

# Introduction to Solid State Physics Notes

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## Introduction:

Notes written while following the upper-level undergraduate course taught at the University of Pittsburgh in the Fall 2015 semester by Sergey Frolov. The course is based on Steven Simon's "Oxford Solid State Basics" textbook. If any errors are found in the notes, feel free to email me at [tobias.faehndrich@gmail.com](mailto:tobias.faehndrich@gmail.com). Overleaf formatting was copied from Rio W.

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## 2 Quantum Review

- Harmonic oscillator distance between energy levels is always the same.
- wavefunctions allows for tail going past classically allowed area.
  - exponential decay

- **Particle in a Box (PIB)**

$$E = \frac{n^2 \hbar^2}{8mL^2}, \quad n = 1, 2, 3...$$

$$\Delta E = (2n + 1) \frac{\hbar^2}{8mL^2}$$

- **Harmonic Oscillator (HO)**

$$E = \hbar\omega\left(\frac{1}{2} + n\right), \quad n = 0, 1, 2, 3...$$

$$\Delta E = \hbar\omega$$

- **Coulomb Potential (Hydrogen 1p+1e)**

$$U(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

–

$$\Psi(r)\Phi(\theta, \varphi)$$

- eigenvalues are possible energies
- radial quantum number  $n_r = 0, 1, 2...$
- principle quantum number  $n \equiv n_r + l + 1$
- S family orbitals ( $l=0$ )
- 2 types of particles that make large differences in behaviour @  $T = 0$  and low  $E$ .

1. **Bosons:**

- occupation number can take any value
- ex: photons, mesons, composite particle with integer spin (ex.  $\text{Li}^7$ )
- even total number of proton/electron/neutron

2. **Fermions:**

- occupation number can be zero or one (Pauli exclusion principle).
- ex. electrons, protons, neutrons, composite particles with half-integer spin
- odd number of proton/electron/neutron

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$$\beta = \frac{1}{kT}$$

$$\bar{n}_s = \frac{1}{\exp(\beta(\epsilon_s - \mu)) - 1}$$

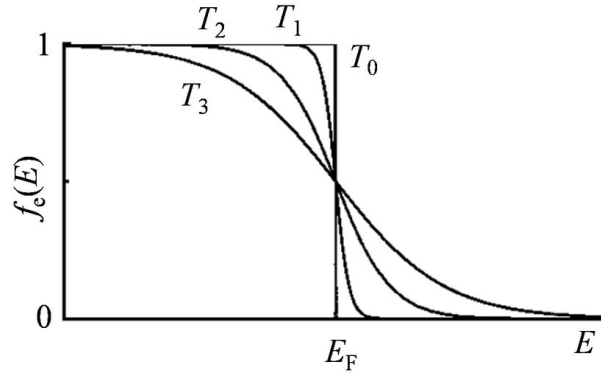


Figure 2.1: Temperature dependence of Fermi-Dirac distribution

### 3 Einstein & Debye Models of a solid

- Heat Capacities of Solids:

- rate of change of energy with temp (@const Volume)

$$C = \frac{dE}{dT}$$

- @  $T \gg 0$ ,  $C = 3Nk$
- Law of Dulong & Petit
- Classically: Law of equipartition
  - \*  $C = \frac{k}{2}$  for each DOF in material.
- $C_V \propto \alpha T^3 + \gamma T$ 
  - \* Insulators:  $\gamma = 0$
  - \* Conductors:  $\gamma \neq 0$

- Einstein model of Solid

- each atom in crystal vibrates independantly
- assumed these were Harmonic Oscillators  $E_n = \hbar\omega_E(n + \frac{1}{2})$
- partition function

$$Z = \frac{\exp(-\beta\hbar\omega_E/2)}{1 - \exp(-\beta\hbar\omega_E)}$$

$$Z = \sum_r \exp(-\beta E_r)$$

$$\bar{E} = -\frac{1}{Z} \frac{dZ}{d\beta}$$

$$C_V = \left( \frac{\partial \bar{E}}{\partial T} \right)_V$$

- Result

$$C_V = 3Nk(\beta\hbar\omega_E)^2 \frac{e^{\beta\hbar\omega_E}}{(e^{\beta\hbar\omega_E} - 1)^2}$$

- $T \rightarrow \infty, \quad C_V = 3Nk$
- $T \rightarrow 0, \quad C_V = 0$
- real solids go  $T^3$  instead of exponentially
- partially successful model  $\rightarrow$  shape behaviour @ low temp was incorrect.

- **Debye's Model**

- atoms coupled to each other in a solid
- atoms vibrations generate sound waves
- quantize! (can use planck's results for light quantization)
- "phonons" vs photons
  - \* described by wavevector  $k$
  - \* longitudinal and transverse modes possible for phonons
- Debye Temp  $\theta = \frac{\hbar\omega_D}{k}$

$$C_V = \frac{12\pi^4}{5} Nk \left( \frac{T}{\theta_D} \right)^3$$

$$E \propto T^4 \quad \therefore C_V \propto T^3$$

- still not fully complete

## 4 Drude & Sommerfeld Theories of electrons in solids

- **Drude (1900):** kinetic gas, classical ideas

- **Principles of Drude Theory:**

1. electrons have an average scattering time  $\tau$ .  $\rightarrow$  phenomenological parameter (based on observable facts)
2. after scattering event occurs, electron returns from some  $p$  to momentum  $p=0$ .
- 3.

$$F = -e(\vec{E} + \vec{v} \times \vec{B})$$

Between events, electron responds as a free particle to applied  $\vec{E}$  &  $\vec{B}$  fields.

- **Steady State:**  $\frac{dp}{dt} = 0$

- \* **conductivity:**

$$\sigma = \frac{ne^2\tau}{m}$$

from current density

$$\vec{j} = \sigma \vec{E}$$

- \* **resistivity:**

$$\rho = \frac{m}{ne^2\tau}$$

- **With Magnetic Field:** In semiconductor  $m \rightarrow m^*$  (mass is replaced by an effective mass).  
"non-local"

$$V_y = \rho_{xy} I_x$$

"local"

$$V_x = \rho_{xx} I_x$$

Hall coefficient

$$R_H = \frac{\rho_{xy}}{|B|} = -\frac{1}{ne}$$

- **Sommerfeld theory (1920):** assumed fermionic behaviour

## 5 1D models of vibrations

- monatomic chain (restricted to longitudinal motion for now.)
- $a$ : lattice constant and  $k$ : spring constant
- equilibrium position for the  $n$ th atom and displacement.

$$x_n^{eq} = na$$

$$\delta x_n = x_n - x_n^{eq}$$

- Hooke's Law:

$$F_n = k(\delta x_{n+1} - \delta x_n) - k(\delta x_n - \delta x_{n-1})$$

- Newton's Law  $\rightarrow$  equations of motion (EoM) make ansatz:

$$\delta x_n = A e^{-ikna + i\omega t}$$

- Plug ansatz into Newton:

$$\omega = 2\sqrt{\frac{k}{m} \left| \sin\left(\frac{ka}{2}\right) \right|}$$

- $A$ : amplitude and  $k$ : wave vector (related to momentum).
- Point with  $k=0$ ; Reciprocal Lattice points  $G_m$  and Positions of atoms of along the chain  $x_n$ .

$$G_n = \frac{2\pi n}{a}, \quad n = -2, -1, 0, 1, 2, \dots$$

- Reciprocal lattice  $\leftrightarrow$  Direct lattice

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$$e^{iG_m x_n} = 1$$

- 1st Brillouin Zone: unit cell centered around  $k=0$  with boundaries @  $k = \pm \frac{\pi}{a}$  in reciprocal lattice. All allowed cases contained in 1st. 2nd 3rd etc can be helpful but not needed.
- for finite length:

$$k = \frac{2\pi n}{L}$$

### Phonons

$$E_n = \left(\frac{1}{2} + n\right)h\omega$$

- each excitation of harmonic oscillators corresponding to vibrations in a material  $\rightarrow$  bosons (which phonons are).
- number of phonons is  $\therefore$  given by Bose distribution.

$$n_B(\beta\hbar\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}$$

- Diatomic chain + excitations with multiple branches  $\rightarrow$  leads to increase in possible modes of vibrations.

