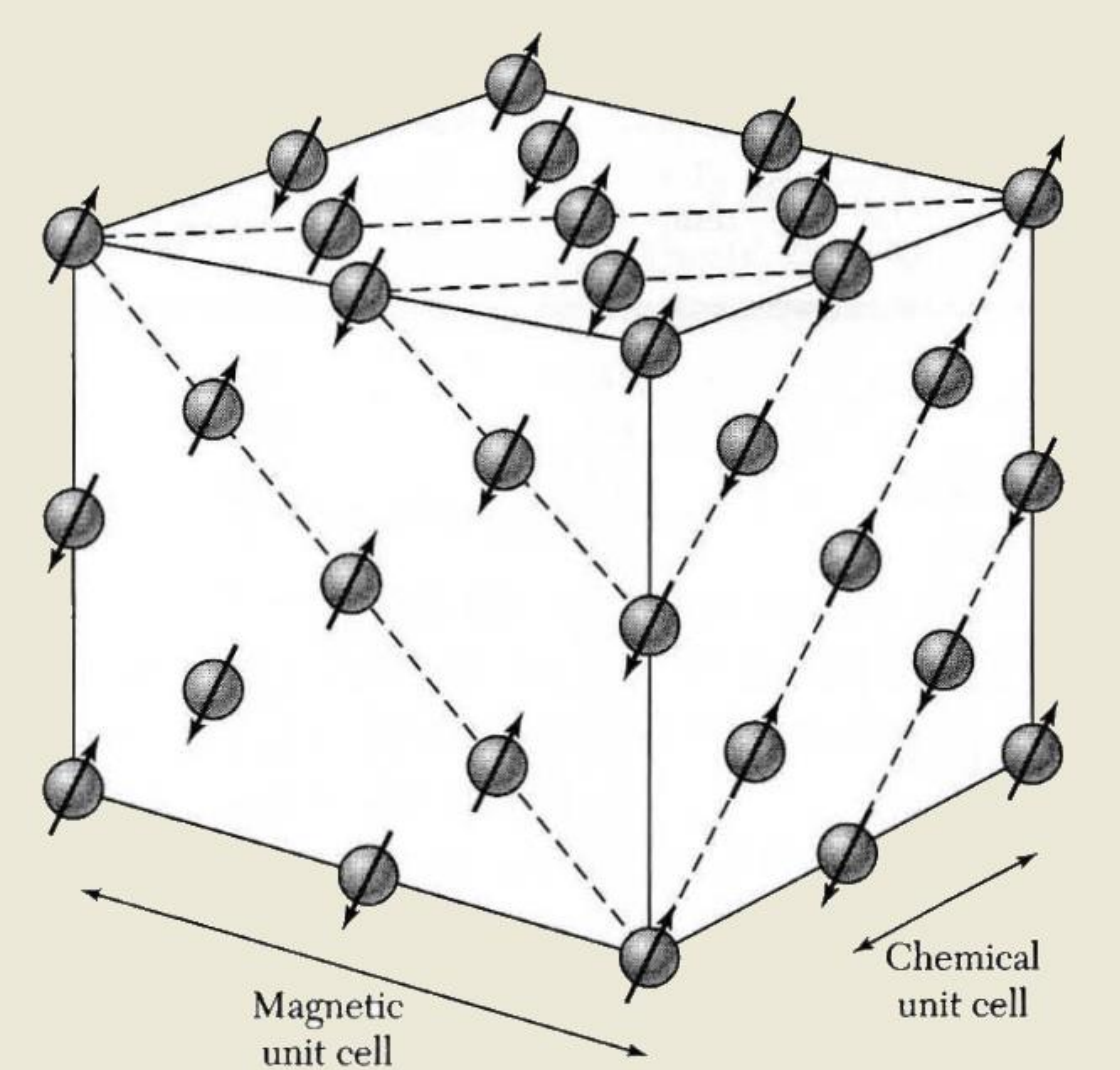


Figure 18
Ordered arrangements of spins of the Mn^{2+} ions in manganese oxide, MnO, as determined by neutron diffraction. The O^{2+} ions are not shown.

Chapter 12: Ferromagnetism and Antiferromagnetism

Magnetic Force Microscopy

- The success of the scanning tunneling microscope (STM) stimulated the development of related scanning probe devices, of which the scanning magnetic force microscope is one of the most effective.
- A sharp tip of a magnetic material, such as nickel, is mounted on a cantilever lever.
- Forces from the magnetic sample act on the tip and cause a change, such as a deflection, in the cantilever status, and an image is formed by scanning the sample relative to the tip.
- The magnetic force microscope (MFM) is the only magnetic imaging technique that can provide high resolution (10-100 nm) with little surface preparation.
- An important application is to thc study of magnetic recording media.

Chapter 12: Ferromagnetism and Antiferromagnetism

Magnetic Force Microscopy

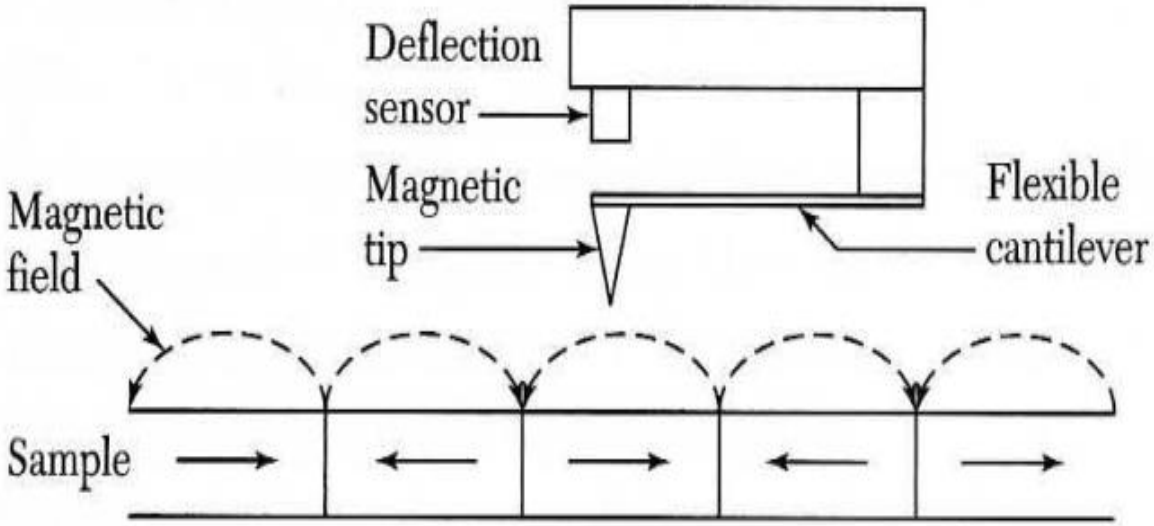


Figure 34 Basic concept of magnetic force microscopy. A magnetic tip attached to a flexible cantilever is used to detect the magnetic field produced by the regions of alternating magnetization in the plane of the sample. (After Gruetter, Mamin, and Rugar, 1992.)

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 09

Chapter 10:
Superconductivity

Prof. Nasser S. Alzayed

Chapter 10: Superconductivity

Superconductivity:

TOPICS:

1. Introduction
2. Destruction of S.C. by mag. F. & flux Quantization
3. Meissner effect
4. Heat Capacity
5. Energy Gap
6. Isotope Effect
7. London Equations
8. Coherence Length

2nd week

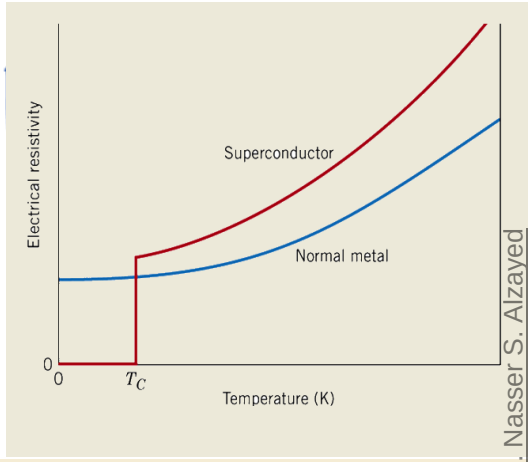
1. BCS Theory
3. Type II sup. Cond
4. Single Particle Tunn.
5. Josephson Junctions
   - DC effect
   - AC "
6. Macroscopic Quantum Interference.

Chapter 10: Superconductivity

Introduction

① Introduction

* Superconductivity takes place when the conductor is cooled below $T_c \Rightarrow \rho = 0$
* Onnes noticed this on 1911. ρ
* $\Rightarrow$ Persistent Current can Run forever.



Chapter 10: Superconductivity

Introduction

* File & Mills studied the decay of persistent current using N.M.R $\Rightarrow$ > 100,000 years.

* magnetic properties are more than if R = 0

* If B_a is weak $\Rightarrow$ $B_{inside} = 0$

  $\Rightarrow$ Perfect diamagnet

* If Cooling was done after B_a is applied then $T \rightarrow T_c \Rightarrow$ B will be ejected

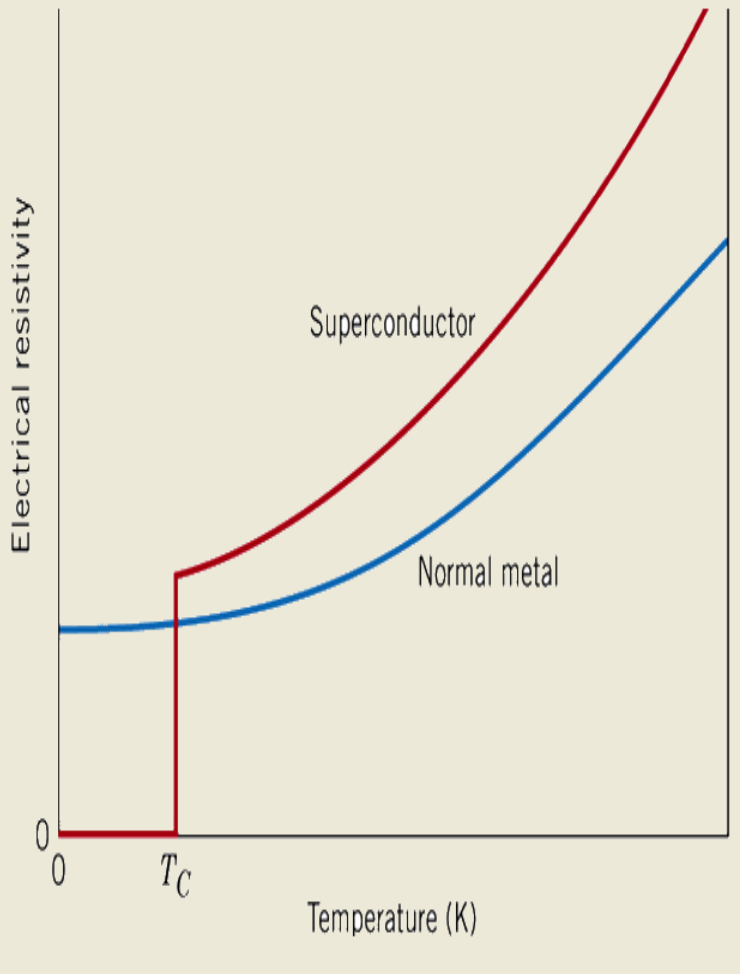
* superconductivity is an ordered state

* in sup. e's $\Rightarrow$ 2e (Cooper Pairs)

Chapter 10: Superconductivity

Introduction

- The electrical resistivity of many metals and alloys drops suddenly to zero when the specimen is cooled to a sufficiently low temperature, often a temp. in the liquid helium range.
- This phenomenon, called superconductivity, was observed first by Kamerlingh Onnes in Leiden in 1911.
- At a critical temperature T_c the specimen undergoes a phase transition from a state of normal electrical resistivity to a superconducting state



Chapter 10: Superconductivity

EXPERIMENTAL SURVEY

- In the superconducting state the dc electrical resistivity is zero, or so close to zero that persistent electrical currents have been observed to flow without attenuation in superconducting rings for more than a year.
- The decay of supercurrents in a solenoid was studied by File and Mills using precision nuclear magnetic resonance methods to measure the magnetic field associated with the supercurrent. They concluded that the decay time of the supercurrent is not less than 100,000 years
- The magnetic properties exhibited by superconductors are as dramatic as their electrical properties. The magnetic properties cannot be accounted for by the assumption that a superconductor is a normal conductor with zero electrical resistivity

Chapter 10: Superconductivity

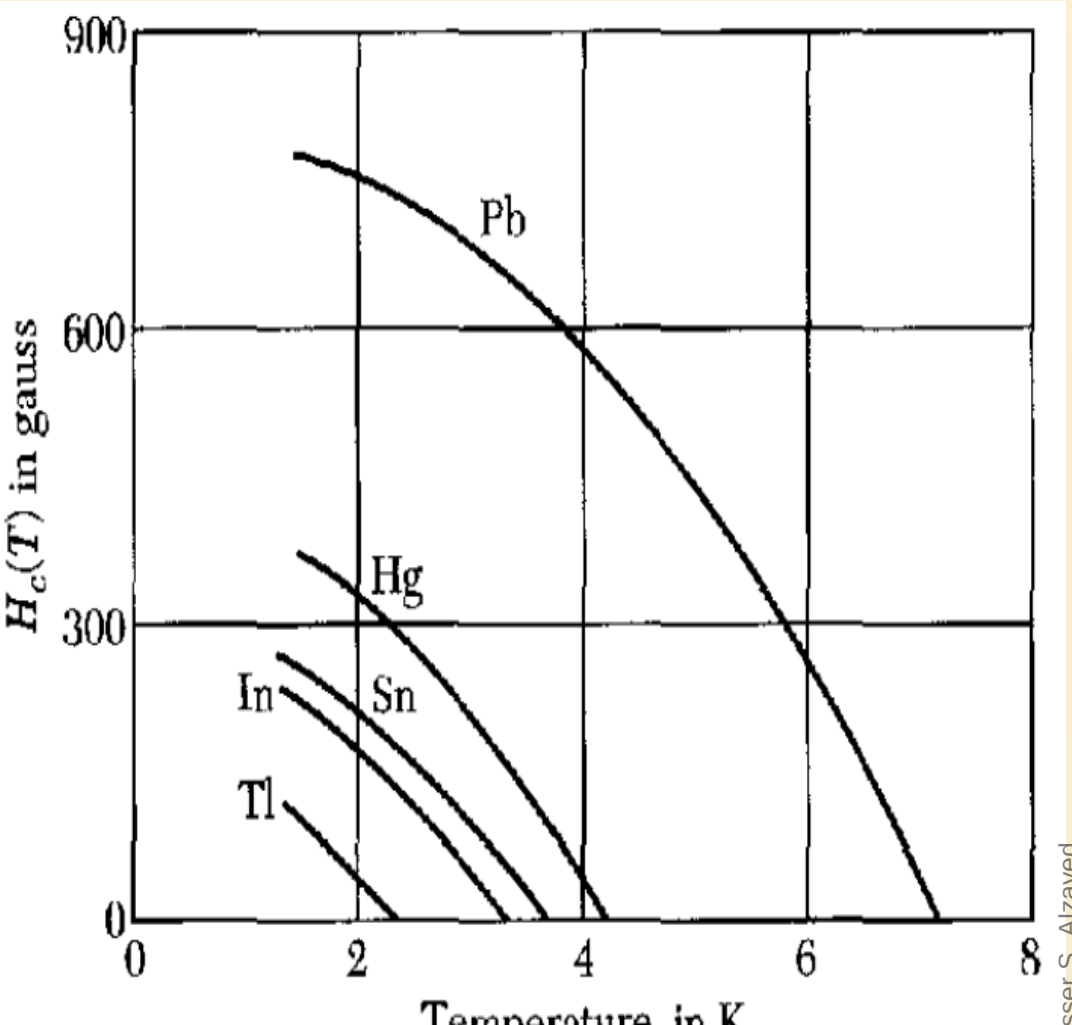
EXPERIMENTAL SURVEY

- It is an experimental fact that a bulk superconductor in a weak magnetic field will act as a perfect diamagnet, with zero magnetic induction in the interior.
- When a specimen is placed in a magnetic field and is then cooled through the transition temperature for superconductivity, the magnetic flux Originally present is ejected from the specimen
- The superconducting state is an ordered state of the conduction electrons of the metal
- The order is in the formation of loosely associated pairs of electrons
- The electrons are ordered at temperatures below the transition temperature, and they are disordered above the transition temperature

Chapter 10: Superconductivity

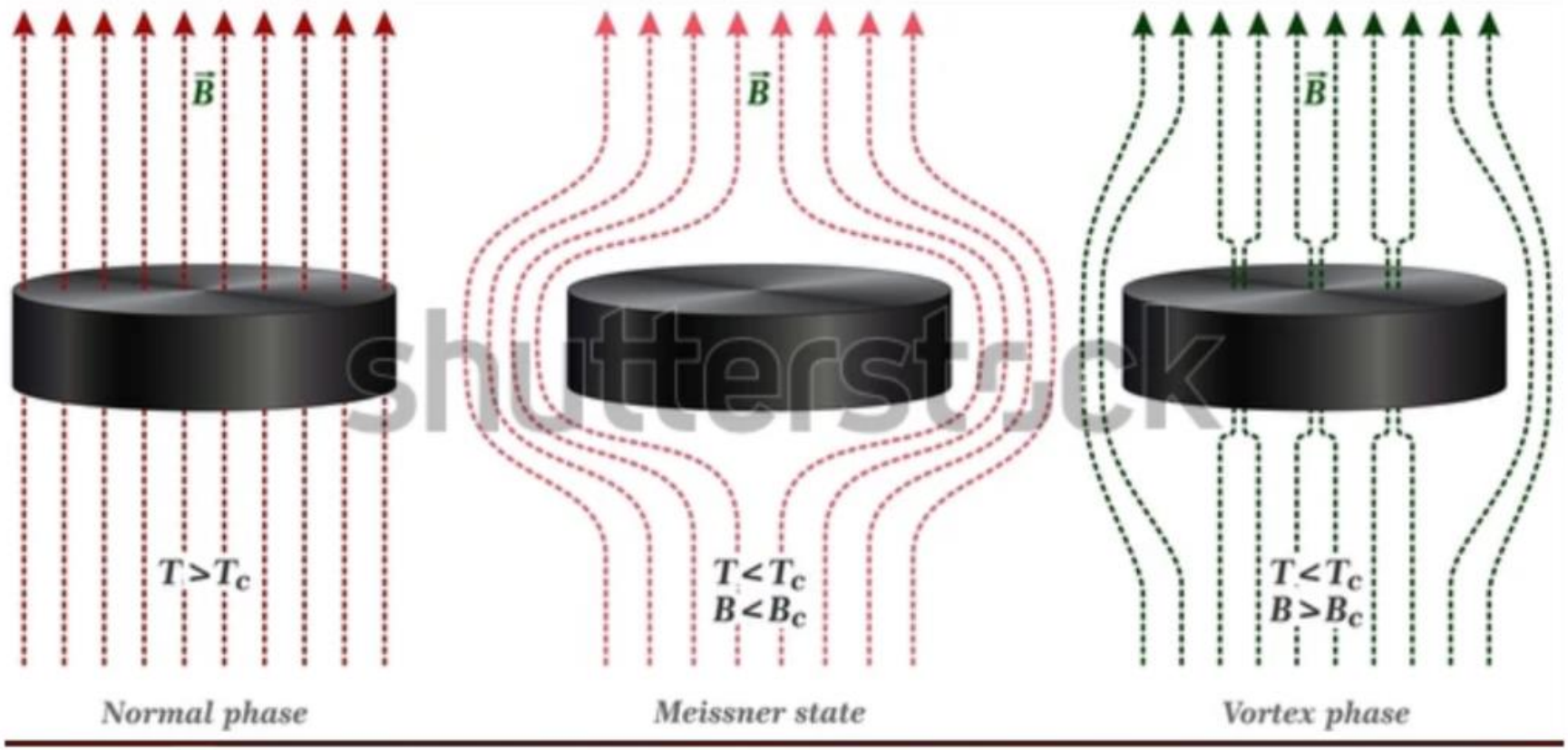
Destruction of Superconductivity by Magnetic Fields

- A sufficiently strong magnetic field will destroy superconductivity
- The threshold or critical value of the applied magnetic field for the destruction of superconductivity is denoted by $H_c(T)$ and is a function of the temperature
- At the critical temperature the critical Field is zero; $H_c(t) = 0$



Chapter 10: Superconductivity

Meissner Effect



$$\therefore B = B_a + 4\pi M = 0$$

$$\Rightarrow B_a = -4\pi M \quad \cdots \quad (1) \qquad [M = -H]$$

$$\chi = \frac{dM}{dH} = -1 \quad \cdots \quad (2)$$

-1 is the maximum value possible for χ

$\rho = 0$ does not Implement $B = 0$

In other words: $\rho = 0$ is not enough to $\Rightarrow B = 0$

* Ohm's Law: $\vec{E} = \rho \vec{J}$

if $\rho \to 0$ and $J \neq c \Rightarrow \vec{E} = 0$ not $\vec{B}$

* Also: from max. eq.

$$\vec{\nabla} \times \vec{E} + \frac{\partial B}{\partial t} = 0$$

if $\vec{E} \to 0 \Rightarrow \frac{\partial B}{\partial t} \to 0$ not $\vec{B}$.