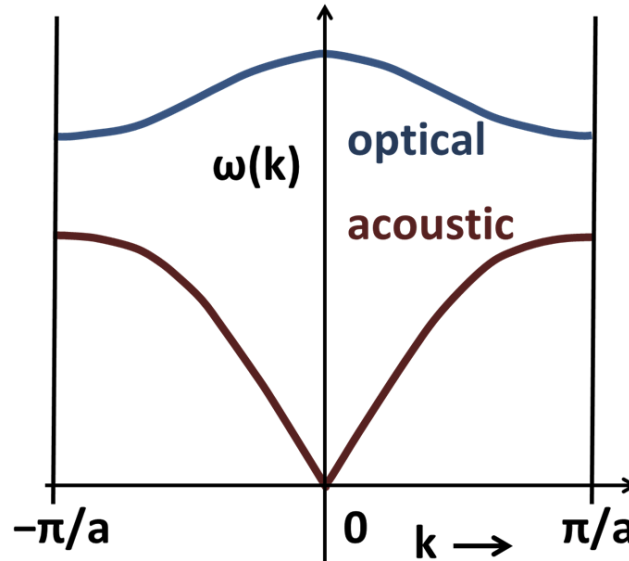


Figure 5.1: Caption

- Again assume coupled according to Hooke's Law (and easier if we let  $m_1=m_1$ )
- Sol. Newton:

$$\begin{cases} m \frac{d^2(\delta x_n)}{dt^2} = k_2(\delta y_n - \delta x_n) + k_1(\delta y_{n-1} - \delta x_n) \\ m \frac{d^2(\delta y_n)}{dt^2} = k_2(\delta x_n - \delta y_n) + k_1(\delta x_n - \delta y_n) \end{cases}$$

- Ansatz: Plug into the matrix form of EoM.

$$\begin{cases} \delta x_n = A_x e^{-ikna + i\omega t} \\ \delta y_n = A_y e^{-ikna + i\omega t} \end{cases}$$

- solve for  $\omega$ . plus or minus solutions or multiple solutions will give a E-k diagram and thus the Single Brillouin Zone. The top one in this case is Optical phonons and the bottom is Acoustic phonons (which are nuanced names. Photons can interact only with the "optical" phonons.

$$\omega = 2\sqrt{\frac{k}{m}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

- **Extended zone scheme**

- shifts the optical to the second brillouin zone and leaves the acoustic in the first.
- makes it easier to see the change from diatomic to monatomic.

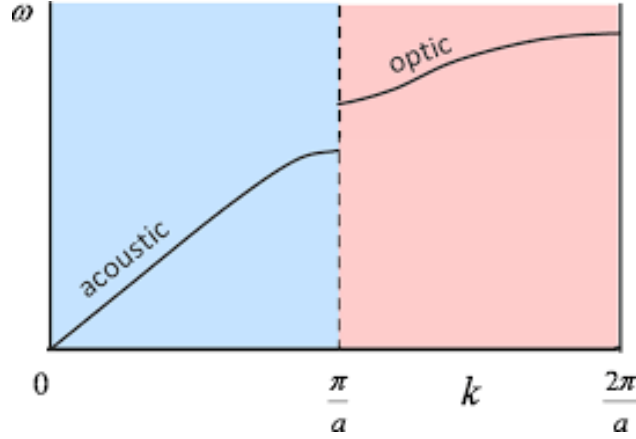


Figure 5.2: extended zone scheme

## 6 The 1D Tight Binding Model for Electrons

- "Hopping of an electron along a 1D lattice.
- each atom has 1 orbital denoted by  $n$ 
  - orthogonal to each other  $n|m = \delta_{n,m}$  although the true Kronecker-Delta function result is only really true if the atoms are far enough away from each other.
- Wave function of the electron in the basis of the orbitals is:

$$\Psi = \sum_n c_n n$$

- Model of linear combination of atomic orbitals (LCAO)
- Time Independent Schrodinger Equation (TISE):

$$H\Psi = E\Psi$$

- Hamiltonian only couples nearest neighbour sites so we say:

$$n|H|m = \begin{cases} \epsilon_0, & n = m \leftarrow \text{staying in atom} \\ -J, & n = m \pm 1 \leftarrow \text{hop by 1 site is way more probable} \\ 0, & \text{otherwise} \leftarrow \text{than hopping by several atoms.} \end{cases}$$

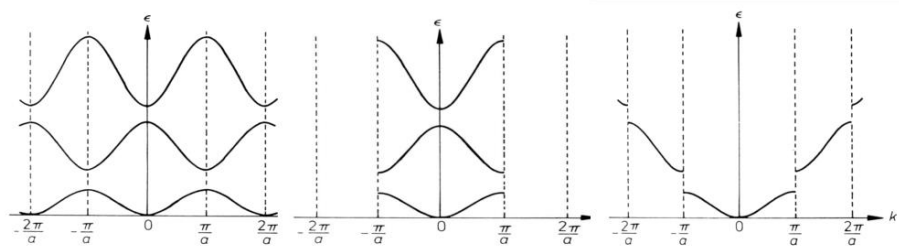
$$n|H|m = \begin{bmatrix} \epsilon & -J & & 0 \\ -J & \epsilon & -J & \\ & -J & \ddots & \ddots \\ 0 & & \ddots & \ddots \end{bmatrix}$$

$$n|\mathcal{H}|m = \epsilon_0 \delta_{n,m} - J(\delta_{n,m+1} + \delta_{n,m-1})$$

$$\sum_m H_{n,m} c_m = E c_n$$



## Extended, reduced and periodic Brillouin zone schemes



Periodic Zone

Reduced Zone

Extended Zone

All allowed states correspond to  $k$ -vectors in the first Brillouin Zone.

Can draw  $E(k)$  in 3 different ways

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Figure 6.1: Caption

TISE:

$$\epsilon_0 c_n - J(c_{n-1} + c_{n+1}) = E c_n$$

Plug-in Ansatz (without time dependency):

$$c_n = \frac{e^{-ikna}}{\sqrt{N}}$$

Relationship to phonons – obtain dispersion relation:

$$E = \epsilon_0 - 2J \cos(ka)$$

We get single band because we chose to have 1 orbital per site with our current model.

- **Phonons in monatomic chain** → **diatomic or more complex crystals** similar to
- **Band Diagram in 1 orbital per site** → **multiple orbitals per site**
- We can represent **band structure** (energy ranges and  $k$ -dependence of multiple bands.
- Reduced zone scheme vs Extended zone scheme
- Typically many bands in solids with 2 relevant bands
- no solutions for any energy in this gap which relates to insulators, conductors, semiconductors etc.
- energy gap = band gap, and occurs at edge of Brillouin zone for the extended zone scheme.
- **Bandwidth** effective mass and crystal momentum

- width of the band energy depends of nuclei spacing
- N lattice sites + one orbital  $\rightarrow$  N states for electron.
- $\frac{2\pi}{aN}$  spacing is so incredibly small for all particle solids so we therefore assume band structure is continuous.

- **Band Shape**

Approximate for  $k \ll 1$  we see parabolic near  $k=0$  for free particle  $E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$ .

$$E = \epsilon_0 - 2J \cos(ka)$$

$$E \approx \epsilon_0 - 2J \left(1 - \frac{(ka)^2}{2}\right)$$

$$E \approx \epsilon_0 - 2J + Ja^2 k^2$$

$$E = \frac{\hbar^2 k^2}{2m^*} + \text{Const.}$$

$$\frac{\hbar^2 k^2}{2m^*} = Ja^2 k^2$$

Effective Mass (determined by J: hopping parameter/ tunnelling amplitude):

$$m^* = \frac{\hbar^2}{2Ja^2}$$

### Filling Bands and the Fermi Surface

- atoms with one valence electron, expect donate to collection moving in band.
- electrons have 2 spin ( $\uparrow, \downarrow$ ) which gives room for 2N electrons in band.
- at low temp ( $T \ll T_f$ ), half filled band involves states being filled up to the Fermi Energy.
- system has fermi surfaces (here only 2 points) k points where the filled meets unfilled region.
- $c \propto T$ : heat capacity propto temp
- **Metal**: the fermi surface is in the middle of a band.
- applied external electrical field, electrons can accelerate to higher values of k  $\rightarrow$  current flows in material. (backward and forward moving).
- **Band Insulator**: if band is filled, fermi surface is at the edge of the Brillouin Zone, then there are no states available in band for electrons to move into by an electrical field. (almost never carries current)
- **Energy Gap**
  - $\rightarrow$  if it's large enough it's not possible for electron to be pushed to higher band.
  - $\rightarrow$  if  $BG \geq 4eV$  then material is an (band) insulator.
  - $\rightarrow$  if  $BG < 4eV$  then electrons can be transferred to higher bands either @ **finite temperatures** or with **applications of fields**  $\rightarrow$  material can then be a semiconductor.
- Many materials with **2 valence electrons** are insulators  $\rightarrow$  some can form metals if interatomic spacing is small enough (two bands merge). See E bands vs atomic spacing.
- **Opposite** many materials with 1 valence electron are metals  $\rightarrow$  some are special type of Insulator: "Mott Insulator"

- too much energy to have 2 electrons (ex. NiO & CoO) on one site.
- Simple band model also doesn't fully describe when system has magnetic properties (ferro, antiferro, & ferro) spin alignment.
- kwant simulation library in PYTHON is a cool resource.

## 7 Crystal Structure

- crystals: periodic arrangements of atoms in a lattice
- Penrose tiles are quasi crystal.
- **Lattice:** repeating structure defined as an infinite set of points, which can be constructed as sums of set of linearly independent **primitive lattice vectors**.

$$\vec{R} = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3, \quad n \in \{0, \pm 1, \pm 2, \dots\}$$

- Points in the form of:  $2\vec{a}_1 + \vec{a}_2$  notated as  $[2, 1]$
- Square Lattice:  $\varphi = 90$ ,  $|a_1| = |a_2|$
- Hexagonal Lattice (or Triangular):  $\varphi = 120$ ,  $|a_1| = |a_2|$
- choice of primitive lattice vectors for a lattice is not unique  $\rightarrow$  must be able to get to any spot/point on the lattice with a linear combination.
- **Unit cell:** a region of space chosen so that you could tile/ fill all of space.
- **Primitive Unit Cell:** Unit cell with exactly one lattice point inside (conventional/convenient unit cell is when it is not primitive). Can also add fractions of points to add up to 1 full point for PUC (i.e.  $4 * 1/4 = 1$ ).
- **Wigner-Seitz Unit Cell:** is a way to construct a primitive unit cell that is always possible.
  1. Draw lines to connect a given lattice point to all nearby lattice points
  2. At the midway points, normal to these lines, draw new-lines or planes.
    - (smallest volume enclosed in this way is the Wigner-Seitz primitive cell. All space may be filled by these cells.)
    - **notice:** not all lines from the method need to be used in the end.
- **Crystal with Multiple Atom Types:**
  - Unit cell can have more than one atom
  - periodic for each atom type or for some region in space repeated periodically.
  - Define a basis for example for the large atom and for the small atom.
- **Simple Cubic 3D:** very improbable in nature cause there is so much empty space where crystal could configure in a more efficient manner.
  - can be **unit cell (a)**, **tetragonal** ( $a = b \neq c$ ) or **orthorhombic** ( $a \neq b \neq c$ )
- Cesium Chloride (CsCl): is simple cubic with basis Cs  $[0,0,0]$  and Cl  $[1/2, 1/2, 1/2]$
- **Unit Cell of Body Centered Cubic Lattice (BCC):**
  - Much more probable
  - Simple cubic with basis also Body centered cubic (BCC):
- **Face Centered Cubic (FCC):**
  - nature likes even more (probable!), for ex: NaCl Salt or C Diamond.

- The full list of all possible 3D crystal types (**The 14 Bravais Lattice Types**)
  - **4 types of Unit Cells**
    - \* P = primitive
    - \* I = Body-centered
    - \* F = Face-centered
    - \* C = side-centered
  - **with 7 crystal classes**
    1. Cubic
    2. Tetragonal
    3. Orthorhombic
    4. Hexagonal
    5. Trigonal
    6. Monoclinic
    7. Triclinic
- GaAs is a zincblende FCC Basis atom1 (0,0,0) and atom2 (1/4, 1/4, 1/4).

## 8 Reciprocal Lattices

space in which waves live

not only electron or vibrational waves – also waves of light travelling through a crystal

X-rays are used very often to study crystals

**Recall Reciprocal Lattice in 1D**

$$\sigma x_n = A e^{i\omega t - i k n a}$$

where:

a = lattice const (direct, in real space)

any system that is periodic in space (a) is also periodic in k space (or reciprocal space) with period  $2\pi/a$

Points equivalent to k=0:

$$G_n = \frac{2\pi n}{a}$$

where n = ... -2, -1, 0, 1, 2, ...

Space	...	n=-2	n=-1	n=0	n=1	n=2	...
$x_n =$	...	-2a	-a	0	a	2a	...
$G_n =$	...	$-2(\frac{2\pi}{a})$	$-(\frac{2\pi}{a})$	0	$(\frac{2\pi}{a})$	$2(\frac{2\pi}{a})$	...

We find a relationship between the spaces:

### Reciprocal-Direct Lattice Relationship

$$e^{iG_n x_n} = 1 \quad (8.1)$$

### Reciprocal Lattice now in 3D

Real:

$$\mathbf{R} = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3, \quad n_i \in \{0, \pm 1, \pm 2, \pm 3, \dots\}$$

Reciprocal:

$$\mathbf{G} = m_1 \mathbf{b}_1 + m_2 \mathbf{b}_2 + m_3 \mathbf{b}_3, \quad m_i \in \{0, \pm 1, \pm 2, \pm 3, \dots\}$$

Conditions to find vectors of the reciprocal lattice:

$$e^{\mathbf{G} \cdot \mathbf{R}} = 1 \quad (8.2)$$

construct primitive lattice vectors for the reciprocal lattice  $\mathbf{b}_i$ , using the property that

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi \delta_{ij} \quad (8.3)$$

Ways to determine the reciprocal lattice vectors:

- Using a Fourier Transformation of the original lattice (not so intuitive):

$$\rho(x) = \sum_n \delta(x - na)$$

$$\mathcal{F}(\rho(x)) = \int dx e^{ikx} \rho(x)$$

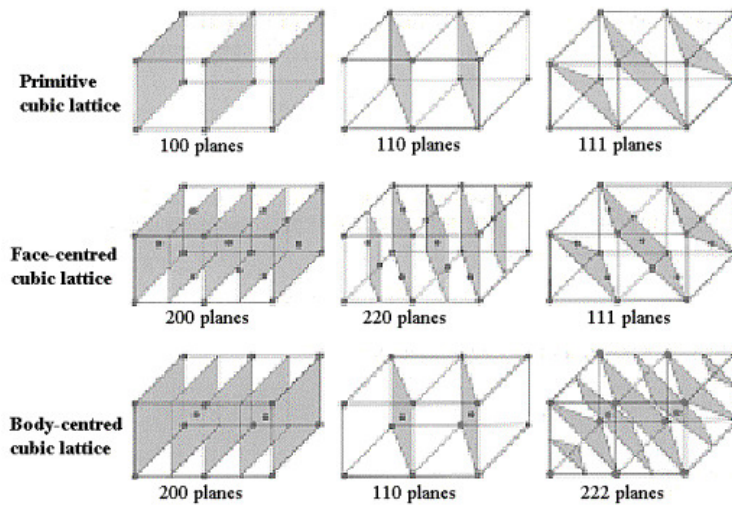
$$\begin{aligned}
 &= \sum_n e^{ikan} \\
 &= \frac{2\pi}{a} \sum_m \delta\left(k - \frac{2\pi}{a}m\right)
 \end{aligned}$$

- Geometric Interpretation: see it as the set of vectors that are normal to the families of lattice planes (infinite set of equidistant parallel lattice planes which as a family contain all of the points of the lattice).

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- Mathematical Way (minute 1:10 on L8 YT)

Must be equidistant planes and must include ALL points in a crystal.



Miller indices for three types of cubic lattices.

Figure 8.1: Lattice Planes

**Family of lattice planes:** an infinite set of equidistant parallel lattice planes, which as a family contain all of the points of the lattice.

No extra planes can occur.

**Index System for Crystal Planes – Miller Indices:**

1. Express the intercepts of the plane with the crystal axes in units of lattice constants  $a_1, a_2, a_3$ .
2. Take the reciprocal of these numbers.
3. Reduce them to integers of the same ratio:  $(h,k,l)$ .

- round brackets  $()$  - reciprocal space
- square brackets  $[]$  - real space
- plane parallel to an axis will result in a 0 in the Miller Indices

For some experiments it is important to know the distance between the lattice planes

General Distance formula:

$$d_{hkl} = \frac{n}{\sqrt{\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2}}} \quad (8.4)$$

Distance for cubic lattice (simpler):

$$d = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \quad (8.5)$$

- bar over top of miller indice indicates negative number; ex  $(11\bar{2})$



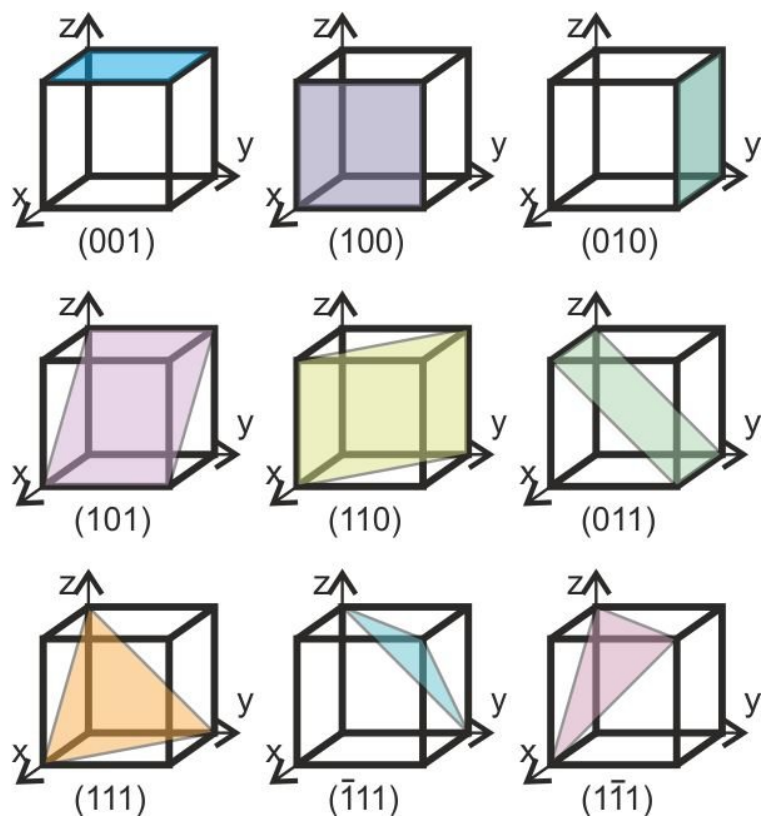


Figure 8.2: miller indices

## 9 Scattering Experiments (X-ray diffraction)

Shining of wave on a crystal and detecting the scattered particles/radiation

- x-rays, electrons and neutrons
- wavelength of radiation should be comparable to a typical inter atomic distance of a few Å.

$$E = h\nu = \frac{hc}{\lambda}$$

$$\lambda(\text{\AA}) = 12398/E(eV)$$

- a few keV is needed for a wavelength of around 1 angstrom.

### X-Ray

- $\lambda = 1\text{\AA}$
- $E = 10^4 eV$
- interact with electron
- penetrating

### Neutron

- $\lambda = 1\text{\AA}$
- $E = 0.08 eV$
- interact with nuclei
- Highly penetrating

### Electron

- $\lambda = 2\text{\AA}$
- $E = 150 eV$
- interact with electron
- Less penetrating

- X-ray is great for bulk investigation - Electron is great for surface investigation (checking surfaces with MBE)

### The Bragg Law

$$2d \cdot \sin(\theta) = m\lambda \quad (9.1)$$

- Ignores some things but gives a good rough estimate with a simple model
- Diffraction occurs for:

$$\vec{k} + \vec{G} = \vec{k}'$$

The larger the indices, the smaller the spacing between the planes.

- Single slit diffraction gives Fraunhofer Diffraction Pattern - This is a Fourier transform of the slit (or periodic crystal structure)

- Atomic Form Factor increases with atomic charge.
- Some planes are absent in X-ray diffraction and some show:

The missing orders follow rules depending on which type of lattice it is –

- **Simple Cubic (sc):** any (hkl)
- **Body-centred cubic (bcc):** h+k+l=even
- **Face-centred cubic (fcc):** h, k and l all odd or all even.

Lattice Type			
Miller Indices	sc (P)	bcc (I)	fcc (F)
100	Y	N	N
110	Y	Y	N
111	Y	N	Y
200	Y	Y	Y
210	Y	N	N
211	Y	Y	N
220	Y	Y	Y
310	Y	Y	N
311	Y	N	Y

N = will not give a diffraction pattern for these planes (due to interference). Y = will give ...