∴ Meissner Effect ⇒ Perfect diamagnetism is an essential Property of sup. state.

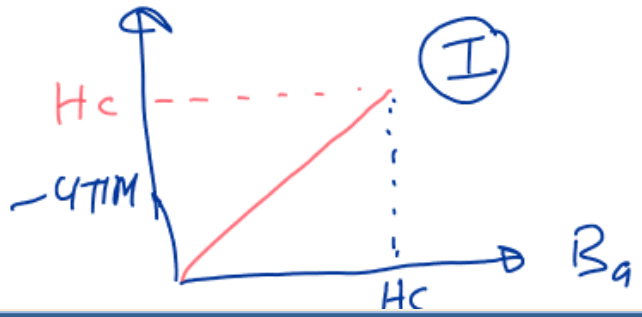
* sup. c. vs Perfect Cond.:

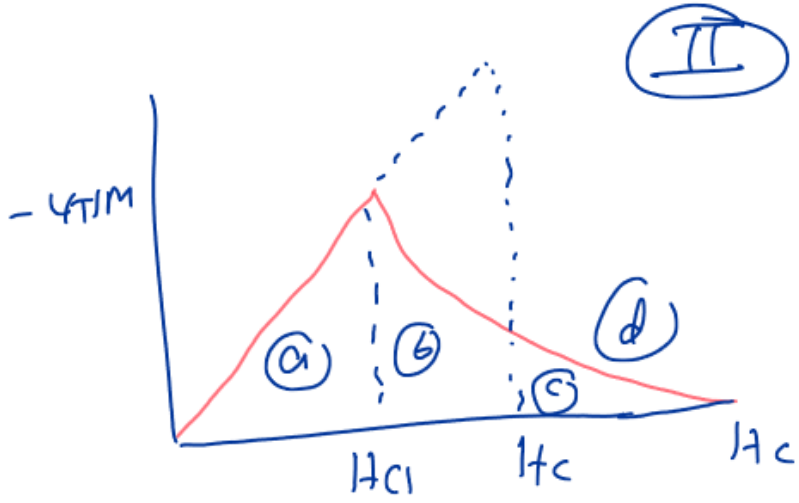
Perfect Cond.: Infinite mean free path

if subjected to external mag. field ⇏ Permanent eddy Current

" S.C " " " " " ⇒ persistent Curr.

* Type I vs Type II:





in Type (I):

at $B_a = H_c \Rightarrow$ superconductivity disappears

in Type (II): domins (a) full superconductivity state

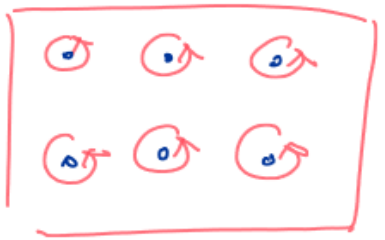
" (b) + (c) vortex state ($H_{c1} \rightarrow H_{c2}$)
(partial sup. state)

or (d) Normal state. $H > H_{c2}$

Between $H_{c1} \rightarrow H_{c2}$: $B \neq 0$, Meissner is Incomplete

" " " : vortex state

H_{c2} as high as 56 T has been Reported.



Chapter 10: Superconductivity

Meissner Effect

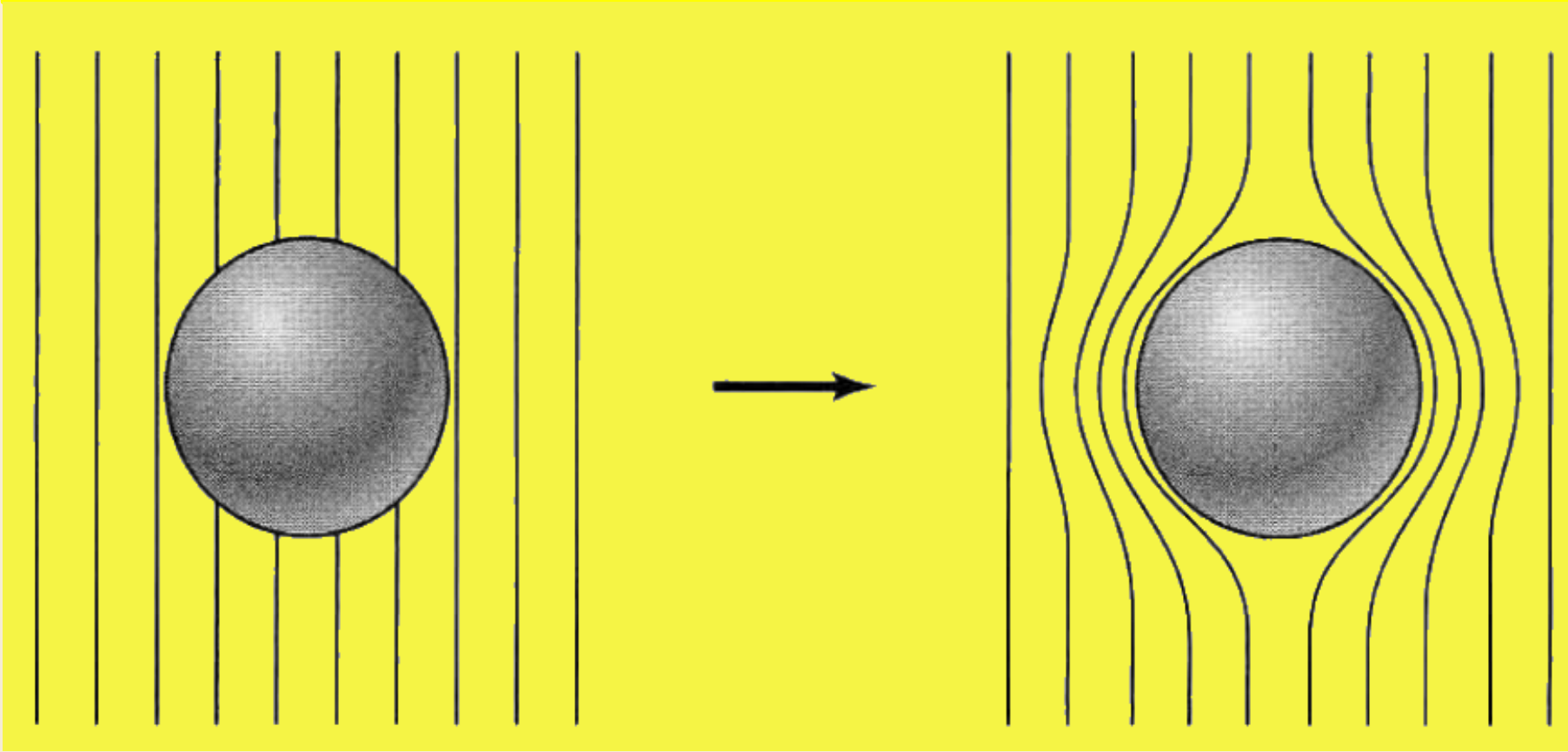
when Meissner effect is complete

$\Rightarrow$ magnetic levitation

Chapter 10: Superconductivity

Meissner Effect

- Meissner and Ochscnfeld (1933) found that if a superconductor is cooled in a magnetic field to below the transition temperature, then at the transition the lines of induction *B* are pushed out



Chapter 10: Superconductivity

Meissner Effect

- The Meissner effect shows that a bulk superconductor behaves as if $B = 0$ inside the specimen

$$B = B_a + 4\pi M = 0$$

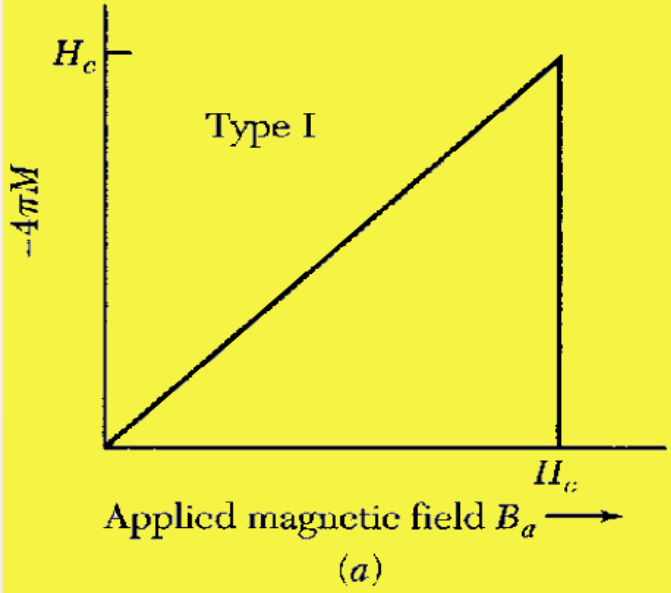
$$\therefore B_a = -4\pi M \qquad (1)$$

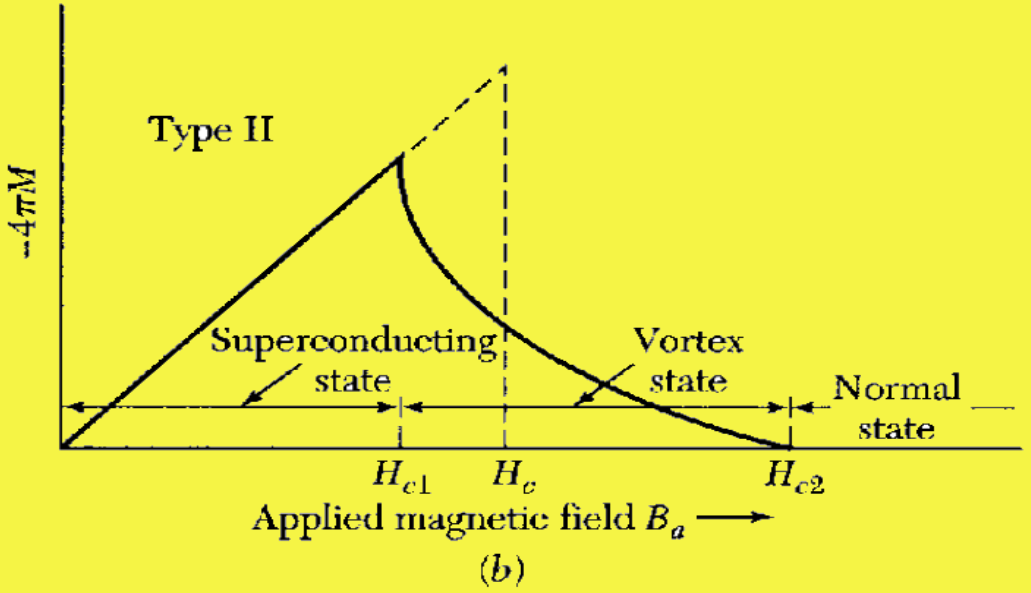
- The result $B = 0$ cannot be derived from the characterization of a superconductor as a medium of zero resistivity.
- From Ohm's law, $\mathbf{E} = \rho\mathbf{j}$, we see that if the resistivity ρ goes to zero while $\mathbf{j}$ is held finite, then $\mathbf{E}$ must be zero.
- By a Maxwell equation $d\mathbf{B}/dt$ is proportional to $\nabla\times\mathbf{E}$, so that zero resistivity implies $d\mathbf{B}/dt = 0$, but not $\mathbf{B} = 0$
- The Meissner effect suggests that perfect diamagnetism is an essential property of the superconducting state.

Chapter 10: Superconductivity

Meissner Effect

- We expect another difference between a superconductor and a perfect conductor, defined as a conductor in which the electrons have an infinite mean free path. When the problem is solved in detail, it turns out that a perfect conductor when placed in a magnetic field cannot produce a permanent eddy current screen: the field will penetrate about 1 cm in an hour.
- We have two types of superconductors: Type I & Type II.





Chapter 10: Superconductivity

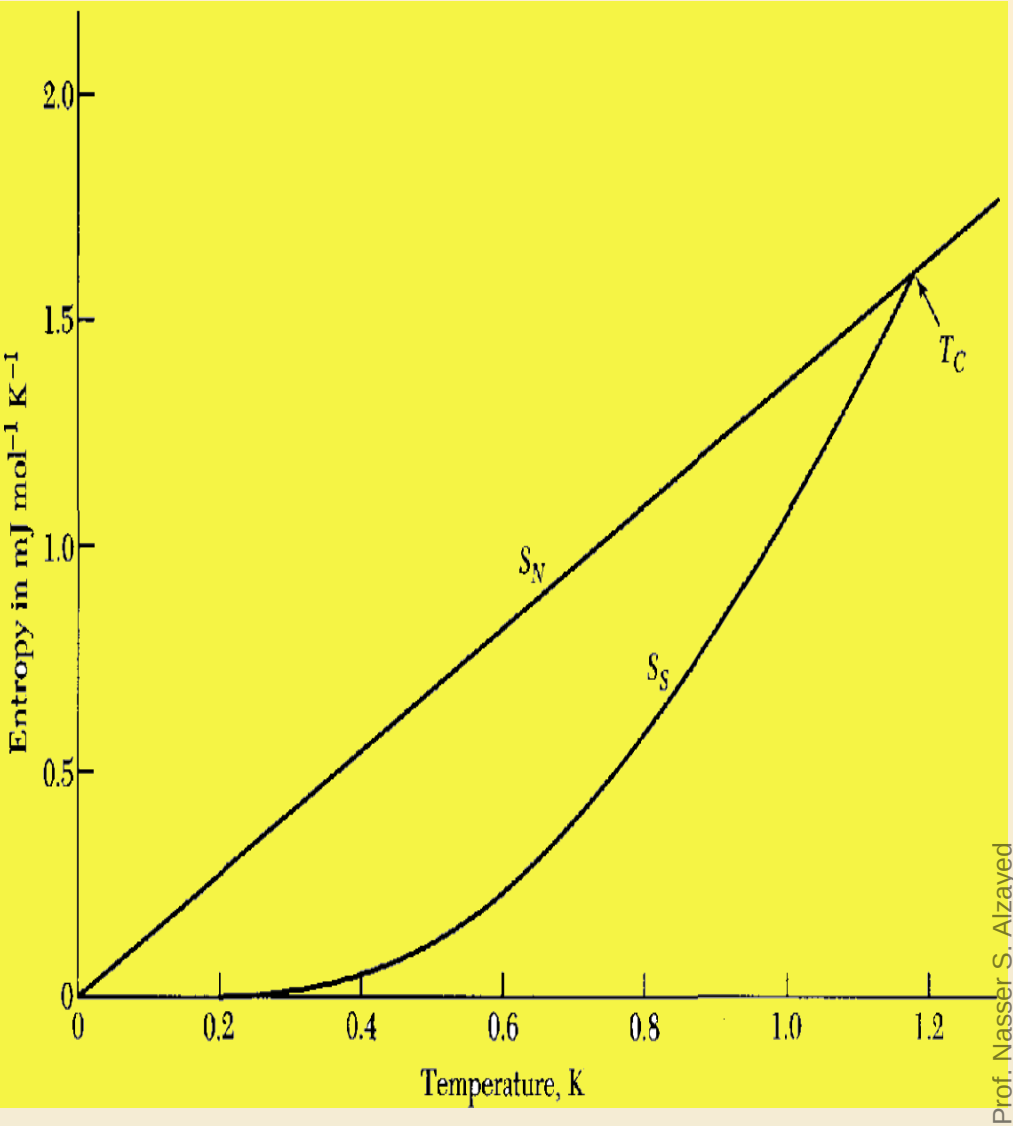
Meissner Effect

- Type II superconductors have superconducting electrical properties up to a field denoted by H_{c2} . Between the lower critical field H_{c1} and the upper critical field H_{c2} the flux density $B \neq 0$ and the Meissner effect is said to be incomplete.
- In the region between H_{c1} and H_{c2} the superconductor is threaded by flux lines and is said to be in the **vortex state**.
- A field H_{c2} of 41 Tesla has been attained in an alloy of Nb, Al, and Ge at the boiling point of helium, and 54 Tesla has been reported for $PbM0_6S_8$
- Commercial solenoids wound with a hard superconductor produce high steady fields over 10 Tesla. Such materials have an important medical application in magnetic resonance imaging (MRI). They can also be used in large accelerators as well as in the Tokamak (fusion reactors)

Chapter 10: Superconductivity

Heat Capacity

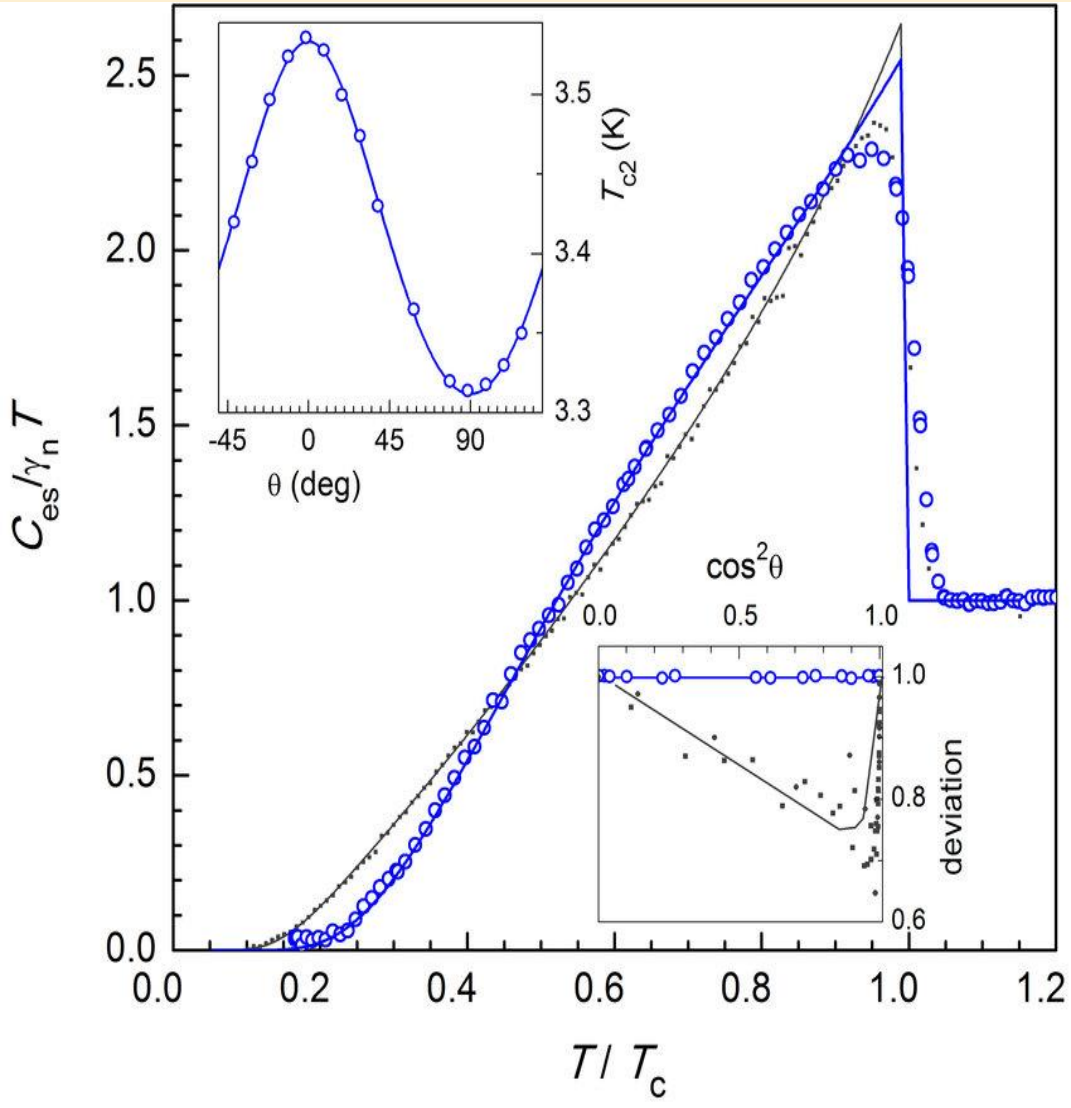
- In all superconductors the entropy decreases markedly on cooling below T_c
- The decrease in entropy between the normal state and the superconducting state tells us that the superconducting state is more ordered than the normal state
- Some or all of the electrons thermally excited in the normal state are ordered in the superconducting state.



Chapter 10: Superconductivity

Heat Capacity

- The heat capacity of NbS_2 is plotted in Fig. shows that the electronic contribution to the heat capacity in the sup. state is an exponential form with an argument proportional to -1/T, suggestive of excitation of electrons across an energy gap. A corresponding single-gap α-model fit



Chapter 10: Superconductivity

Energy Gap

- The energy gap of superconductors is of entirely different origin and nature than the energy gap of insulators
- In an insulator the energy gap is caused by the electron-lattice interaction. This interaction ties the electrons to the lattice.
- In a superconductor the important interaction is the electron-electron interaction which orders the electrons in k space with respect to the Fermi gas of electrons.
- The argument of the exponential factor in the electronic heat capacity of a superconductor is found to be $-E_g/2k_BT$ and not $-E_g/k_BT$
- The transition in zero magnetic field from the sup. state to the normal state is observed to be a ***second-order*** phase transition.
- The energy gap decreases continuously to zero as the temperature is increased to the transition temperature T_c

Chapter 10: Superconductivity

Energy Gap

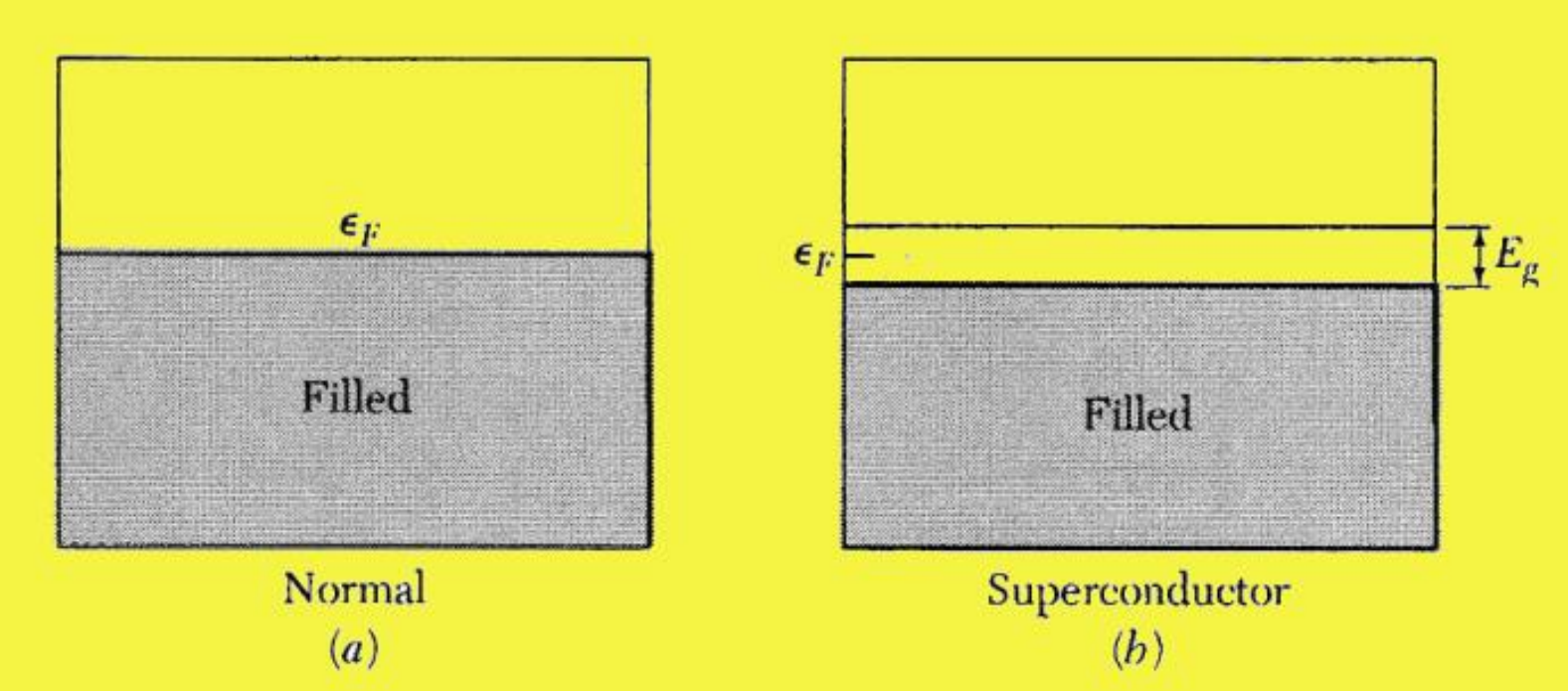


Figure 9 (a) Conduction band in the normal state: (b) energy gap at the Fermi level in the superconducting state. Electrons in excited states above the gap behave as normal electrons in rf fields: they cause resistance; at dc they are shorted out by the superconducting electrons.

Chapter 10: Superconductivity

Isotope Effect

- It has been observed that the critical temperature of superconductors varies with isotopic mass
- The experimental results within each series of isotopes may be fitted by a relation of the form:

$$M^{\alpha} T_c = \text{Constant} \qquad (1)$$

- From the dependence of T_c on the isotopic mass we learn that lattice vibrations and hence electron-lattice interactions are deeply involved in superconductivity.
- This was a fundamental discovery: there is no other reason for the superconducting transition temperature to depend on the number of neutrons in the nucleus.
- The original BCS model gave the result $T_c \ \alpha \ \theta_{Debye} \ \alpha \ M^{1/2}$, so that $\alpha = 1/2$ in (2).

Chapter 10: Superconductivity

London Equation

London assumes that not only $\frac{dB}{dt} = 0$ but $B \to 0$

$\therefore J = J_n + J_s \quad - - - - (1)$

for J_n: Ohm's law $\Rightarrow J_n = \sigma E$

But for J_s:

we will apply Current density in Q. M.

def. $J(r) = \frac{qh}{4\pi m i}\left[\psi^* \nabla \psi - \nabla \psi^* \psi\right] \quad - - - (2)$

solution: $\psi = \Phi e^{i\phi(r)} \quad - - - - (3)$

$q = 2e \quad m = 2m_e \quad \phi$: phase angle

③ → $\psi^* = \Phi^* e^{-i\varphi}$

$\Rightarrow \psi\psi^* = |\psi|^2 = \Phi\Phi^* e^{i\varphi} e^{-i\varphi} = \Phi\Phi^*$ - ④

1st term in ②:

$\psi^* \nabla\psi = [\Phi^* e^{-i\varphi}][\Phi' e^{i\varphi} + i\Phi e^{i\varphi} \nabla\varphi)$

$= \Phi^*\Phi' + i\Phi^*\Phi\nabla\varphi$ ---⑤

2nd term in ②:

$\nabla\psi^*\psi = [\Phi^{*\prime} e^{-i\varphi} - \Phi^* i e^{-i\varphi} \nabla\varphi] \Phi e^{i\varphi}$

$= \Phi^{*\prime}\Phi - \Phi^*\Phi i\nabla\varphi$ ---⑥

If ⑤ & ⑥ in ② ⇒

$$J(r) = \frac{2e\hbar}{4\pi \cdot 2mi}\left[\Phi^{*}\nabla\Phi + i\Phi^{*}\Phi\nabla\Phi - \Phi^{*}\nabla\Phi + \Phi^{*}\Phi i\nabla\Phi\right]$$

$$\Rightarrow J(r) = \frac{e\hbar}{4\pi m i}\left[2i\Phi^{*}\Phi\nabla\Phi\right] \quad (2)$$

$$\boxed{J(r) = \frac{e\hbar}{m}|\psi(r)|^{2}\nabla\varphi(r)} \quad * \quad ---(7)$$

Now: we apply Coupling with ext. mag. Field:

$$\bar{\nabla} \longrightarrow \bar{\nabla} + \frac{ie}{\hbar}A \quad ----(8)$$

with $\bar{B} = \bar{\nabla}\times\bar{A}$ ---(9)

$\therefore$ (7) $\Rightarrow$

$$J_s(\vec{r}) = \frac{e\hbar}{m}|\psi|^2 \nabla\varphi - \frac{2e^2}{m} A |\psi|^2 \quad \text{--(10)}$$

(1) (2)

$\because B = 0$

$\Rightarrow |\psi|^2 = \text{constant}$

let $|\psi|^2 = n_s$ (No. of super pairs)

term (1) in (10) $= 0$

$$\Rightarrow J_s = -\frac{2e^2 n_s}{m} A \quad \text{----(11)}$$

Now: take $\nabla\times$ for Both Sides.

London Equation

$$\nabla \times J_s = -\frac{2 n_s e^2}{m} \nabla \times A$$

$$\Rightarrow \nabla \times J_s + \frac{2 n_s e^2}{m} \nabla \times A = 0$$

$$\Rightarrow \nabla \times J_s + \frac{2 n_s e^2}{m} B = 0$$

$$\Rightarrow \nabla \times J_s + \frac{1}{\mu_0 \lambda^2} B = 0 \quad \text{--- (12)}$$

(12) is London Eq.

λ is penetration depth

$$\lambda^2 = \frac{m^2}{2 \mu_0 n_s e^2}$$

for $n_s = 10^{28} \rightarrow \lambda \sim 52 \text{ Å}$

Chapter 10: Superconductivity

London Equation

- Meissner effect implies a magnetic susceptibility:

$$\because B_a = -4\pi M$$

$$\therefore \chi = \frac{M}{B_a} = -\frac{1}{4\pi}$$

London Assumed That not only $\frac{dB}{dt} = 0$ but Also: $B = 0$

$$\because J = J_n + J_s$$

For $J_n = \sigma E$ (Ohm's Law)

For J_s, We use current density in QM:

$$J(r) = \frac{qh}{4\pi M i}\left[\psi^*(r)\nabla\psi(r) - \nabla\psi^*(r)\psi(r)\right] \qquad (*)$$

Solution: $\psi(r) = \Phi(r)e^{i\phi(r)}$ (3)

- ϕ is the phase angle. q=2e and M=2m_e

Chapter 10: Superconductivity

London Equation

$$\because \psi^*(r) = \Phi^*(r) e^{-i\phi(r)}$$

$$\therefore \psi(r)\psi^*(r) = |\psi(r)|^2 = \Phi(r)\Phi^*(r) e^{i\phi(r)} e^{-i\phi(r)} = \Phi(r)\Phi^*$$

1st term in (*):

$$\psi^*(r)\nabla\psi(r) = \left[\Phi^* e^{-i\phi(r)}\right]\left[\Phi' e^{i\phi(r)} + i\,\Phi e^{i\phi(r)}\nabla\phi\right]$$

$$= \left[\Phi^*\Phi'(r) + i\,\Phi^*\Phi\nabla\phi(r)\right] \qquad (4)$$

2nd term in (*):

$$\nabla\psi^*(r)\psi(r) = \left[\Phi^{*'} e^{-i\phi(r)} - \Phi^* i e^{-i\phi(r)}\nabla\phi\right]\Phi e^{i\phi(r)}$$

$$= \left[\Phi^{*'}\Phi - \Phi^*\Phi i\,\nabla\phi\right] \qquad (5)$$

(4) & (5) in (*):

$$J(r) = \frac{2eh}{4\pi 2mi}\left[2i\,\Phi^*(r)\Phi(r)\nabla\phi(r)\right]$$

$$= \frac{e\hbar}{m}|\psi(r)|^2\nabla\phi(r) \qquad (6)$$

Chapter 10: Superconductivity

London Equation

❑ Due to coupling with the external magnetic field:

$$\nabla \rightarrow \nabla + \frac{ie}{\hbar} A \qquad (7)$$

Where: $B = \nabla \times A$

$\therefore (6) \rightarrow$:

$$J_s(r) = \frac{e\hbar}{m} |\psi(r)|^2 \nabla\phi(r) - \frac{2e^2}{m} A |\psi(r)|^2 \qquad (8)$$

$\because \mathrm{B} = 0$

$\therefore |\psi(r)|^2 = const.$

Let: $|\psi(r)|^2 = n_s$ (density of superpairs)

$\therefore$ 1st term in (8)=0

$$\therefore J_s(r) = -\frac{2e^2}{m} A |\psi(r)|^2$$

$$\therefore J_s(r) = -\frac{2n_s e^2}{m} A \qquad (9)$$

❑ (8) is the general form of London Equation

Chapter 10: Superconductivity

London Equation

- By taking $\nabla\times$ for both sides:

$$\nabla\times J_s(r) = -\frac{2n_s e^2}{m}\nabla\times A$$

$$\therefore \nabla\times J_s(r) + \frac{2n_s e^2}{m}\nabla\times A = 0$$

$$\therefore \nabla\times J_s(r) + \frac{2n_s e^2}{m}B = 0$$

$$\Rightarrow \nabla\times J_s(r) + \frac{1}{\mu_o\lambda^2}B = 0 \qquad (10)$$

- Equation (10) is called: London Equation. λ is called: London penetration depth. For $n_s = 10^{28} \rightarrow \lambda \sim 500$Å

$$\lambda^2 = \frac{m}{2\mu_o n_s e^2} \qquad (11)$$

Chapter 10: Superconductivity

London Equation

❑ We do more treatment starting from Maxwell Equation:

$$\nabla \times B = \mu_o J \quad (Max.Eq.) \tag{12}$$

$\nabla \times$ for both sides:

$$\nabla \times \nabla \times B = \mu_o \nabla \times J \tag{13}$$

(10) *in* (13) $\Rightarrow$:

$$\nabla \times \nabla \times B + \frac{1}{\lambda^2} B = 0 \tag{14}$$

$$\because \nabla \times \nabla \times B = \nabla(\nabla . B) - \nabla^2 B$$

But $\nabla . B = 0$

$$\Rightarrow \nabla^2 B = \frac{1}{\lambda^2} B \tag{15}$$

$$\Rightarrow B(r) = B(0) e^{-r/\lambda} \tag{16}$$

Chapter 10: Superconductivity

London Equation

❑ So that London Equation leads to Meissner effect:

$$\because \lambda^2 = \frac{m}{2\mu_o n_s e^2} \qquad (11)$$

$as\ T \to T_c$

$n_s \to \infty$

$\lambda \to 0$

$$\Rightarrow \frac{-r}{\lambda} \to \infty$$

$$\Rightarrow B \to 0$$

$as\ T \to \infty$

$n_s \to 0$

$\lambda \to \infty$

$$\Rightarrow \frac{-r}{\lambda} \to 0$$

$$\Rightarrow e^{-\frac{r}{\lambda}} \to 1$$

Chapter 10: Superconductivity

London Equation

- Eq. (15) is seen to account for the Meissner effect because it does not allow a solution uniform in space, so that a uniform magnetic field cannot exist in a superconductor. That is, B(r) = B(0) = constant is not a solution of (15) unless the constant field B(0) is identically zero.
- Eq. (12) ensures that J = 0 in a region where B = 0.
- In the pure superconducting state the only field allowed is exponentially damped as we go in from an external surface

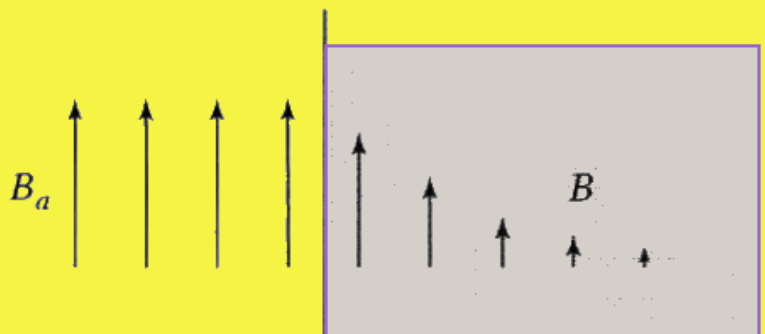


Figure 13 Penetration of an applied magnetic field into a semi-infinite superconductor. The penetration depth λ is defined as the distance in which the field decreases by the factor e^{-1}. Typically, $\lambda \approx 500$ Å in a pure superconductor.