#### X-Ray Diffraction (XRD) Methods:

- Laue: not that good
- Rotating Crystal: meh
- Powder: to get lattice parameters, polycrystal (powdered), monochromatic beam, variable angle.
  - Debye-Scherrer cone
  - beam comes through holes

#### XRD Procedure

- Measure angle
- $d = \frac{\lambda}{2 \sin \theta}$
- bigger angle gives smaller d
- small d corresponds to higher miller indices
- scale d's by the first one (get d=1 for first)
- scale all d by an clever choice of integer N
- $N = h^2 + k^2 + l^2$
- hkl
- $a = d \sqrt{h^2 + k^2 + l^2}$  (hopefully getting the same a for all)

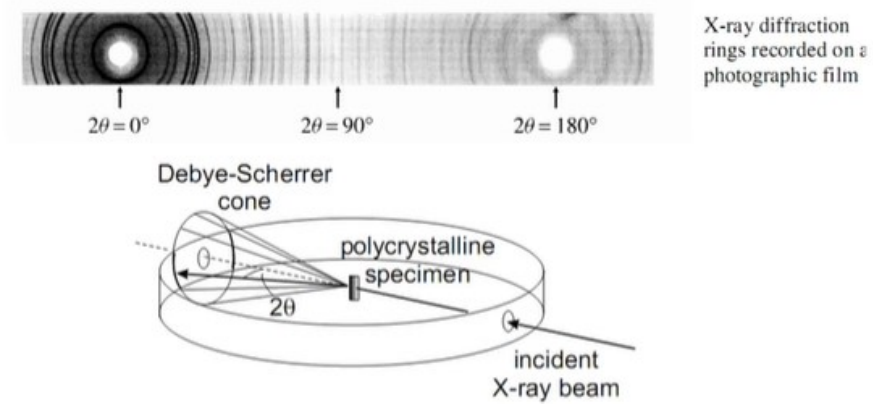


Figure 9.1: XRD

Scattering Selection Rules					
hkl	$N = h^2 + k^2 + l^2$	Multiplicity	sc (P)	bcc (I)	fcc (F)
100	1	6	*		
110	2	12	*	*	
111	3	8	*		*
200	4	6	*	*	*
210	5	24	*		
211	6	24	*	*	
—	7	—			
220	8	12	*	*	*
221,300	9	24+6	*		
310	10	24	*	*	
311	11	24	*		*
222	12	8	*	*	*
320	13	24	*		
321	14	48	*	*	
—	15	—			
400	16	6	*	*	*

**XRD Identification of SC,BCC, FCC:**

- P (SC):  $N = 1,2,3,4,5,6,8,9,\dots$  (=all integers excluding 7,15,23,...)
- I (BCC):  $N = 2,4,6,8,10,12,14,\dots$  (=even integers excluding 28, 60,...)
- F (FCC):  $N = 3,4,8,11,12,16,19,20,\dots$

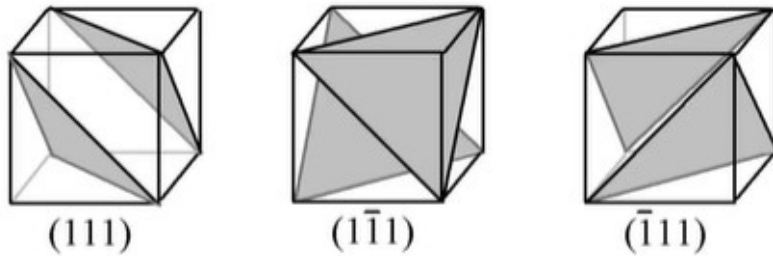


Figure 10.1: 111

## 10 Electron waves in crystals

Multiplicity: some families of lattice planes have the same spacing, and thus would be indistinguishable in an XRD experiment.

ex: 111 signifies all (111) ( $1\bar{1}1$ ) and ( $\bar{1}\bar{1}1$ ) in the so called '111' class. They all diffract with the same angle and thus the line will have a stronger intensity reading compared to other classes without the negative miller indices.

Most common basis structure is sodium chloride NaCl and zinc blende ZnS.

- you can use pattern in XRD or neutron scattering data (i.e. odd peaks ( $h+k+l=\text{odd}$ ) are big and even are small) can tell you which basis it is from.

### Refresher of Brillouin Zones

- You can perform Wigner-Seitz (closest lines drawn, then half way points draw perpendicular lines/planes) method to find 1st, 2nd, 3rd, etc Brillouin Zones on a lattice. - first is for the reciprocal lattice point  $G=0$ .

- each Brillouin zone has the same area

**Band Structure in 3D** - labelling convention to indicate points of symmetry in the Brillouin Zone. Allows us to show structure on a 2D graph.

- $\Gamma$  point is the where for  $k=0$
- X points at  $(0, 2\pi/a, 0)$
- L point
- $\Sigma$  point
- $\Delta$  point
- W point

**Correspondence** == $\hookrightarrow$  if we start with a FCC lattice in REAL space, then RECIPROCAL lattice will be the BCC lattice.

$\therefore$

1st Brillouin Zone of an FCC lattice = same shape as Wigner Seitz cell of a BCC lattice.

1st Brillouin Zone of a BCC lattice = same shape as Wigner Seitz cell of an FCC lattice.

- Electron and Phonon Structure can be related to the important points of the Brillouin Zone.

### Nearly-Free electron model

- Drude and Sommerfeld models assume free electrons. - Here we instead impose the crystal structure on a gas of free electrons (and get bands).

$$H_0 = \frac{p^2}{2m}$$

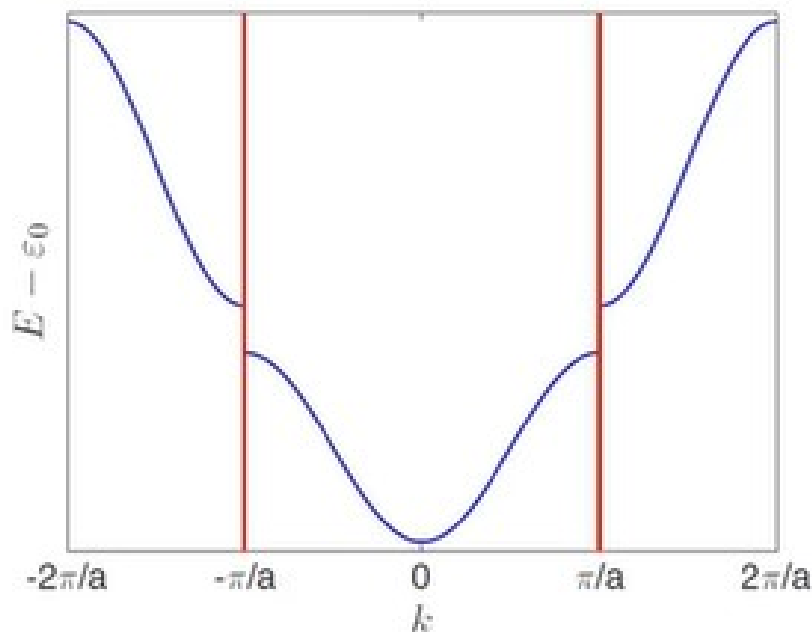


Figure 10.2: BZ

$$E_0(k) = \frac{\hbar^2 k^2}{2m}$$

- Perturbation Theory allows you to find complicated Hamiltonian solutions if we find a known similar system with solution and say there is an additional small perturbation.

**Bloch's Theorem** - perturbation theory only helps if period potential is weak. - Felix Bloch studied periodic potential Schrodinger equation solutions. - He showed in 1928 that particles in a periodic potential will behave just like free particles except that it is their crystal momentum that is conserved in collisions rather than regular linear momentum.

Bloch's Theorem is that a particle in a periodic potential has eigenstates of the form:

**Bloch's Theorem**

$$\psi_{\mathbf{k}}^{\alpha}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{\mathbf{k}}^{\alpha}(\mathbf{r}) \quad (10.1)$$

where  $\mathbf{k}$  can be chosen to be within the first Brillouin zone, and the function  $u_{\mathbf{k}}^{\alpha}(\mathbf{r})$  is a periodic function with period equal to the lattice spacing, which depends on a band index  $\alpha$  and on  $\mathbf{k}$ .