Chapter 10: Superconductivity

Coherence Length

- The London penetration depth λ is a fundamental length that characterizes a superconductor.
- The **coherence length** ξ is a measure of the distance within which the superconducting electron concentration cannot change drastically in a spatially-varying magnetic field.
- **coherence length** can be derived as:

$$\xi = \frac{2\hbar v_F}{\pi E_g} \qquad (17)$$

Metal	Intrinsic Pippard coherence length ξ_0, in 10^{-6} cm	London penetration depth λ_L, in 10^{-6} cm	λ_L/ξ_0
Sn	23.	3.4	0.16
Al	160.	1.6	0.010
Pb	8.3	3.7	0.45
Cd	76.	11.0	0.14
Nb	3.8	3.9	1.02

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 10

Chapter 10:
Superconductivity

Prof. Nasser S. Alzayed

Chapter 10: Superconductivity

BCS Theory of Superconductivity

- ❑ BCS Theory
- ❑ Flux Quantization
- ❑ Singl Particle Tunneling
- ❑ DC JS Effect
- ❑ AC JS Effect
- ❑ Macroscopic Quantum Interference
- ❑

Prof. Nasser S. Alzayed

BCS Theory

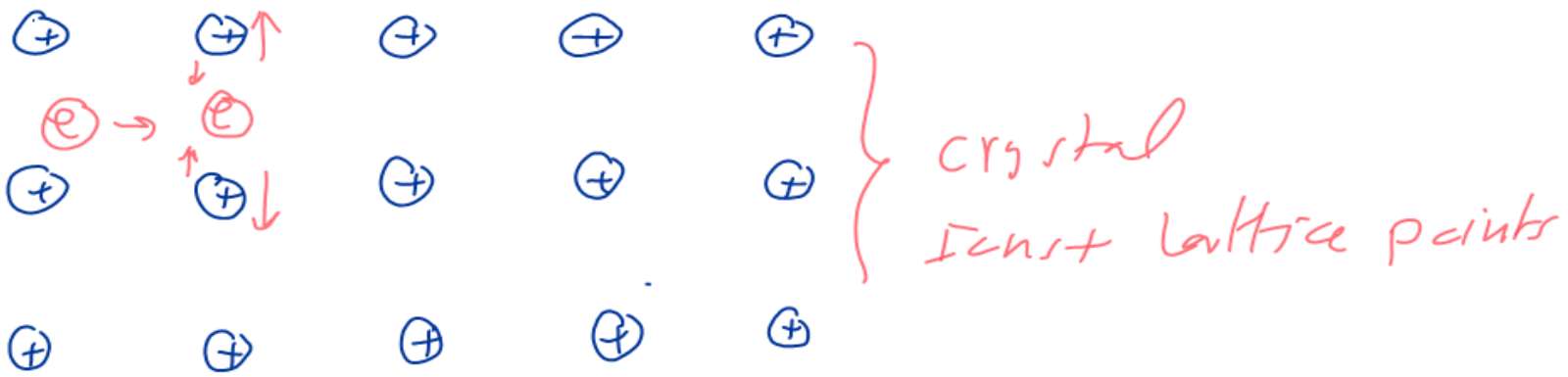
① Isotope effect:

$T_c \propto \frac{1}{\sqrt{M}}$

where M is the mass of atom.

⇒ T_c depends on mass of atom. ?

Isotope effect ⟹ that electrons Interact with Lattice.



Steps:
1. e No. 1 go Between Ions
2. they will be attracted by e
3. after e leaves ⇒ Restoration of Ionic ⇒ good chance for e #2 to step in ⇒ the pair will continue moving. #

This leads to effect of M of ions.

$\Rightarrow$ Isotope effect

* The maximum phonon energy due to vibrations that are caused by electrons passing is:

$$\hbar\omega_D = k_B \Theta_D \simeq 0.01 - 0.02 \text{ eV}.$$

ω_D: Debye freq.

Θ_D: " Temp.

$$\omega_D \propto \frac{1}{\sqrt{M}} \Rightarrow T_c \propto \frac{1}{\sqrt{M}} \quad \#$$

2 electrons are paired together by pairing Strength $\Delta \simeq \hbar\omega_D$

Relaxation time for ions to get Back to original location is $\tau = \frac{2\pi}{\omega_D}$

the distance between the pair is:

$$\xi = v_f \cdot \tau = v_f \cdot \frac{2\pi}{\omega_D} \approx 100 - 500 \text{ nm} \#$$

↳ Fermi velocity

ξ is called Coherence length

Binding energy of one cooper pair:

$$\Delta = 2\hbar\omega_D e^{-\frac{1}{V_0 N(\epsilon_F)}}$$

Where: V_0: Interaction potential

ϵ_F: Fermi Energy

Δ can be approximated as:

$$\Delta \approx 1.76 K_B T_c \qquad -\frac{1}{V_0 N(\epsilon_F)} \qquad -\frac{1}{V_c N(\epsilon_F)}$$

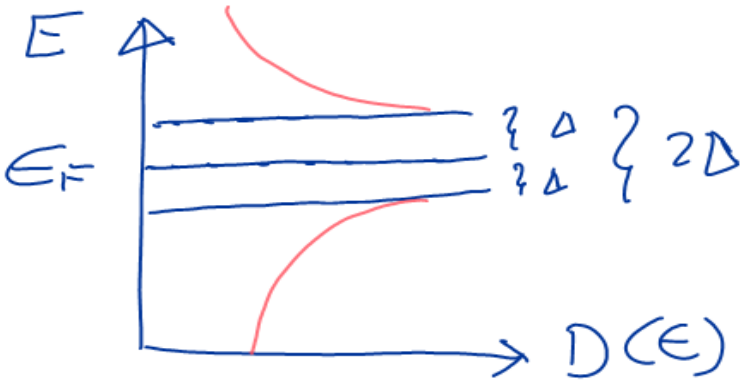
$$\Rightarrow K_B T_c = \frac{2}{1.76} \hbar\omega_D e \qquad = 1.14 \hbar\omega_D e$$

$$\therefore T_c = \frac{1.14 \hbar \omega_D}{K_B} e^{-\frac{1}{V_0 N(\epsilon_F)}}$$

$$\therefore T_c \propto \omega_D$$

$$\therefore \omega_D \propto \frac{1}{\sqrt{M}} \quad \text{Debye Model}$$

$$\Rightarrow T_c \propto \frac{1}{\sqrt{M}} \quad \not\quad \text{Isotope Effect}$$



When $T \longrightarrow T_c$

⇒ all electrons get into pairs

⇒ No single electrons exist.

⇒ No electrons from: $\epsilon_F - \Delta \longrightarrow \epsilon_F + \Delta$

⇒ Gap.

⇒ Jump in Specific Heat

∴ we don't need one wave function for each electron

Instead; we can use one function.

$$\psi = \psi_0 e^{i\phi}$$

ϕ is the phase

with $|\psi_0|^2 = n_s$ ∴ No. of Cooper Pairs.

ψ is for 2 electrons $k\uparrow$ and $-k\downarrow$

ψ is called: S-wave

the Gap is S.C. is Behined.

1. critical field H_c
2. specific heat Jump.
3. Any other electromag. property.
4. flux quantization dependson $2e$

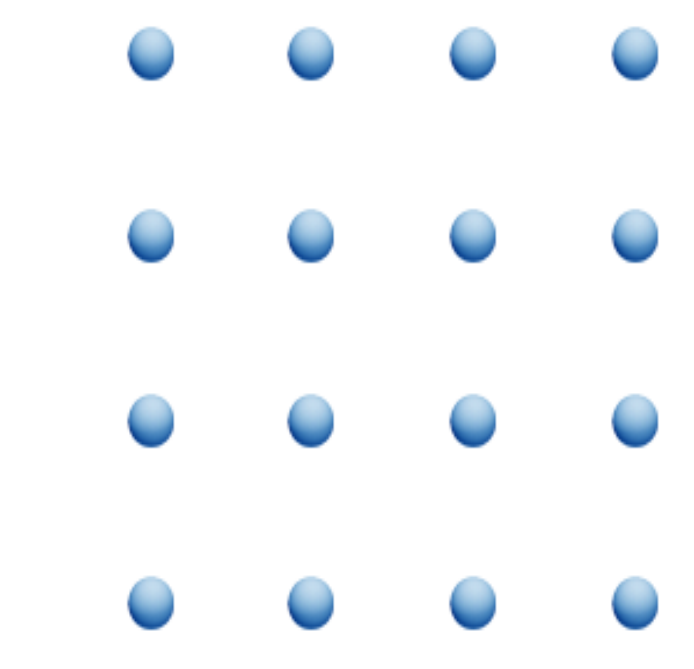
Chapter 10: Superconductivity

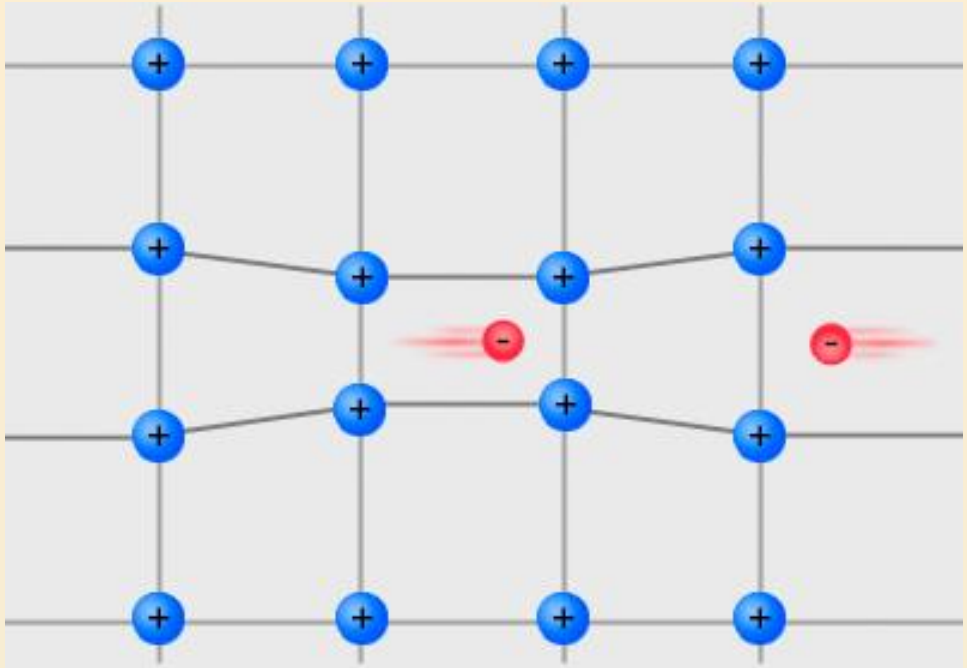
BCS Theory of Superconductivity

- It was developed by 3 professors: Bardeen, Cooper and Schrieffer in 1957.
- It has been used ever since to explain for superconductivity, Low T_c as well as High T_c, Type I as well as Type II.
- This theory assumes BCS wavefunction composed of two electrons: Cooper Pair $\mathbf{k}\uparrow$ and $-\mathbf{k}\downarrow$
- Sometimes we call this pairing s-wave pairing.
- An attractive interaction between electrons can lead to a ground state separated from excited states by an energy gap. The critical field, the thermal properties, and most of the electromagnetic properties are consequences of the energy gap.
- The electron-lattice-electron interaction leads to an energy gap of the observed magnitude. The indirect interaction proceeds when one electron interacts with the lattice and deforms it; a second electron sees the deformed lattice and adjusts itself to take advantage of the deformation to lower its energy. Thus the second electron interacts with the first electron via the lattice deformation.
- Magnetic flux through a superc. ring is quantized and the effective unit of charge is 2e rather than e. The BCS involves pairs of electrons; thus flux quantization in terms of the pair charge 2e is a consequence of the theory.

Chapter 10: Superconductivity

BCS Ground State

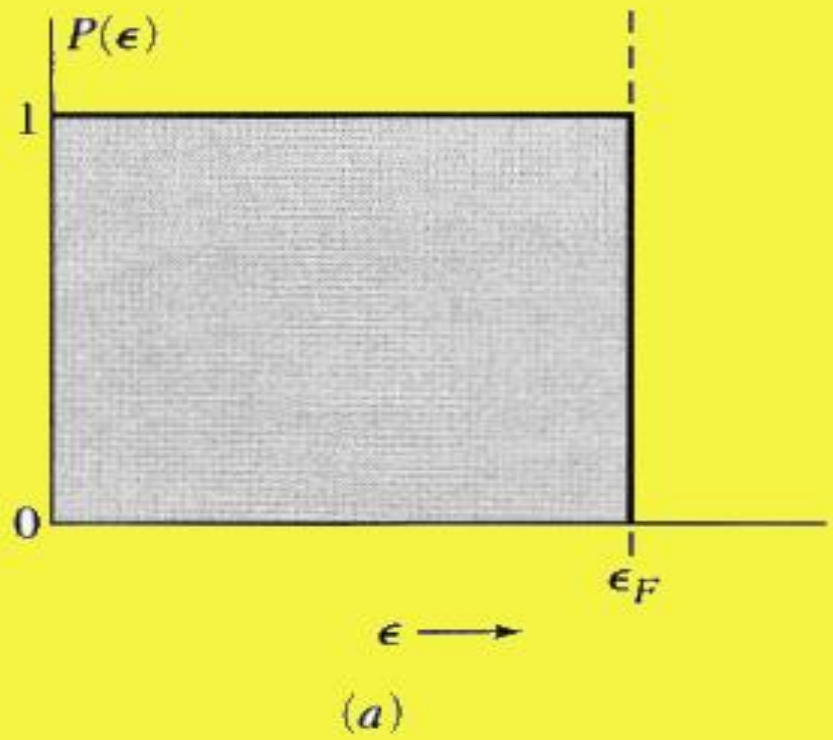


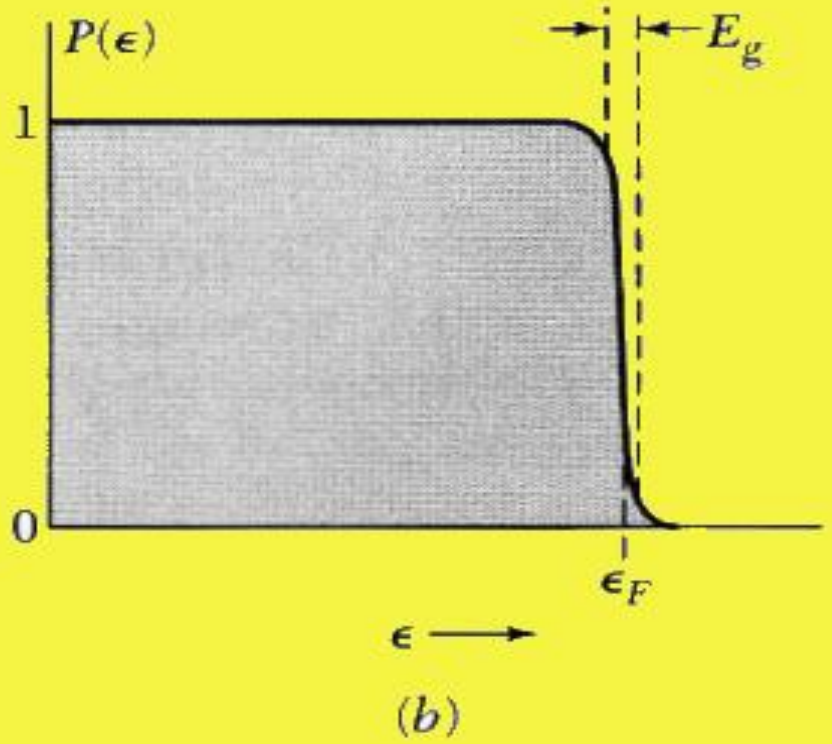


Cooper Pair The electron-lattice-electron interaction leads to an energy gap of the observed magnitude. The indirect interaction proceeds when one electron interacts with the lattice and deforms it; a second electron sees the deformed lattice and adjusts itself to take advantage of the deformation to lower its energy. Thus the second electron interacts with the first electron via the lattice deformation.

Chapter 10: Superconductivity

BCS Ground State





❑ **Figure 15** (a) Probability *P* that an orbital of kinetic energy ε is occupied in the ground state of the noninteracting Fermi gas; (b) the BCS ground state differs from the Fermi state in a region of width of the order of the energy gap E_g. Both curves are for absolute zero.

Chapter 10: Superconductivity

BCS Theory of Superconductivity

- Excited state cab take place by taking an electron from the Fermi surface and raising it just above the Fermi surface.
- The BCS theory shows that with an appropriate attractive interaction between electrons, the new ground state is superconducting and is separated by a finite energy E_g from its lowest excited state.
- The formation of the BCS ground state is suggested by **Fig. 15**. The BCS state in (b) contains admixtures of one-electron orbitals from above the Fermi energy ε_F.
- At first sight the BCS state appears to have a higher energy than the Fermi state: the comparison of (b) with (a) shows that the kinetic energy of the BCS state is higher than that of the Fermi state. But the attractive potential energy of the BCS state, although not represented in the figure , acts to lower the total energy of the BCS state with respect to the Fermi state.
- The central feature of the BCS state is that the one-particle orbitals are occupied in pairs: if an orbital with wavevector **k** and spin up is occupied, then the orbital with wavevector -**k** and spin down is also occupied. If $\mathbf{k}\uparrow$ is vacant, then $-\mathbf{k}\downarrow$ is also vacant. The pairs are called ***Cooper pairs.***

Chapter 10: Superconductivity

Flux Quantization in a Superconducting Ring

- We prove that the total magnetic flux that passes through a superconducting ring may assume only quantized values, integral multiples of flux quantum:

$$\Phi_0 = \frac{2\pi\hbar c}{2e}$$

- We prove that the total magnetic flux that passes through a superconducting ring may assume only quantized values, integral multiples of flux quantum.
- We first show that a charged boson gas obeys the London equation. Let $\psi(r)$ be the particle probability amplitude. We suppose that the pair concentration $n = \psi^* \psi$ = constant. At absolute zero n is one-half of the concentration of electrons in the conduction band, for n refers to pairs.
- Then we may write:

$$\left.\begin{aligned} \psi &= \sqrt{n} e^{i\varphi(r)} \\ \psi^* &= \sqrt{n} e^{-i\varphi(r)} \end{aligned}\right\} \qquad (19)$$

- φ is the phase angle.

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Flux Quantization in a Superconducting Ring

- The velocity of a particle is, from the Hamilton equation of mechanics:

$$v = \frac{1}{m}\left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right) = \frac{1}{m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)$$

- The particle flux is given by:

$$\begin{aligned}\psi^* v \psi &= \sqrt{n}e^{-i\varphi(r)}\left[\frac{1}{m}\left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)\right]\sqrt{n}e^{i\varphi(r)} \\ &= \frac{n}{m}e^{-i\varphi(r)}\left[\left(-i\hbar(i\nabla\varphi) - \frac{q}{c}\mathbf{A}\right)\right]e^{i\varphi(r)} \\ &= \frac{n}{m}\left(\hbar\nabla\varphi - \frac{q}{c}\mathbf{A}\right) \qquad (20)\end{aligned}$$

- so that the electric current density is:

$$\because I = \frac{\pi R^2 ne\ell}{t} = A.q\frac{\ell}{t} = A.qv \Rightarrow J_s = \frac{I}{A} = qv$$

Chapter 10: Superconductivity

Flux Quantization in a Superconducting Ring

- Hence, current density is:

$$\Rightarrow J_s = q\psi^* v\,\psi = \frac{nq}{m}\left(\hbar\nabla\varphi - \frac{q}{c}\mathbf{A}\right) \qquad (21)$$

- We may take the curl of both sides to obtain the London equation:

$$\nabla\times J_s(r) = \nabla\times\left[\frac{nq}{m}\left(\hbar\nabla\varphi - \frac{q}{c}\mathrm{A}\right)\right]$$

$$\therefore \nabla\times J_s(r) = \frac{nq}{m}\hbar\left(\nabla\times\nabla\varphi\right) - \frac{nq}{m}\frac{q}{c}\nabla\times\mathrm{A}$$

$$\therefore \nabla\times J_s(r) = 0 - \frac{nq^2}{mc}B$$

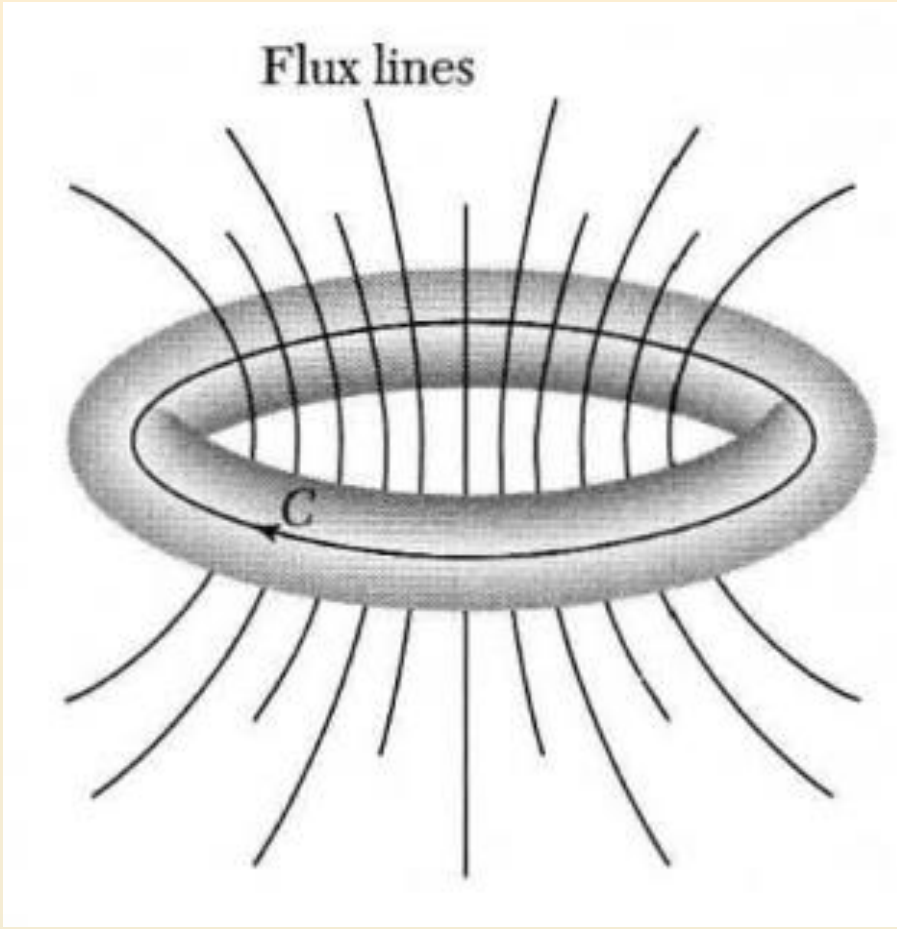
$$\Rightarrow \nabla\times J_s(r) + \frac{nq^2}{mc}B = 0 \qquad (22)$$

- Hence, we are back to the London equation again.
- Quantization of the magnetic flux through a ring is a dramatic consequence of Eq. (21).

Chapter 10: Superconductivity

Flux Quantization in a Superconducting Ring

- Let us take a closed path C through the interior of the superconducting material, well away from the surface (Fig. 16). The Meissner effect tells us that B and j are zero in the interior.



- **Figure 16** Path of integration *C* through the interior of a superconducting ring. The flux through the ring is the sum of the flux Φ_{ext} from external sources and the flux Φ_{sc} from the superconducting currents which flow in the surface of the ring; $\Phi = \Phi_{ext} + \Phi_{sc}$ The flux Φ is quantized. There is normally no quantization condition on the flux from external sources, so that Φ_{sc} must adjust itself appropriately in order that Φ assume a quantized value

Chapter 10: Superconductivity

Flux Quantization in a Superconducting Ring

- The Meissner effect tells us that B and J are zero in the interior.

$$(21) \Rightarrow \quad 0 = \frac{nq}{m}\left(\hbar\nabla\varphi - \frac{q}{c}\mathbf{A}\right)$$

$$\Rightarrow \quad \hbar\nabla\varphi - \frac{q}{c}\mathbf{A} = 0$$

$$\therefore \quad \hbar c\nabla\varphi = q\mathbf{A} \qquad (23)$$

- Using Stokes' theorem:

$$\hbar c\oint \nabla\varphi . d\ell = q\oint \mathbf{A} . d\ell = q\int_s \nabla\times\mathbf{A} . d\sigma = q\int_s B . d\sigma = q\Phi \qquad (25)$$

$$\because \mathrm{q} = -2\,\mathrm{e}$$

$$\because \oint \nabla\varphi . d\ell = 2\pi s$$

$$\therefore \Phi = \frac{2\pi\hbar c}{2\,\mathrm{e}}s \qquad (26)$$

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Flux Quantization in a Superconducting Ring

- Thus the flux through the ring is quantized.
- Flux quantum is:

$$\Phi_0 = \frac{2\pi\hbar c}{2e} \approx 2.07\times10^{-15}\ \mathrm{Tm}^2 \qquad (27)$$

- Flux quantum is called: fluxoid of fluxon.
- The flux through the ring is the sum of the flux Φ_{ext} from external sources and the flux Φ_{sc} from the persistent superconducting currents which flow in the surface of the ring: $\Phi = \Phi_{ext} + \Phi_{sc}$
- The flux Φ is quantized.
- There is normally no quantization condition on the flux from external sources
- so that Φ_{sc} must adjust itself appropriately in order that Φ assume a quantized value.
- Flux quantization indeed follows from the fact that the current is the result of a phase gradient.
- the superconducting ring thus reads variation between magnetic fields by small amount such as one flux quantum (fluxoid)

Chapter 10: Superconductivity

Type II superconductors

- There is no difference in the mechanism of superconductivity in type I and type II superconductors.
- Both types have similar thermal properties at the superconductor-normal transition in zero magnetic field.
- But the Meissner effect is entirely different.
- A good type I superconductor excludes a magnetic field until superconductivity is destroyed suddenly, and then the field penetrates completely.
- A good type II superconductor excludes the field completely up to a field H_{c1} Above H_{c1} the field is partially excluded, but the specimen remains electrically superconducting. At a much higher field, H_{c2} , the flux penetrates completely and superconductivity vanishes.
- An important difference in a type I and a type II superconductor is in the mean free path of the conduction electrons in the normal state.
- If the coherence length ξ is longer than the penetration depth λ, the superconductor will be type I.
- Most metals are type I, with $\lambda/\xi < 1$.

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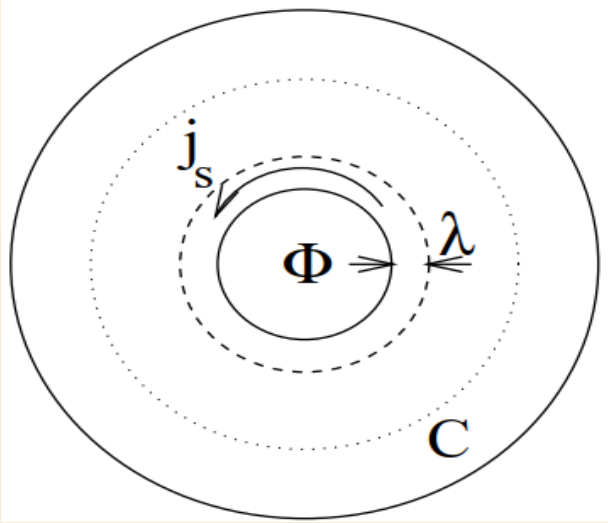
Type II superconductors

- But, when the mean free path is short, the coherence length is short and the penetration depth is great.
- This is the situation when $\lambda/\xi > 1$, and the superconductor will be type II.
- The theory of type II superconductors was developed by Ginzburg, Landau, Abrikosov, and Gorkov.
- Estimation of H_{c1} and H_{c2} :

$$H_{c1} \simeq \frac{\Phi_0}{\pi\lambda^2} \qquad (30)$$

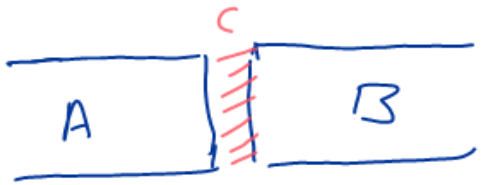
$$H_{c2} \simeq \frac{\Phi_0}{\pi\xi^2} \qquad (31)$$



- The larger the ratio λ/ξ , the larger the ratio: H_{c2}/H_{c1}

Single Particle tunneling

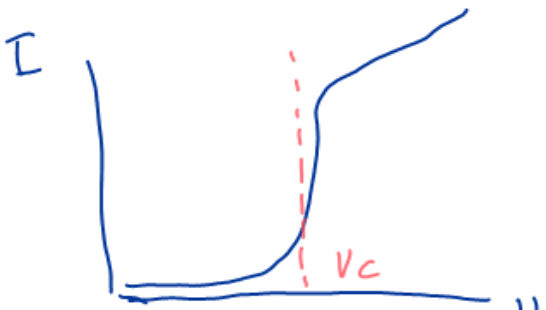
if we have two conductors A and B with thin Insulator between them: e from A could tunnel to B.



c: thin layer (10 – 20 Å)
Could be oxide layer

A and B: could be metals
or superconductors
or mixture of them

A & B are metals



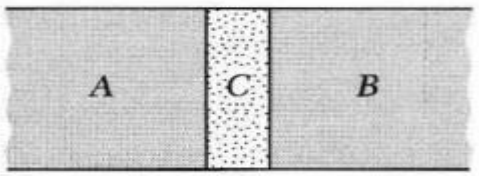
A: metal B: S.C.

I – V characteristic

Chapter 10: Superconductivity

Single Particle Tunneling

- Consider two metals separated by an insulator, as in Fig. 20. The insulator normally acts as a barrier to the flow of conduction electrons from one metal to the other.



- If the barrier is sufficiently thin (less than 10 or 20 Å) there is a significant probability that an electron which impinges on the barrier will pass from one metal to the other.
- This is called tunneling.
- In many experiments the insulating layer is simply a thin oxide layer formed on one of two evaporated metal films. Or it could be even a weak link.
- When both metals are normal conductors, the current-voltage relation of the sandwich or tunneling junction is ohmic at low voltages, with the current directly proportional to the applied voltage.
- Giaever (1960) discovered that if one of the metals becomes superconducting the current-voltage characteristic changes from the straight line of Fig. 22a to the curve shown in Fig. 22b.

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Single Particle Tunneling

Figure 22 (a) Linear current-voltage relation for junction of normal metals separated by oxide layer; (b) current voltage relation with one metal normal and the other metal superconducting.

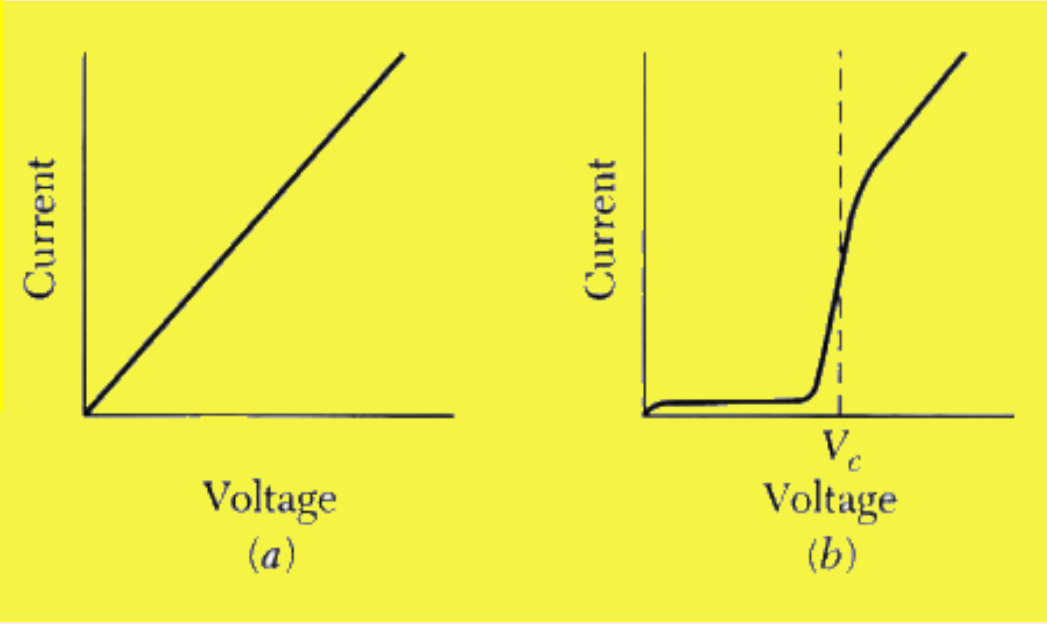
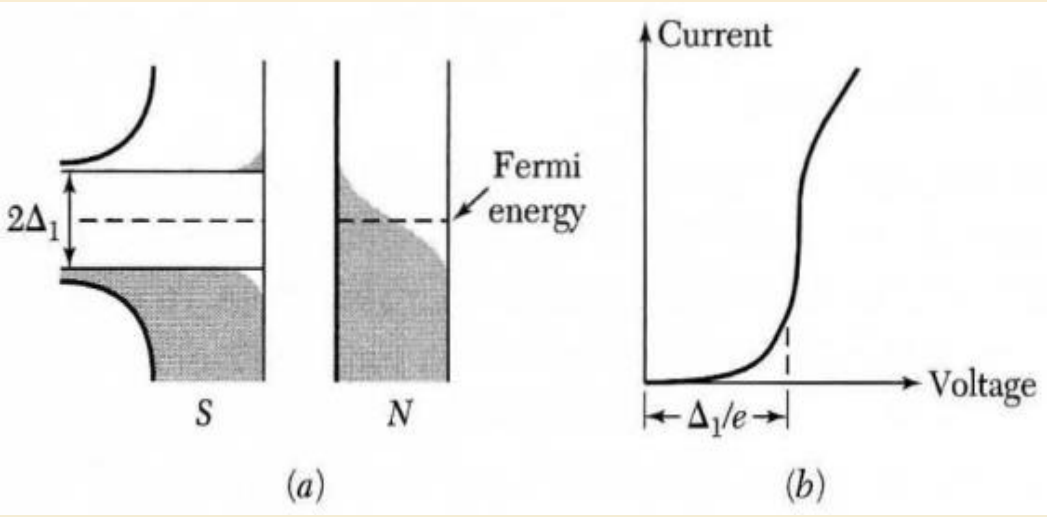


Figure 23 The density of orbitals and the current-voltage characteristic for a tunneling junction.
In (a) the energy is plotted on the vertical scale and the density of orbitals on the horizontal scale. One metal is in the normal state and one in the superconducting state. (b) I versus V; the dashes indicate the expected break at T = 0.



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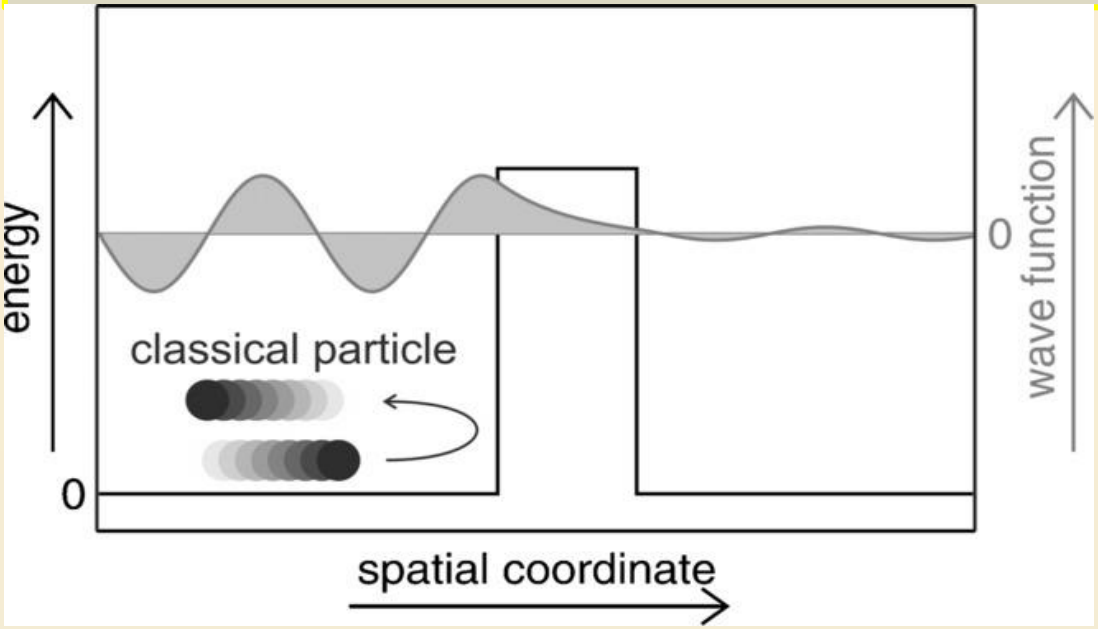
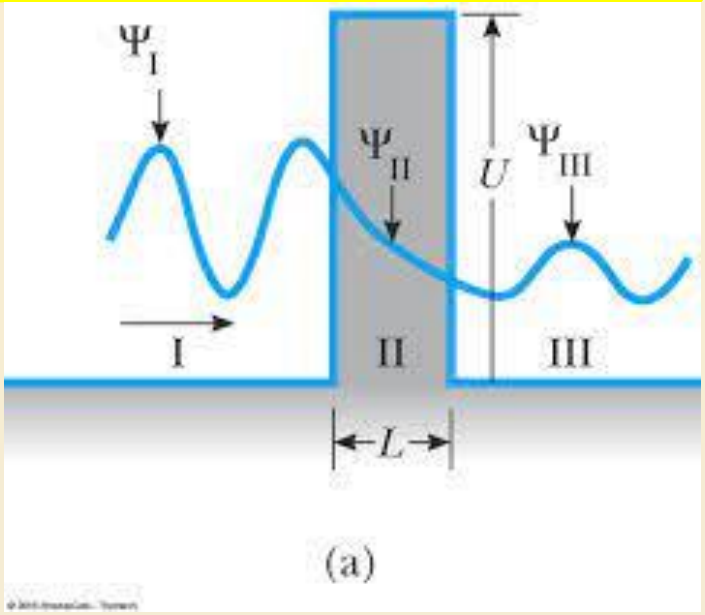
Single Particle Tunneling

- Figure 23a contrasts the electron density of orbitals in the superconductor with that in the normal metal. In the superconductor there is an energy gap centered at the Fermi level. At absolute zero no current can flow until the applied voltage is $V = E_g/2e = \Delta/e$.
- The gap E_g corresponds to the break-up of a pair of electrons in the superconducting state, with the formation of two electrons , or an electron and a hole, in the normal state.
- The current starts when $eV = \Delta$.