- **electron motion in crystals is similar to a plane waves! BLOCH WAVES! even if the electrons are strongly bound by the crystal.**

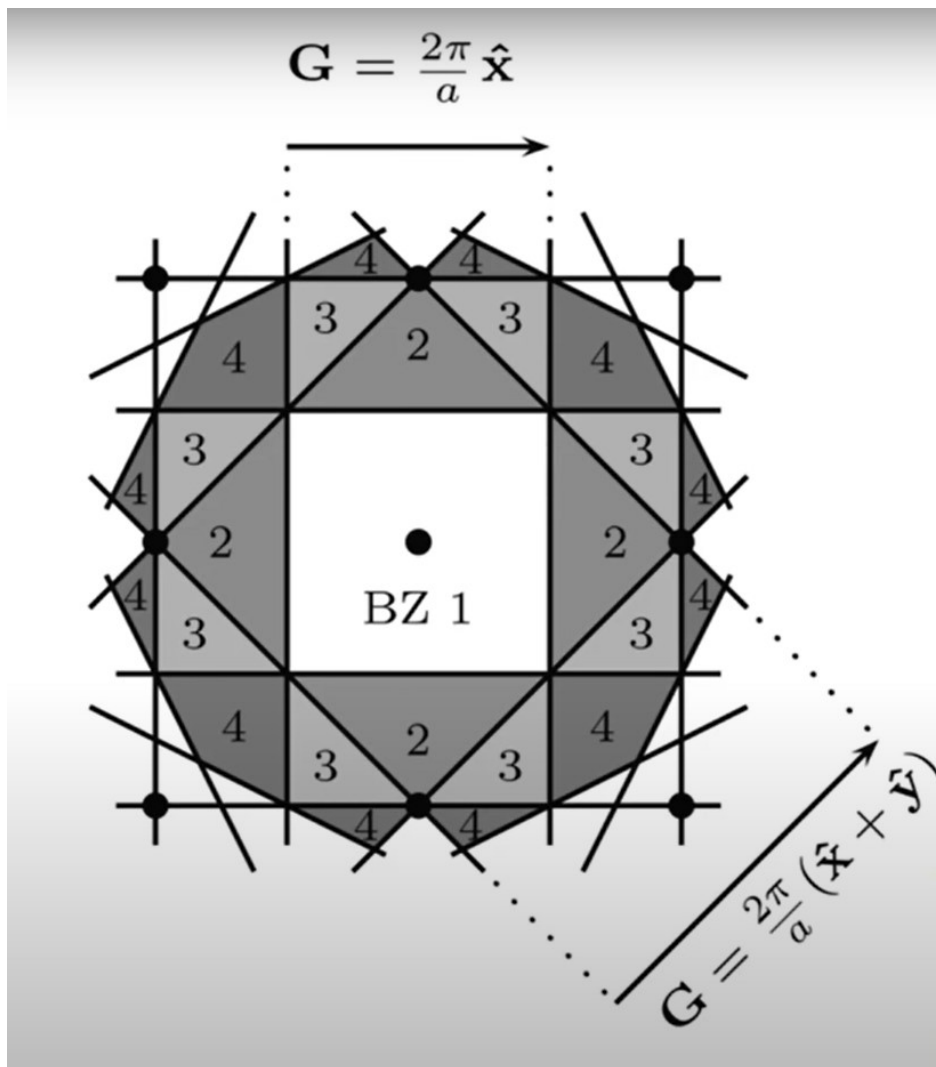


Figure 10.3: zones

### Nearly-free electron model results

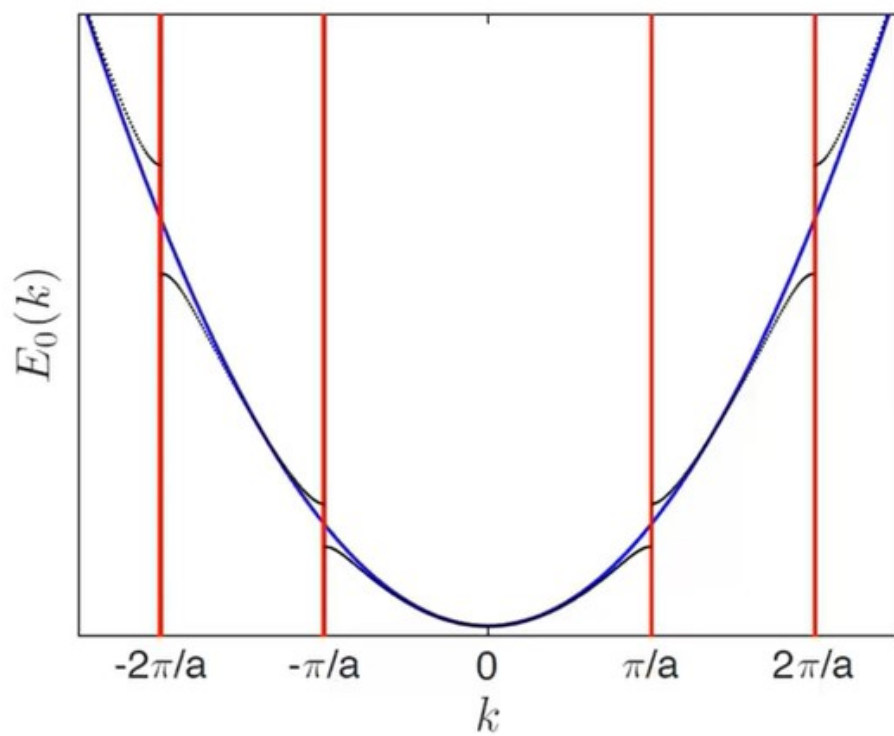


Figure 10.4: nearly



## 11 Band Structure of Electrons in Solids

### Band structure representation for 1D

- Reduced zone scheme
- Extended zone scheme

$$E = \epsilon_0 - 2J \cos(ka)$$

- for Both we see energy band gaps
  - At low temp a half filled band involves states being filled up to the Fermi Energy
  - **fermi surface** is the points or planes in k where the filled meets the unfilled region
  - **fermi energy** is the line in E where the filled meets the unfilled region
  - **Unfilled band** allows electric field to shift electrons in band ==> conducting
  - **Filled band** has no available states to move into and thus (almost) never carries a current.
  - **Band filling and Fermi surfaces in 2D**
  - fills up in same way → lowest energy first, each level with at most one electron in each spin state.
- 2D hopping/tight-binding model for cubic lattice, we get energy:

$$E = \epsilon_0 - 2J \cos(k_x a) - 2J \cos(k_y a) \quad (11.1)$$

- highest unfilled band is the conduction band
- valence band is the bands that are filled.

from  $\frac{p^2}{2m}$ :

**lighter effective mass** → sharper parabola in band

**heavier effective mass** → wider parabola in band

**Band theory does not consider interactions between electrons!** – cannot explain:

- Magnetism
- Mott insulators
- Superconductivity

- **Band insulators:** cannot absorb photons with smaller energy than the bandgap. Instead they pass through and it is transparent to them - if BG > 3.2eV, then they are transparent with visible light (ex: Quartz, diamond, sapphire (aluminium oxide)).

- **Semiconductors:** smaller bandgaps can absorb for ex. violet and blue light and transmit red and green (like CdS). - Other smaller (<1.7eV) BGs may transmit in the IR but appear black cause they absorb visible light (ex. Si, Ge, GaAs).

- **Direct band gap:** VB max and CB min are at the same k value.
- **Indirect band gap:** VB max and CB min are not at the same k value.

-indirect band gap makes it hard for material to absorb light because you need an increase in crystal momentum (which again is hard)! Not good for optical applications for lasers (but rather for electronics like silicon).