Chapter 10: Superconductivity

Josephson Superconductor Tunneling

- Under suitable conditions we observe remarkable effects associated with the tunneling of superconducting electron pairs from a superconductor through a layer of an insulator into another superconductor. Such a junction is called a weak link.
- **Dc Josephson effect.** A *dc current* flows across the junction in the absence of any electric or magnetic field.
- **Ac Josephson effect**. A *dc voltage* applied across the junction causes rf current oscillations across the junction. This effect has been utilized in a precision determination of the value of $\hbar/e$.
- Our discussion of Josephson junction phenomena follows the discussion of flux quantization.
- Let ψ_1, be the probability amplitude of electron pairs on one side of a junction, and let ψ_2 be the amplitude on the other side.
- For simplicity, let both superconductors be identical.
- For the present we suppose that they are both at zero potential.
- Next, we derive the equations describing this effect.

Chapter 10: Superconductivity

Dc Josephson effect

- The time-dependent Schrodinger equation for both sides of the barrier:

$$\left.\begin{aligned} i\hbar\frac{\partial\Psi_1}{\partial t} &= \hbar T\,\Psi_2 \\ i\hbar\frac{\partial\Psi_2}{\partial t} &= \hbar T\,\Psi_1 \end{aligned}\right\} \qquad (38)$$

- $\hbar T$ is for the transfer interaction across the insulator.
- T is a measure of the leakage of ψ_1 into region 2, and of ψ_2 into the region 1.
- If the insulator is very thick, *T* is zero and there is no pair tunneling.

$$\left.\begin{aligned} \psi_1 &= \sqrt{n_1}\,e^{i\varphi_1(r)} \\ \psi_2 &= \sqrt{n_2}\,e^{i\varphi_2(r)} \end{aligned}\right\} \Rightarrow$$

$$\frac{\partial\Psi_1}{\partial t} = \frac{1/2}{\sqrt{n_1}}e^{i\varphi_1(r)}\frac{\partial n_1}{\partial t} + i\Psi_1\frac{\partial\varphi_1(r)}{\partial t} = -iT\Psi_2 \qquad (39)$$

$$\frac{\partial\Psi_2}{\partial t} = \frac{1/2}{\sqrt{n_2}}e^{i\varphi_2(r)}\frac{\partial n_2}{\partial t} + i\Psi_2\frac{\partial\varphi_2(r)}{\partial t} = -iT\Psi_1 \qquad (40)$$

$$(39)\times\sqrt{n_1}e^{-i\varphi_1(r)} \Rightarrow$$

$$\sqrt{n_1}e^{-i\varphi_1(r)}\times\frac{1/2}{\sqrt{n_1}}e^{i\varphi_1(r)}\frac{\partial n_1}{\partial t}+\sqrt{n_1}e^{-i\varphi_1(r)}\times\left(i\sqrt{n_1}e^{i\varphi_1(r)}\frac{\partial\varphi_1(r)}{\partial t}\right)=\sqrt{n_1}e^{-i\varphi_1(r)}\times\left(-iT\sqrt{n_2}e^{i\varphi_2(r)}\right)$$

$$\therefore\frac{1}{2}\frac{\partial n_1}{\partial t}+in_1\frac{\partial\varphi_1}{\partial t}=-iT\sqrt{n_1n_2}e^{i\delta} \qquad (41)$$

$$(40)\times\sqrt{n_2}e^{-i\varphi_2(r)} \Rightarrow$$

$$\therefore\frac{1}{2}\frac{\partial n_2}{\partial t}+in_2\frac{\partial\varphi_2}{\partial t}=-iT\sqrt{n_1n_2}e^{-i\delta} \qquad (42)$$

$$\delta=\varphi_2-\varphi_1$$

Taking real and imagenary parts together:

$$\frac{\partial n_1}{\partial t}=2T\sqrt{n_1n_2}\sin\delta;\qquad\frac{\partial n_2}{\partial t}=-2T\sqrt{n_1n_2}\sin\delta \qquad (43)$$

$$\frac{\partial\varphi_1}{\partial t}=-T\sqrt{\frac{n_2}{n_1}}\cos\delta;\qquad\frac{\partial\varphi_2}{\partial t}=-T\sqrt{\frac{n_1}{n_2}}\cos\delta \qquad (44)$$

❑ If $n_1 = n_2$ as for identical superconductors 1 and 2: (44)➔

$$\left.\begin{aligned} &\frac{\partial \varphi_1}{\partial t} = \frac{\partial \varphi_2}{\partial t} \\ &\therefore \frac{\partial}{\partial t}\left(\varphi_2 - \varphi_1\right) = 0 \end{aligned}\right\} \qquad (45)$$

$(43) \rightarrow$

$$\frac{\partial n_1}{\partial t} = -\frac{\partial n_2}{\partial t} \qquad (46)$$

❑ Since current J is dependent on $\partial n_2/\partial t$ or $\partial n_1/\partial t$, then we must have:

$$\because \frac{\partial n_1}{\partial t} = 2T\sqrt{n_1 n_2}\sin\delta$$

$$\therefore J = J_0 \sin\delta$$

$$\therefore J = J_0 \sin\left(\varphi_2 - \varphi_1\right) \qquad (47)$$

$$J_0 = 2T\sqrt{n_1 n_2}$$

❑ J_0 is the maximum zero-voltage current that can be passed by the junction

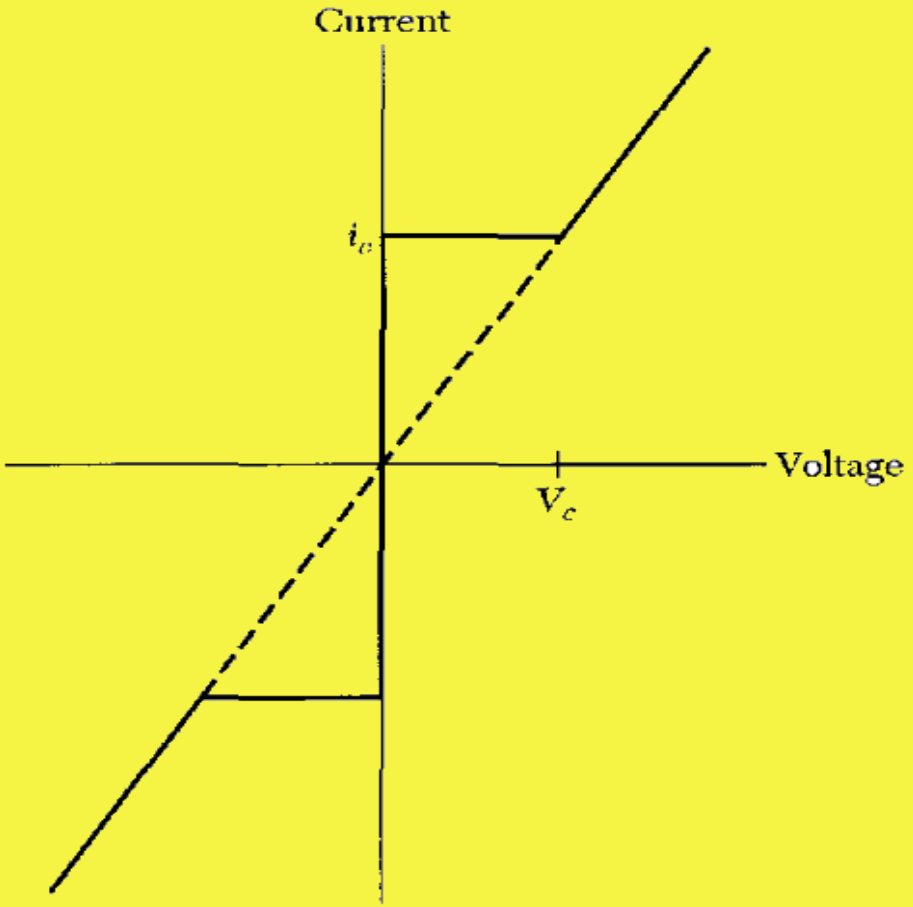
Chapter 10: Superconductivity

Josephson Superconductor Tunneling

❑ With no applied voltage a dc current will flow across the junction (Fig. 24), with a value between J_o and - J_o according to the value of the phase difference $\varphi_2 - \varphi_1$, This is the dc Josephson effect.

Figure 24:

- Current-voltage characteristic of a Josephson junction. Dc currents flow under zero applied voltage up to a critical current i_o: this is the dc Josephson effect.
- At voltages above V_c the junction has a finite resistance, but the current has an oscillatory component of frequency $\omega = 2eV/\hbar$,
- this is the ac Josephson effect.



Chapter 10: Superconductivity

Ac Josephson effect

- Let a dc voltage V be applied across the junction. We can do this because the junction is an insulator. An electron pair experiences a potential energy difference qV on passing across the junction, where $q = -2e$. We can say that a pair on one side is at potential energy $-eV$ and a pair on the other side is at eV. The equations of motion that replace (38) are:

$$\left.\begin{aligned} i\hbar\frac{\partial\Psi_1}{\partial t} &= \hbar T\Psi_2 - eV\Psi_1 \\ i\hbar\frac{\partial\Psi_2}{\partial t} &= \hbar T\Psi_1 + eV\Psi_2 \end{aligned}\right\} \qquad (48)$$

$$\left.\begin{aligned} \psi_1 &= \sqrt{n_1}\,e^{i\varphi_1(r)} \\ \psi_2 &= \sqrt{n_2}\,e^{i\varphi_2(r)} \end{aligned}\right\} \Rightarrow$$

$$\frac{\partial\Psi_1}{\partial t} = \frac{1/2}{\sqrt{n_1}}e^{i\varphi_1(r)}\frac{\partial n_1}{\partial t} + i\Psi_1\frac{\partial\varphi_1(r)}{\partial t} = -iT\Psi_2 + i\frac{eV}{\hbar}\Psi_1 \qquad (48a)$$

$$\frac{\partial\Psi_2}{\partial t} = \frac{1/2}{\sqrt{n_2}}e^{i\varphi_2(r)}\frac{\partial n_2}{\partial t} + i\Psi_2\frac{\partial\varphi_2(r)}{\partial t} = -iT\Psi_1 - i\frac{eV}{\hbar}\Psi_2 \qquad (48b)$$

$$(48a)\times\sqrt{n_1}e^{-i\varphi_1(r)} \Rightarrow$$

$$\sqrt{n_1}e^{-i\varphi_1}\times\frac{1/2}{\sqrt{n_1}}e^{i\varphi_1}\frac{\partial n_1}{\partial t}+\sqrt{n_1}e^{-i\varphi_1}\times\left(i\sqrt{n_1}e^{i\varphi_1}\frac{\partial\varphi_1}{\partial t}\right)$$

$$=\sqrt{n_1}e^{-i\varphi_1}\times\left(-iT\sqrt{n_2}e^{-i\varphi_2}\right)+\sqrt{n_1}e^{-i\varphi_1}\times i\frac{eV}{\hbar}\sqrt{n_1}e^{i\varphi_1}$$

$$\therefore\frac{1}{2}\frac{\partial n_1}{\partial t}+in_1\frac{\partial\varphi_1}{\partial t}=i\frac{eVn_1}{\hbar}-iT\sqrt{n_1n_2}e^{-i\delta}$$

$$(48b)\times\sqrt{n_2}e^{-i\varphi_2} \Rightarrow$$

$$\therefore\frac{1}{2}\frac{\partial n_2}{\partial t}+in_2\frac{\partial\varphi_2}{\partial t}=-i\frac{eVn_2}{\hbar}-iT\sqrt{n_1n_2}e^{-i\delta} \qquad (49)$$

❑ Like we did before, splitting real and imaginary parts.

$$\frac{\partial n_1}{\partial t}=2T\sqrt{n_1n_2}\sin\delta;\qquad\frac{\partial n_2}{\partial t}=-2T\sqrt{n_1n_2}\sin\delta \qquad (50)$$

❑ This result is the same for the case V=0.

Chapter 10: Superconductivity

Ac Josephson effect

❑ For the imaginary part:

$$\frac{\partial \varphi_1}{\partial t} = \frac{eV}{\hbar} - T\sqrt{\frac{n_2}{n_1}}\cos\delta; \qquad \frac{\partial \varphi_2}{\partial t} = -\frac{eV}{\hbar} - T\sqrt{\frac{n_1}{n_2}}\cos\delta \qquad (51)$$

❑ So here we added a new term: $eV/\hbar$

(41) becomes:

$$\frac{1}{2}\frac{\partial n_2}{\partial t} + in_2\frac{\partial \varphi_2}{\partial t} = -i\frac{eVn_2}{\hbar} - iT\sqrt{n_1 n_2}e^{-i\delta} \qquad (52)$$

$$\therefore \frac{1}{2}\frac{\partial n_2}{\partial t} + in_2\frac{\partial \varphi_2}{\partial t} = -i\frac{eVn_2}{\hbar} - iT\sqrt{n_1 n_2}\left(\cos\delta - i\sin\delta\right)$$

$$\therefore \frac{1}{2}\frac{\partial n_2}{\partial t} + in_2\frac{\partial \varphi_2}{\partial t} = -i\frac{eVn_2}{\hbar} - iT\sqrt{n_1 n_2}\cos\delta - T\sqrt{n_1 n_2}\sin\delta$$

$$\therefore \frac{\partial n_2}{\partial t} = -2T\sqrt{n_1 n_2}\sin\delta \qquad (53)$$

$$\& \frac{\partial \varphi_2}{\partial t} = -\frac{eV}{\hbar} - T\sqrt{\frac{n_1}{n_2}}\cos\delta \qquad (54)$$

Chapter 10: Superconductivity

Ac Josephson effect

❑ If $n_1 = n_2$ as for identical superconductors 1 and 2: (51 & 54)➔

$$\frac{\partial \varphi_1}{\partial t} = \frac{eV}{\hbar} - T\cos\delta; \qquad \frac{\partial \varphi_2}{\partial t} = -\frac{eV}{\hbar} - T\cos\delta$$

$$\therefore \frac{\partial \varphi_2}{\partial t} - \frac{\partial \varphi_1}{\partial t} = -2\frac{eV}{\hbar}$$

$$\frac{\partial}{\partial t}\left(\varphi_2 - \varphi_1\right) = -2\frac{eV}{\hbar} \qquad (55)$$

$$\therefore \int \partial\delta = -2\frac{eV}{\hbar}\int \partial t$$

$$\Rightarrow \delta(t) - \delta(0) = -2\frac{eV}{\hbar}t$$

$$\therefore \delta(t) = \delta(0) - 2\frac{eV}{\hbar}t \qquad (56)$$

$$\because J = J_0 \sin\left(\varphi_2 - \varphi_1\right) \qquad (47)$$

$$\therefore J = J_0 \sin\left(\delta(0) - 2\frac{eV}{\hbar}t\right) \qquad (57)$$

Chapter 10: Superconductivity

Ac Josephson effect

- Hence, current J oscillate with frequency:

$$\omega = \frac{2eV}{\hbar} \qquad (58)$$

- This is the **ac Josephson effect**.
- A dc voltage of 1 μV produces a frequency of 483.6 MHz.
- The relation (58) says that a photon of energy ħω= 2eV is emitted or absorbed when an electron pair crosses the barrier.
- By measuring the voltage and the frequency it is possible to obtain a very precise value of e/ħ

Chapter 10: Superconductivity

Macroscopic Quantum Interference

- As we have shown before:

$$\varphi_2 - \varphi_1 = 2\pi s \qquad (24)$$

$$\Phi = \frac{\hbar c}{2\mathrm{e}} 2\pi s \qquad (26)$$

or :

$$\Phi = \frac{\hbar c}{2\mathrm{e}}\left[2\pi\left(\varphi_2 - \varphi_1\right)\right]$$

$$\therefore \left(\varphi_2 - \varphi_1\right) = \frac{2\mathrm{e}}{\hbar c}\Phi \qquad (59)$$

- We consider two Josephson junctions in parallel, as in Fig. 25. No voltage is applied.
- Let the phase difference between points 1 and 2 taken on a path through junction *a* be δ_a.
- When taken on a path through junction *b,* the phase difference is δ_b
- In the absence of a magnetic field these two phases must be equal
- Now let the flux Φ pass through the interior of the circuit. We do this with a straight solenoid normal to the plane of the paper and lying inside the circuit.

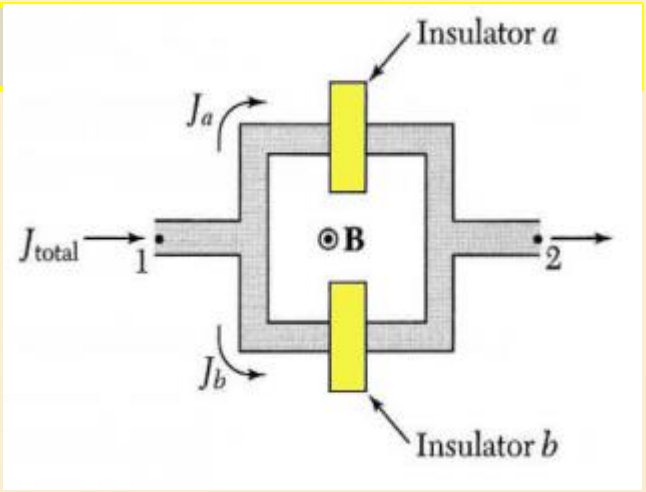
Chapter 10: Superconductivity

Macroscopic Quantum Interference

❑ From Equation (59) we have:

$$\left(\delta_b - \delta_a\right) = \frac{2\,\mathrm{e}}{\hbar c}\Phi \qquad (59^*)$$

$$\left.\begin{aligned} \therefore\ \delta_b &= \delta_0 + \frac{\mathrm{e}}{\hbar c}\Phi \\ \&\ \delta_a &= \delta_0 - \frac{\mathrm{e}}{\hbar c}\Phi \end{aligned}\right\} \qquad (60)$$



❑ Note that if we use (60) (both equations) we get back (59*).
❑ The total current is the sum of J_a and J_b
❑ (47) and (59*) give the total current:

$$J_{total} = J_0\left[\sin\left(\delta_0 + \frac{\mathrm{e}}{\hbar c}\Phi\right) + \sin\left(\delta_0 - \frac{\mathrm{e}}{\hbar c}\Phi\right)\right]$$

$$J_{total} = J_0\left[\sin\delta_0\cos\frac{\mathrm{e}\Phi}{\hbar c} + \cos\delta_0\sin\frac{\mathrm{e}\Phi}{\hbar c} + \sin\delta_0\cos\frac{\mathrm{e}\Phi}{\hbar c} - \cos\delta_0\sin\frac{\mathrm{e}\Phi}{\hbar c}\right]$$

$$\therefore J_{total} = J_0\left(2\sin\delta_0\cos\frac{\mathrm{e}\Phi}{\hbar c}\right) = 2\left(J_0\sin\delta_0\right)\cos\frac{\mathrm{e}\Phi}{\hbar c} \qquad (60^*)$$

- The current varies with Φ and has maxima when:

$$\because J_{total} = 2\left(J_0 \sin\delta_0\right)\cos\frac{e\Phi}{\hbar c}$$

$$\therefore J_{max} = 2\left(J_0 \sin\delta_0\right)\cos(s\pi)$$

$$at: \frac{e\Phi}{\hbar c} = s\pi \qquad (61)$$

$$s = \text{integer}$$

- The periodicity of the current is shown in Fig. 26.
- The short period variation is produced by interference from the two junctions, as predicted by (61).
- The longer period variation is a diffraction effect and arises from the finite dimensions of each junction.
- This causes Φ to depend on the particular path of integration

Chapter 10: Superconductivity

Macroscopic Quantum Interference

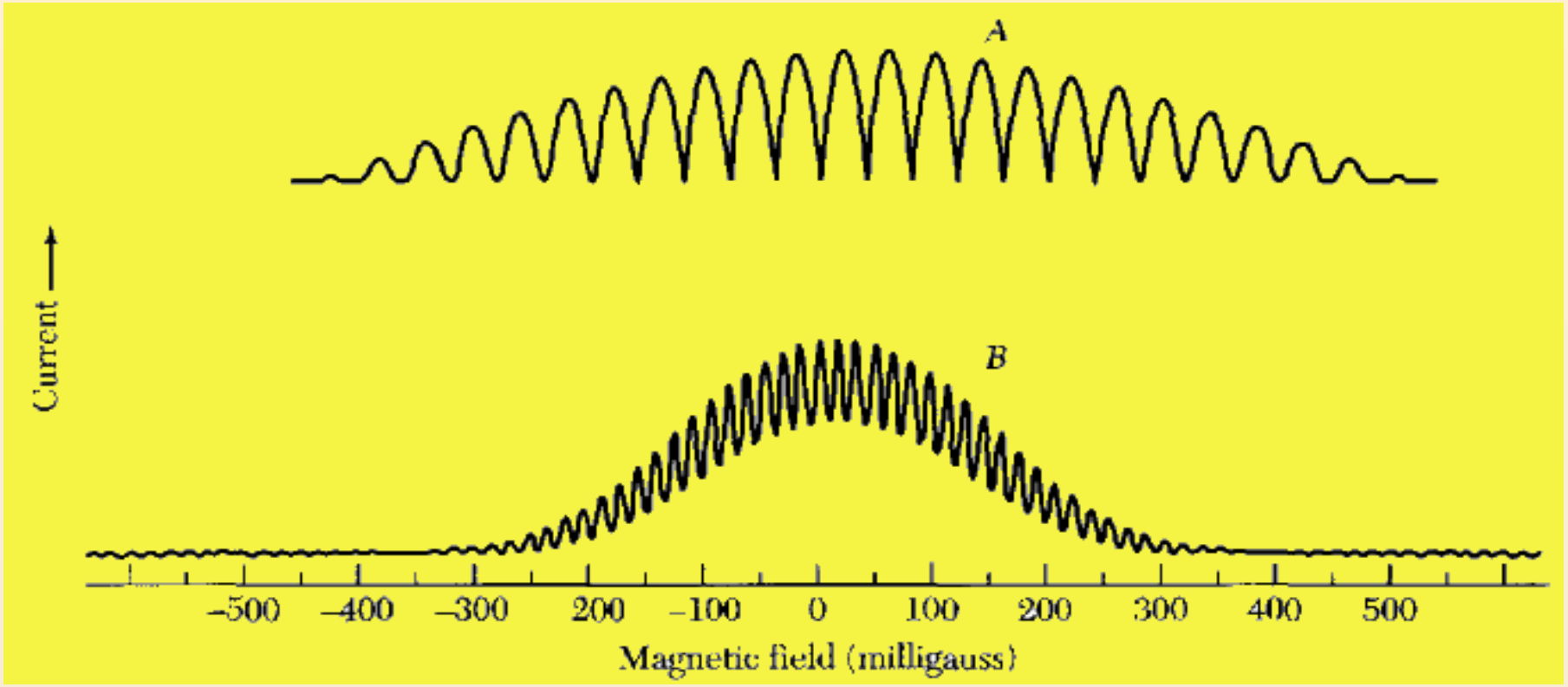


Figure 26 Experimental trace of J_{max} versus magnetic field showing interference and diffraction effects for two junctions A and B. The field periodicity is 39.5 and 16 mG for *A* and *B,* respectively. Approximate maximum currents are 1 mA (*A*) and 0.5 mA (*B)*. The junction separation is 3 mm and junction width 0.5 mm for both cases. The zero offset of *A* is due to a background magnetic field

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2021/2022

Lecture No. 11

Chapter 13:
Magnetic Resonance

Prof. Nasser S. Alzayed

Chapter 13: Magnetic Resonance

Introduction

- NMR: nuclear magnetic resonance
  NQR: nuclear quadruple resonance
  EPR or ESR: electron paramagnetic or spin resonance
  FMR: ferromagnetic resonance
  SWR: spin wave resonance (ferromagnetic films)
  AFMR: antiferromagnetic resonance
  CESR: conduction electron spin resonance
- A great impact of NMR has been in organic chemistry and biochemistry, where NMR provides a powerful tool for the identification and the structure determination of complex molecules
- A major medical application of NMR is magnetic resonance imaging (MRI), which allows the resolution in 3D of abnormal growths, configurations, and reactions in the whole body.

Prof. Nasser S. Alzayed

Chapter 13: Magnetic Resonance

NUCLEAR MAGNETIC RESONANCE

- We consider a nucleus that possesses a magnetic moment μ and an angular momentum $\hbar\mathbf{L}$. The two quantities are parallel, and we may write:

$$\mu = \gamma\hbar\mathbf{L} \qquad (1)$$

- Where γ is constant.
- $\mathbf{L}$ denotes the nuclear angular momentum measured in units of $\hbar$.
- The energy of interaction with the applied magnetic field is:

$$U = -\mu.\mathbf{B}_a \qquad (2)$$

$$\text{if } \mathbf{B}_a = B_0\hat{z} \rightarrow$$

$$U = -\mu_z B_0 = -\gamma\hbar B_0 L_z \qquad (3)$$

- The allowed values of Lz are:

$$m_\ell = \ell, \ell-1, ..., -\ell$$

$$\therefore U = -\gamma\hbar B_0 m_\ell \qquad (3b)$$

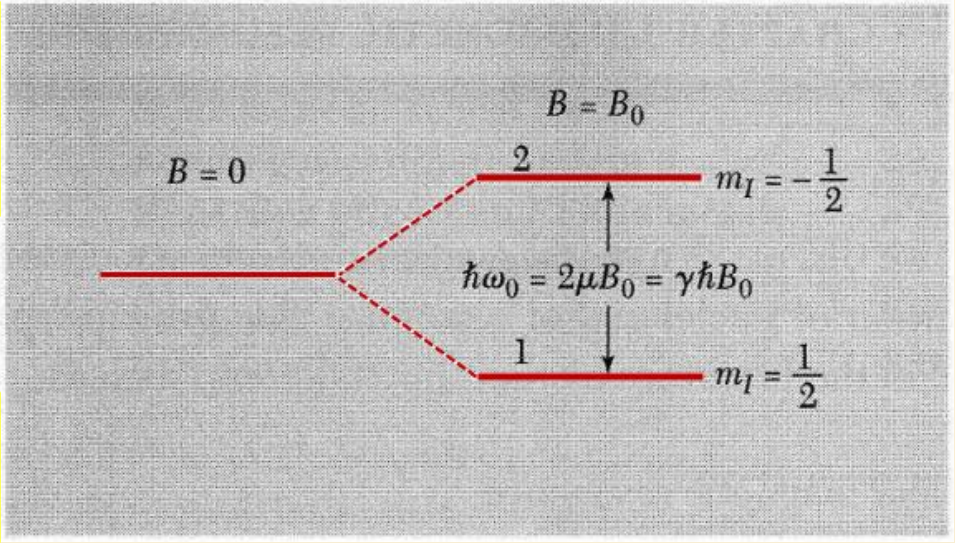
- In a magnetic field a nucleus with S = ½ has two energy levels corresponding to $m_\ell = \pm ½$ as in Fig. 2.

Chapter 13: Magnetic Resonance

NUCLEAR MAGNETIC RESONANCE

- We consider a nucleus that possesses a magnetic moment μ and an angular momentum $\hbar\mathbf{L}$. The two quantities are parallel, and we may write:

- If $\hbar\omega_o$ denotes the energy difference between the two levels, then:



$$\hbar\omega_0 = \gamma\hbar B_0$$

$$\therefore \omega_0 = \gamma B_0 \qquad (4)$$

- This is the fundamental condition for magnetic resonance absorption

- For the proton1 $\gamma = 2.675 \times 10^4$ s^{-1} gauss^{-1} $= 2.675 \times 108$ S-l s^{-1} tesla^{-1} so that: $\nu(MHz) = 42.6B_0$ (tesla)
- For the electron spin, $\nu(GHz) = 28.0B_0$ (tesla)
- It is much larger for the case of electron.

Chapter 13: Magnetic Resonance

Equations of Motion

❑ Equation of motion in case of rotation is, from Newton's laws:

$$\mu = \gamma \hbar \mathbf{L}$$

$$\because \sum \tau = \frac{dL}{dt}$$

$$\because \tau = \mu \times B_a$$

$$\therefore \frac{d\,\hbar \mathbf{L}}{dt} = \mu \times B_a \qquad (5)$$

$$\because \mu = \gamma \hbar \mathbf{L} \Rightarrow \hbar \mathbf{L} = \frac{\mu}{\gamma}$$

$$\therefore \frac{d}{dt}\frac{\mu}{\gamma} = \mu \times B_a$$

$$\rightarrow \frac{d\,\mu}{dt} = \gamma \mu \times B_a \qquad (6)$$

❑ This is a gyroscopic equation. Since the magnetization is the sum of magnetic moments, we can change this to the rate of magnetization change.

Chapter 13: Magnetic Resonance

Equations of Motion

- The nuclear magnetization **M** can be calculated:

$$\because \mathrm{M} = \sum \mu_i$$

$$\therefore (6) \rightarrow$$

$$\frac{d\mathrm{M}}{dt} = \gamma \mathrm{M} \times B_a \qquad (7)$$

$$\text{if: } B_a = B_o \hat{z}$$

$$\therefore M_x = 0; M_y = 0 \; ; M_z = M_o = \chi_o B_a = \frac{CB_o}{T} \qquad (8)$$

- where the susceptibility is χ_o and the Curie constant $C = N\mu^2/3k_B$, as in Chapter 11.
  We can show then that:

$$\frac{d\mathrm{M_z}}{dt} = \frac{\mathrm{M_o}\text{-}\mathrm{M_z}}{T_1} \qquad (10)$$

- In the standard notation T_1 is called the **longitudinal** relaxation time or the spin-lattice relaxation time.

Chapter 13: Magnetic Resonance

Equations of Motion

- If at t = 0 an unmagnetized specimen is placed in a magnetic field B_{oz}, the magnetization will increase from the initial value $M_z = 0$ to a final value $M_z = M_o$
- Integrating both sides in (10):

$$\int_0^{M_z} \frac{dM_z}{M_o - M_z} = \frac{1}{T_1} \int_0^t dt \qquad (11)$$

$$\rightarrow$$

$$\log\left(\frac{M_o}{M_o - M_z}\right) = \frac{t}{T}$$

$$\rightarrow$$

$$\frac{M_o}{M_o - M_z} = e^{\frac{t}{T}} \rightarrow \frac{M_o - M_z}{M_o} = e^{-\frac{t}{T}}$$

$$\therefore M_z = M_o\left(1 - e^{-\frac{t}{T}}\right) \qquad (12)$$

Chapter 13: Magnetic Resonance

Equations of Motion

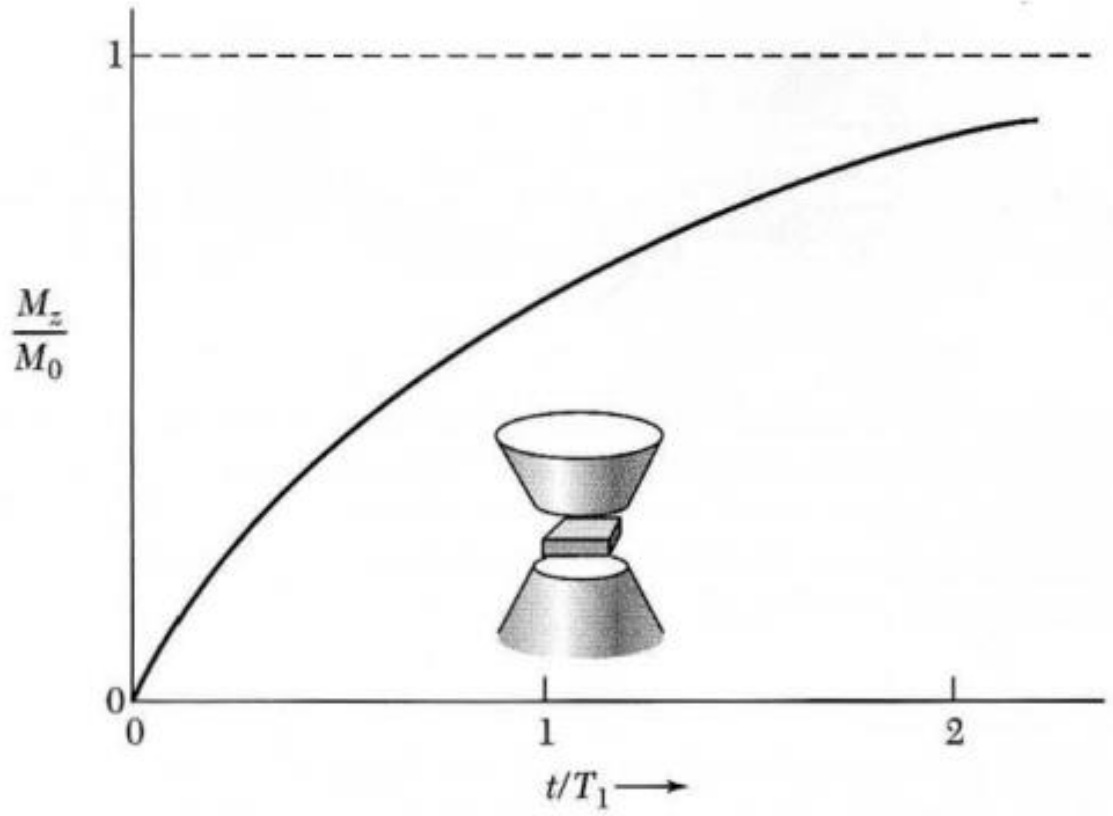


Figure 3 At time $t = 0$ an unmagnetized specimen $M_z(0) = 0$ is placed in a static magnetic field B_0. The magnetization increases with time and approaches the new equilibrium value $M_0 = \chi_0 B_0$. This experiment defines the longitudinal relaxation time T_1. The magnetic energy density $-\mathbf{M} \cdot \mathbf{B}$ decreases as part of the spin population moves into the lower level. The asymptotic value at $t \gg T_1$ is $-M_0 B_0$. The energy flows from the spin system to the system of lattice vibrations; thus T_1 is also called the spin-lattice relaxation time.

Phys 672

Advanced Solid State Physics

Physics & Astronomy
King Saud University
First Term: 2025

Lecture No. 12

Chapter 14:
Plasmons, Polaritons, and Polarons

Prof. Nasser S. Alzayed

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

* Fermi liquid: (F.L.)

F.L. Theory ≡ Landau – Fermi liquid theory 1956

"this Theory: is a theoritical model of Interacting Fermions"

Just as in normal metals at T ~ 0 K

* Theory explains: Why some of the properties of "Interacting Fermion system" are similar to those of the "Fermi Gas"

Fermi-Liquid: electrons Interact

" - Gas : no Interaction

* Examples of F.L.
  ① Liquid He^{-3} ② electrons in normal metals

We have 2 phases of He^{-3}
  ① F.L at Low T
  ② superfluid phase at even lower T

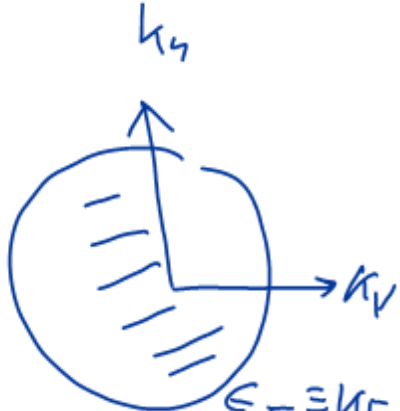
* note that He^{-3}: 2 protons + 1 neutron $\Rightarrow$ Fermion

* Landau approach:
if we have Fermi Gas (non-Interacting e's)
then we "turn on" Interactions slowly

Ground state of F.G $\xrightarrow{\text{adiabatically}}$ Ground state of F.L

(1) $\longrightarrow$ (2)

In F.G. Ground State:
Pauli x.p. $\Rightarrow$ all momentum states are at $k \leq k_F$



⇒ all states inside Fermisphere are occupied

and " " outside " " " un-occupied
higher

* Now: when Interactions are turned on ⇒

spin
charge } for occupied states: Remain the same
→ momentum

However: the mass "m" & magnetic moment:
will be Renormalized to new values

* This is Because of "e-e" Interaction (only Conduction) electron by electrostatic means ⟹ Collisions

this Interaction ⟹ Increase in effective mass

* it is amazing that Crowded electrons in metals that are only 2Å apart ; travel long distance without Collisions.

* mean Free path ~ 10^4 Å (at Room T)
~ 1 cm

Two factors are Behind this Result:

① Pauli exclusion principle

* ② screening of the Coulomb interaction

In Pauli case:

If we have 2 electrons.

e at k_1
collides with } $\Rightarrow k_3 + k_4$
e at k_2

Collision is allowed only if k_3 and k_4 are vacant

If we consider the different Possibilities.

① ϵ_1 outside (sphere)

ϵ_2 inside (r)

if $\mu = 0$ just at Fermi sphere surface

$\Rightarrow$ ϵ_1 + ive

② ϵ_2 - ive

③ states ϵ_3 & ϵ_4 are vacant

④ " " " " are + ive

⑤ Conservation of Energy $\Rightarrow$

$\Rightarrow |\epsilon_1| < \epsilon_2$

$\Rightarrow \quad \epsilon_1 + \epsilon_2 = \epsilon_3 + \epsilon_4$

⑥ $\Rightarrow$ Collisions are possible ..
note that orbital ② is within a shell of
thickness ϵ_1 from μ_0

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **The superfluid phase of helium:**
- is a phase of matter with zero viscosity.
- There are two isotopes of helium that can exhibit superfluidity: He^{-3} and He^{-4}
- He^{-4} enters the superfluid phase below a temperature of about 2.17 Kelvin at atmospheric pressure. In this state, it can flow without friction, seep through tiny cracks and pores that would hold back ordinary fluids, and conduct heat extremely efficiently through a process called second sound.
- He^{-3}, a lighter and rarer isotope, also becomes a superfluid, but at much lower temperatures (thousandths of a Kelvin) and exhibits different properties due to its fermionic nature, as opposed to the bosonic nature of He^{-4}. The superfluidity in He^{-3} is explained by the formation of Cooper pairs and is described by the BCS theory, similar to the theory explaining superconductivity in metals.