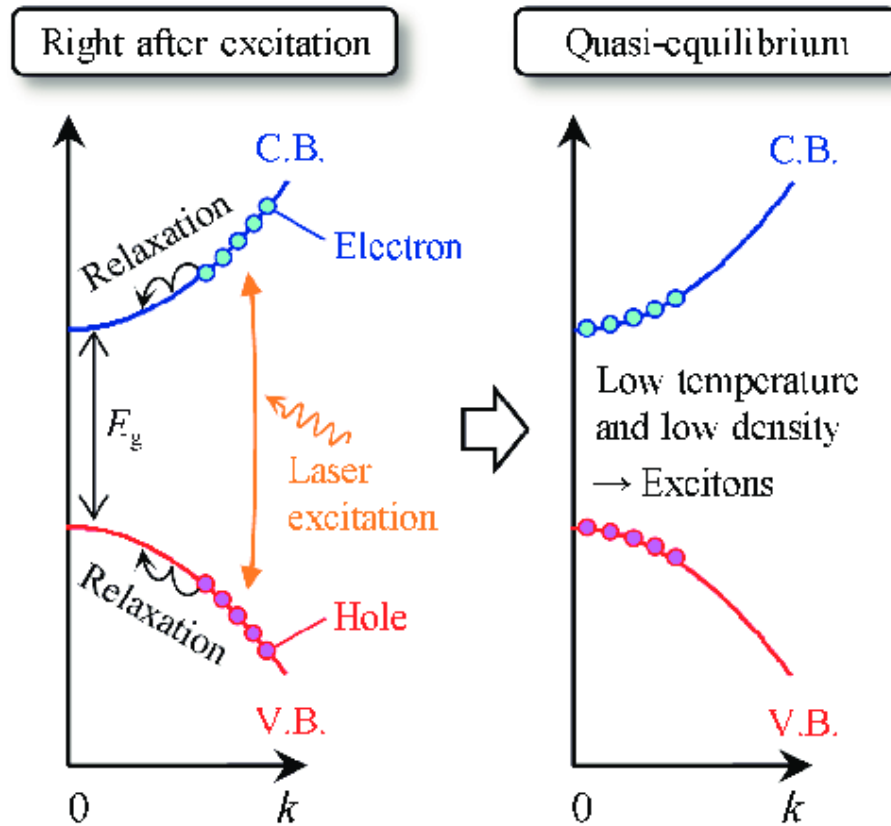


Figure 12.1: electronholes

## 12 Physics of Semiconductors (and metals and insulators)

- InSb is the smallest bandgap in the III-V semiconductor group

### Metals:

- Light will excite electrons, free to move and reemit light so they look shiny. - Conduction band width determines color, gold, copper color etc,

### Impurities:

- crystal color is effected by impurities such as Nitrogen in Diamond making it look yellow or Boron impurity making it look blue.

(area of research – **Nitrogen-Vacancy center in diamond**)

- or oxides (insulator) on shiny metal (conductor) can make it look matte.

### Basic Properties of Semiconductors

#### Electrons and Holes:

- semiconductor with filled VB and excite one electron to the conduction band (photon absorption or thermal excitation).
- **Hole** is then the absence of an electron in VB.

#### Holes

- convenient to keep track of the holes

- effectively act like a positive charge
- moves like a particle
- has charge and mass
- not a real particle → only a quasi-particle
- electrons here with effective mass are actually also quasi-particles
- electron and hole pair attract each other and form another quasi-particle called an exciton
- exciton is a Boson because it is composed of two Fermions (electron and holes). (bose-einstein condensate is a field of research that is not covered in the course).
- electron can fall back, "annihilating" the conduction electron and the hole in the valence band (analogous to electron-positron, particle-antiparticle pair).
- convention to make mass of hole positive, since it takes energy to accelerate the hole from zero vel to finite vel (like pushing a balloon underwater).

$$\frac{\hbar^2}{m_h^*} = -\frac{\partial^2 E}{\partial k^2} = 2\alpha \quad (12.1)$$

### How to Measure the Effective Mass

- Cyclotron Resonance Technique

$$F = \frac{mv^2}{r} = qvB$$

$$f = \frac{qB}{2\pi m}$$

- independent of v and r
- electrons strongly absorb microwaves of that frequency
- only need to measure freq to solve for effective mass.

Electron and hole effective masses					
	Si	Ge	GaAs	InAs	AlAs
$m_n/m_0$	0.26	0.12	0.068	0.023	2
$m_p/m_0$	0.39	0.3	0.5	0.3	0.3

### Doping Semiconductors

- pure ins. or semcond. excite electrons from VB to CB and the density of electrons in the conduction band (n for negative charges) is equal to the density of holes in the valence band (p for positive charges).
- **Intrinsic:** semiconductor without impurities
- **Extrinsic:** when impurities are placed in the SC

### Intrinsic Carrier Concentration:

- Density of States (DoS): how many eigenstates at each energy.

### Law of Mass Action

$$np = 4 \left( \frac{1}{2\pi\hbar^2\beta} \right)^3 (m_e m_h)^{3/2} e^{-\beta E_g} \quad (12.2)$$

intrinsic carrier concentration – Fermi level is inside the gap and the density of holes and electrons are equal then each density is the sqrt of the above expression on the right.

It is often useful to intentionally add impurities.

Consider:

- silicon a semiconductor with a bandgap of 1.1eV
- replace one atom with phosphorus (which has one extra proton and one extra electron)
- VB is filled and so electron must go into the conduction band
- known as donor, **electron donor**, or **n-dopant**, as n is the symbol from the density of electrons in the conduction band.

or instead:

- replace one atom with Aluminium
- provides one fewer electron than silicon
- missing electron from the VB, leaving a hole.
- known as **electron acceptor**, or a **p-dopant**

- semiconductor Fermi energy is in the middle of the band gap, and then dopants shift it up for n-dopant case and down for the p-dopant case.

## 13 Graphene and Carbon Nanotubes

- Carbon is versatile in bonding with other atoms
- Carbon is responsible for all organic chem
- Graphite (like in pencils) most closely related to Graphene
- 2 atom basis, FCC
- pencils (Graphite) are able to write because you can remove one layer (Graphene) at a time quite easily since each layer is bonded with van der Waals forces only.
- Graphene is single hexagonal lattice (not technically a lattice since you can't get to all points with primitive vectors) is exceptionally strong
- Konstantin Novoselov (Manchester) first to get graphene from scotch tape.
- colour change indicated that they had gotten to a monolayer
- solution to the graphene hamiltonian is found with tight binding mode, and by splitting the atoms up into 2 groups of triangular lattices.
- **K and K'** points: where the 2 bands meet each other and touch (no energy gap)
- two seas of electrons but they can't get to each other (K and K' points are separate and different).
- semiconductor has a small bandgap, but graphene has filled valence band and empty conduction band, but the two bands are touching and thus it is considered a metal.
- the dispersion relation where it touches is called a Dirac Cone (ex Graphene)
- area of research here is called "klein tunneling"
- Electrons have extremely fast fermi velocity  $v_F = 8E5m/s$ .

**Carbon Nanotubes!** - rolled up graphene

- Bonds on edge of graphene are happier if rolled around and connected to the other edge (forming a tube).
- can "roll" the graphene in different orientations
- for ex: armchair (up-flat-down), zig-zag (up-down), and chiral (various wrapping).
- Carbon Nanotubes (depending on the rolling vector) can "gap" Graphene (which is normally gap-less).
- Armchair (n,n):  $\theta = 30$  always Metal
- Zig Zag (n,0):  $\theta = 0$  then 2/3 are Metal and 1/3 are Semiconductor (for n multiples of 3)
- Chiral (n,m):  $0 < \theta < 30$ , 2/3 are metal, and 1/3 are semi-conducting, n-m multiple of 3.