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **Fermi Liquid:**
- Fermi liquid theory (also known as Landau–Fermi liquid theory) is a theoretical model of interacting fermions that describes the normal state of most metals at sufficiently low temperatures.
- The phenomenological theory of Fermi liquids was introduced by the Soviet physicist Lev Davidovich Landau in 1956, and later developed by Alexei Abrikosov and I. M. Khalatnikov using diagrammatic perturbation theory.
- The theory explains why some of the properties of an interacting fermion system are very similar to those of the **Fermi gas** (i.e. non-interacting fermions), and why other properties differ.
- Important examples of where Fermi liquid theory has been successfully applied are most notably electrons in most metals and Liquid He^{-3}
- Liquid He^{-3} is a Fermi liquid at low temperatures (but not low enough to be in its superfluid phase.)
- He^{-3} is an isotope of Helium, with 2 protons, 1 neutron and 2 electrons per atom. Because there is an odd number of fermions inside the atom, the atom itself is also a fermion.

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **Fermi Liquid:**
- The electrons in a normal (non-superconducting) metal also form a Fermi liquid, as do the nucleons (protons and neutrons) in an atomic nucleus.
- Strontium ruthenate displays some key properties of Fermi liquids, despite being a strongly correlated material, and is compared with high temperature superconductors like cuprates
- The key ideas behind Landau's theory are the notion of adiabaticity and the exclusion principle.
- *Consider a non-interacting fermion system (a Fermi gas), and suppose we "turn on" the interaction slowly. Landau argued that in this situation, the ground state of the Fermi gas would adiabatically transform into the ground state of the interacting system*.
- By Pauli's exclusion principle, the ground state of a Fermi gas consists of fermions occupying all momentum states corresponding to momentum $K \leq K_F$ with all higher momentum states unoccupied.

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **Fermi Liquid:**
- As interaction is turned on, the spin, charge and momentum of the fermions corresponding to the occupied states remain unchanged, while their dynamical properties, such as their mass, magnetic moment etc. are renormalized to new values.
- Thus, there is a one-to-one correspondence between the elementary excitations of a Fermi gas system and a Fermi liquid system. In the context of Fermi liquids, these excitations are called "quasi-particles".

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **Fermi Liquid:**
- Because of the interaction of the conduction electrons with each other through their electrostatic interaction, the electrons suffer collisions
- Further, a moving electron causes an inertial reaction in the surrounding electron gas, thereby increasing the effective mass of the electron
- The effects of electron-electron interactions are usually described within the framework of the Landau theory of a Fermi liquid
- The object of the theory is to give a unified account of the effect of interactions.
- *A Fermi gas is a system of noninteracting fermions; the same system with interactions is a Fermi liquid*.
- Landau's theory gives a good account of the low-lying single particle excitations of the system of interacting electrons
- These single particle excitations are called quasiparticles; they have a one-to-one correspondence with the Single particle excitations of the electron gas.
- A quasiparticle may be thought of as a Single particle accompanied by a distortion cloud in the electron gas.

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- **Electron-Electron Collisions:**
- It is an astonishing property of metals that conduction electrons, although crowded together only 2 Å apart, travel long distances between collisions with each other.
- The mean free paths for electron-electron collisions are longer than 10^4 Å at room temperature and longer than 10 cm at 1 K
- Two factors are responsible for these long mean free paths, without which the free-electron model of metals would have little value.
- 1-The most powerful factor is the exclusion principle (Fig. 17),
- 2- The screening of the coulomb interaction between two electrons.

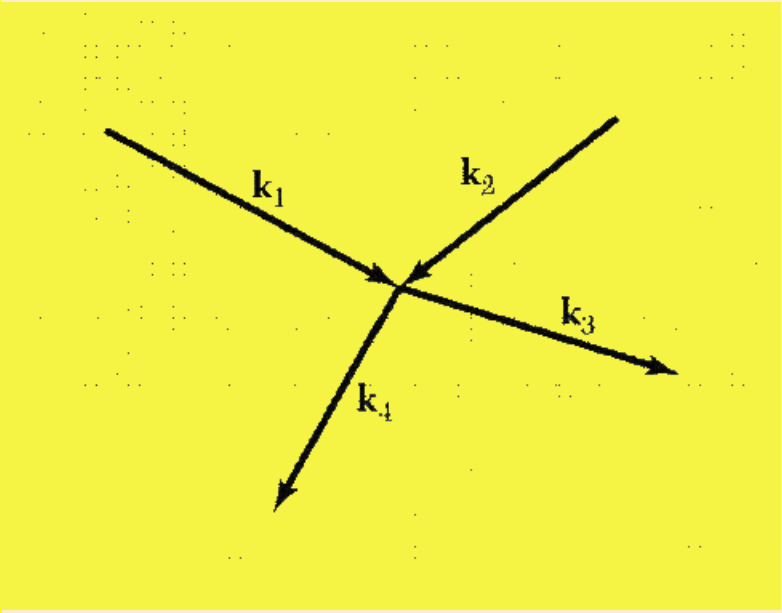


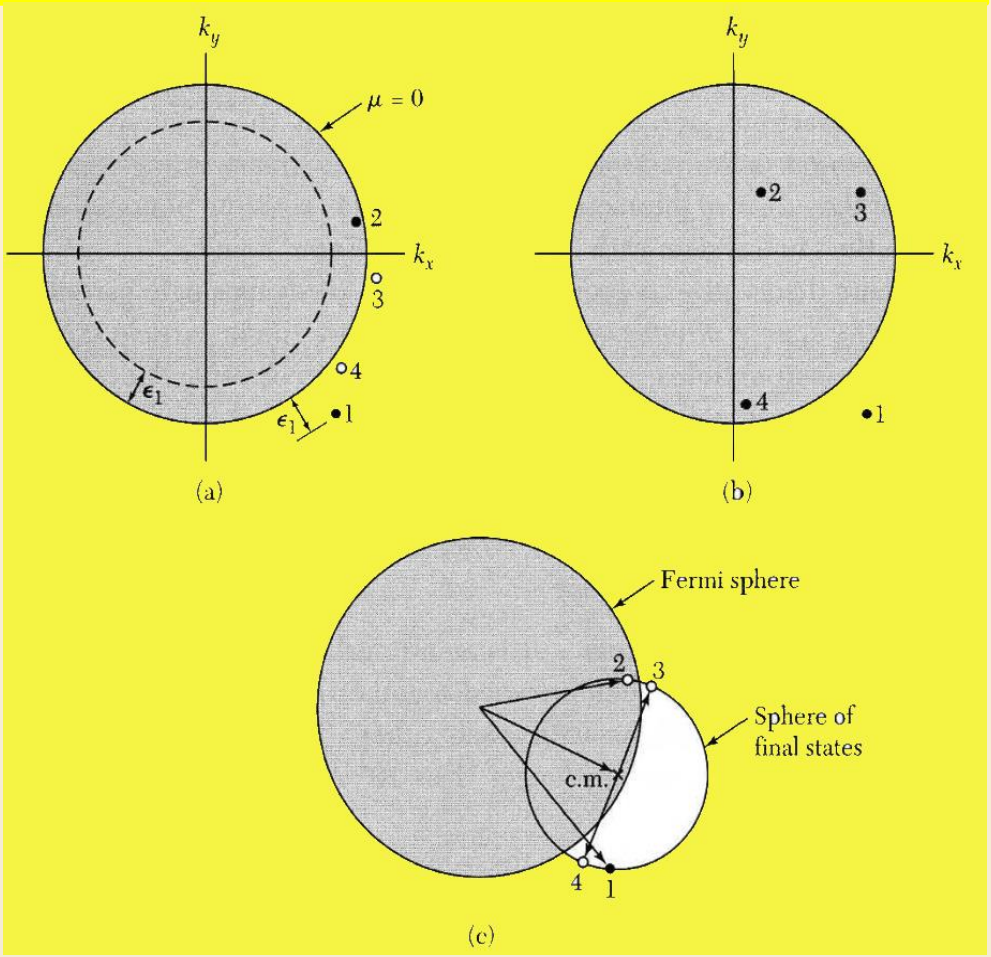
Figure 17: A collision between two electrons of wavevectors $\mathbf{k}_1$ and $\mathbf{k}_2$. After the collision the particles have wavevectors $\mathbf{k}_3$ and $\mathbf{k}_4$. The Pauli exclusion principle allows collisions only to final states $\mathbf{k}_3$, $\mathbf{k}_4$ which were vacant before the collision

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- We show how the exclusion principle reduces the collision frequency of an electron that has a low excitation energy ϵ_1 outside a filled Fermi sphere (Fig. 18)

Figure 18 In (a) the electrons in initial orbitals 1 and 2 collide. If the orbitals 3 and 4 are initially vacant, the electrons 1 and 2 can occupy orbitals 3 and 4 after the collision. Energy and momentum are conserved. In (b) the electrons in initial orbitals 1 and 2 have no vacant final orbitals available that allow energy to be conserved in the collision. Orbitals such as 3 and 4 would conserve energy and momentum, but they are already filled with other electrons. In (c) we have denoted with X the wavevector of the center of mass of 1 and 2. All pairs of orbitals 3 and 4 conserve momentum and energy if they lie at opposite ends of a diameter of the small sphere. The small sphere was drawn from the center of mass to pass through 1 and 2. But not all pairs of points 3, 4 are allowed by the exclusion principle, for both 3, 4 must lie outside the Fermi sphere; the fraction allowed is $\approx \epsilon_1/\epsilon_F$.



Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- We estimate the effect of the exclusion principle on the two-body collision 1 + 2 $\rightarrow$ 3 + 4 between an electron in the excited orbital 1 and an electron in the filled orbital 2 in the Fermi sea.
- It is convenient to refer all energies to the Fermi level μ taken as the zero of energy; thus ϵ_1 will be positive and ϵ_2 will be negative.
- Because of the exclusion principle the orbitals 3 and 4 of the electrons after collision must lie outside the Fermi sphere, all orbitals within the sphere being already occupied; thus both energies ϵ_3, ϵ_4 must be positive referred to zero on the Fermi sphere.
- The conservation of energy requires that $|\epsilon_1| < \epsilon_2$ for otherwise $\epsilon_3 + \epsilon_4 = \epsilon_1 + \epsilon_2$ could not be positive.
- This means that collisions are possible only if the orbital 2 lies within a shell of thickness ϵ_1 within the Fermi surface, as in Fig. 18a.
- Thus the fraction $\approx \epsilon_1/\epsilon_F$ of the electrons in filled orbitals provides a suitable target for electron 1. But even if the target electron 2 is in the suitable energy shell, only a small fraction of the final orbitals compatible with conservation of energy and momentum are allowed by the exclusion principle. This gives a second factor of ϵ_1/ϵ_F.

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- In Fig. 18c we see a small sphere on which all pairs of orbitals 3, 4 at opposite ends of a diameter satisfy the conservation laws, but collisions can occur only if both orbitals 3, 4 lie outside the Fermi sea. The product of the two fractions is $(\epsilon_1/\epsilon_F)^2$. If ϵ_1 corresponds to 1 **K** and ϵ_F to 5 X 10^4 **K**, we have $(\epsilon_1/\epsilon_F)^2 \approx 4 \times 10^{-10}$, the factor by which the exclusion principle reduces the collision rate.
- The argument is not changed for a thermal distribution of electrons at a low temperature such that $k_BT << \epsilon_F$. We replace ϵ_1 by the thermal energy $=k_BT$, and now the rate at which electron-electron collisions take place is reduced below the classical value by $(k_BT/\epsilon_F)^2$, *so that the effective collision cross section* σ *is:*

$$\sigma \approx (k_BT/\epsilon_F)^2 \sigma_0 \qquad (63)$$

- where σ_0 is the cross section for the electron-electron interaction.
- The effect of the electron-gas background in electron-electron collisions is to reduce σ_0 below the value expected from the Rutherford scattering equation for the unscreened coulomb potential

Chapter 13: Plasmons, Polaritons, and Polarons

Electrons-electrons interaction

- At room temperature in a typical metal $k_B T/\epsilon_F$ is ~ 10^{-2} , so that σ ~ $10^{-4}\,\sigma_0$ ~ 10^{-19} cm^2.
- The mean free path for electron-electron collisions is $\ell \approx 1/n\sigma \sim 10^{-4}$ cm at room temperature.
- This is longer than the mean free path due to electron-phonon collisions by at least a factor of 10.
- *So that at room temperature collisions with phonons are likely to be dominant*.
- At liquid helium temperatures a contribution proportional to T^2 has been found in the resistivity of a number of metals.
- This is consistent with the form of the electron-electron scattering cross section (63).
- The mean free path of electrons in indium at 2 K is of the order of 30 cm, as expected from (63).
- *Thus the Pauli principle explains one of the central questions of the theory of metals:*
- *how do the electrons travel long distances without colliding with each other?*

Chapter 13: Plasmons, Polaritons, and Polarons

ELECTRON-PHONON INTERACTION: POLARONS

- The most common effect of the *electron-phonon* interaction is seen in the temperature dependence of the electrical resistivity, which for pure copper is 1.55 microhm-cm at 0°C and 2.28 microhm-cm at l00°C.
- The electrons are scattered by the phonons, and the higher the temperature, the more phonons there are and hence more scattering
- Above the Debye temperature the number of thermal phonons is roughly proportional to the absolute temperature, and we find that the resistivity increases approximately as the absolute temperature in any reasonably pure metal in this temperature region.
- *A more subtle effect of the electron-phonon interaction is the apparent increase in electron mass that occurs because the electron drags the heavy ion cores along with it*.
- In an insulator the combination of the electron and its strain field is known as a **polaron,** Fig. 19.
- The effect is large in ionic crystals because of the strong coulomb interaction between ions and electrons.
- In covalent crystals the effect is weak because neutral atoms have only a weak interaction with electrons.

Chapter 13: Plasmons, Polaritons, and Polarons

ELECTRON-PHONON INTERACTION: POLARONS

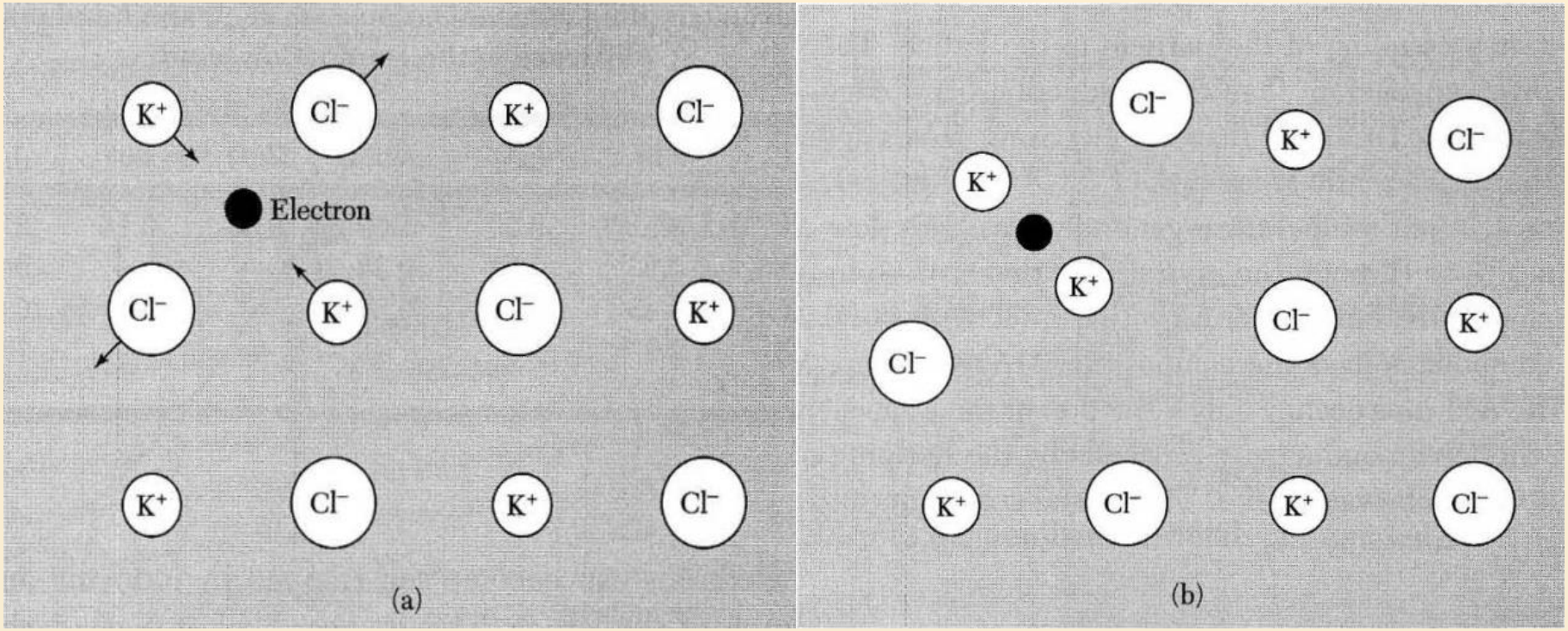


Figure 19 The formation of a polaron. (a) A conduction electron is shown in a rigid lattice of an ionic crystal, KCl. The forces on the ions adjacent to the electron are shown. (b) The electron is shown in an elastic or deformable lattice. The electron plus the associated strain field is called a polaron. The displacement of the ions increases the effective inertia and, hence, the effective mass of the electron; in KCl the mass is increased by a factor of 2.5 with respect to the band theory mass in a rigid lattice. In extreme situations, often with holes, the particle can become selftrapped (localized) in the lattice. In covalent crystals the forces on the atoms from the electron are weaker than in ionic crystals. so that polaron deformations are small in covalent crystals.

Polarons:

(1) electrons will scatter by phonons

(2) ⇒ e will interact with γ (phonon)

⇒ Increase of e mass due to electron drag of the heavy Ion core

(3) **e + strain field ≡ Polaron**

---

so the strength of e-γ interaction is measured by: $\frac{1}{2}\alpha = \frac{\text{deformation Energy}}{\hbar\omega_L}$

ω_L: phonon freq.

So what is the polaron:

1. Fermion
2. quasi-particle
3. ≡ e−γ Interaction
4. mostly exc. in Ionic crystals
5. Its not quantized

Chapter 13: Plasmons, Polaritons, and Polarons

ELECTRON-PHONON INTERACTION: POLARONS

- The strength of the elcctron-latticc interaction is measured by the dimensionless coupling constant *a* given by:

$$\frac{1}{2}\alpha = \frac{deformation\ energy}{\hbar\omega_L} \qquad (64)$$

- where ω_L is the longitudinal optical phonon frequency near zero wavevector.
- We view $\frac{1}{2}\alpha$ as "the number of phonons which surround a slow-moving electron in a crystal."
- It is common to speak of large and small polarons. The electron associated with a large polaron moves in a band, but the mass is slightly enhanced; these are the polarons we have discussed above. The electron associated with a small polaron spends most of its time trapped on a single ion. At high temperatures the electron moves from site to site by thermally activated hopping; at low temperatures the electron tunnels slowly through the crystal, as if in a band of large effective mass.

Thanks