It turns out that there is a formula which tells us if the carbon nanotube will be conducting or not (i.e. if it won't hit the K point)

$$2n_1 + n_2 = 3m \quad m \in \{1, 2, 3, \dots\} \quad (13.1)$$

## 14 Semiconductor Devices

**Heterostructures:** Layers of 2 or more different semiC - band strucutre design.

Lattice mismatch negligile – heterojunction = single crystal with different site occupancies across junction.

3 types of band edge offsets:

1. Normal
2. Staggered
3. Broken Gap

- To make a clean growth of heterostructures you want to match lattice constants (a) very closely
- if it is not matched you will get strain in your sample, and you will get defects in your grown sample.
- **Transmission Electron Microscope (TEM):** send electrons at very high energy all the way through the structure, and pixels represent atomic rows. tells you about the crystallinity of the structure under study.
- **Molecular Beam Epitaxy (MBE):** The structures are gorwn in MBE machines. It generates beams of molecules, and grow layer by layer (epitaxially).
- Stainless steal **ultra high vacuum chamber** so that beams of molecules can go in straight lines and not collide with anything (massive mean free path).
- **Diffusion cells** (molecular guns): buckets containing different materials, heated to a certain temperature where material begins to sublime.
- **Substrate** is the base on which you grown an epitaxial thin film.
- Overlap of for ex. Ga and As shooting at the same time onto the substrate allows for growth of GaAs.
- **Reflection High Energy Electron Diffraction (RHEED):** Shoots electrons at sample which reflect and hit screen while the sample is being grown. Intensity of diffraction pattern oscillates as you're growing. Used to count the layers grown so far.
- RHEED: max diffraction pattern intensity at new layer, min at half layer, max at completion of a layer. layer by layer we can see and count the layers that have been grown so far.
- **Quantum Wells:**

$$E = n^2 \frac{\hbar^2 \pi^2}{2m_e L_z^2} \quad \in n = 1, 2, 3. \quad (14.1)$$

- **Gas LASER:** for ex HeNe works on the atomic transitions within the gas, and uses some kind of pump to bring all the atoms into the excited state and they relax and emit photons all with the same energy. use mirror structure to boost this process.
- **Quantum Well Laser (27:00):** pumping by sending electrical current through.
- **Quantum Cascade Laser:** electrons falls from one QW to the next each time emitting a photon of a specific energy.
- **Field Effect Transistor (HEMT- High electron mobility transistor):** 3 components - source, gate and drain

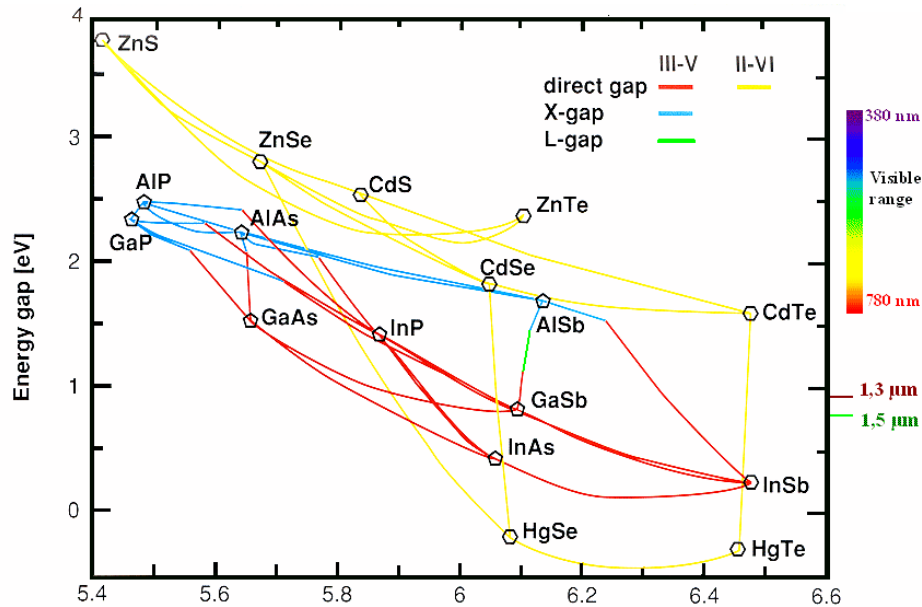


Figure 14.1: bandgap

- **2DEG: Two Dimensional Electron Gas**
- **PN Junction (Diode):** When N-type and P-type dopants are introduced side-by-side in a semiconductor, a PN junction or diode is formed.
- **Rectifier Circuits:** converts an AC voltage into a DC voltage. Sin wave negative values are cut off by diodes unidirectional feature.
- **Light Emitting Diodes (LED):** Recombination in the middle of the PN junction diode of the electron and hole emits a photon. Band gap of the junction determines the colour of the photon.
- Blue LEDs won a nobel prize recently with nitride based diodes.
- **Bandgap Engineering:** Tweaking structures to tune the wavelength and the properties.
- **Solar Cells:** Photon comes in and excites an electron-hole pair in a PN junction. The charges separate and this produces a current.
- **Schottky Barrier:** Metal-SemiC Junction.
- **Metal-Oxide-Semiconductor Transistors:** Most modern digital devices use MOS transistors. Greater density and simpler geometry (easier to make). Switch on and off more slowly.
- Consists of source, drain diffusions, with a gate that controls whether the transistor.
- **MOSFET:** Metal-Oxide Semiconductor Field Effect Transistor.
- Applying positive gate voltage (attracts electrons to gate area, i.e. a conductive path), causes current to flow from source to drain. The more voltage, the more current.
- negative current in MOSFET is like two diodes facing each other (both directions blocked).
- **Complementary MOS Transistors:** Use transistors for logic circuits.

- **Integrated Circuit (IC) chips:** 12 inch semiC wafer printed at INTEL with nanofabrication. out of silicon with n and p doped regions and metal contacts. chopped up into chips to be put into our laptops. They are filled with hundreds of millions of MOSFETS.
- **Electric Field in a CCD:** Charge coupled device. Pixel in our digital camera. Also functions with a P-N junction.



## 15 Paramagnetism and Diamagnetism

### General

- original data storage devices
- only started to understand micro level after advent of QM
- goes past band structure
- treat interactions between particles
- interactions between spins are fundamental to current research: spintronics + quantum technologies using spins.
- phase transitions

### Spinors

$$\alpha\uparrow + \beta\downarrow = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, \quad |\alpha|^2 + |\beta|^2 = 1 \quad (15.1)$$

$$S_z = \frac{1}{2}\hbar\sigma_z, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (15.2)$$

### Bloch sphere representation

$$\Psi = \cos\frac{\theta}{2}\uparrow + \sin\frac{\theta}{2}e^{i\varphi}\downarrow \quad (15.3)$$

### Magnetic Susceptibility

$$M = \chi \frac{\mathbf{B}}{\mu_0} \quad (15.4)$$

### Bohr-van Leeuwen Theorem

$$\mathbf{M} = \lambda \mathbf{L} = 0, \quad \text{according to classical statistics} \rightarrow \text{magnetism obeys quantum statistics} \quad (15.5)$$

### Properties of Magnetism can have three origins,

- Intrinsic angular momentum (Spin).
- Orbital angular momentum about the nucleus
- Change in the dipole moment due to an applied magnetic.
- When electrons are **paired together** their opposite spins cause their magnetic fields to cancel each other. Therefore, **no net magnetic field exists**. Alternatively, materials with some **unpaired electrons** will have a **net magnetic field** and will **react** more to an **external field**.

### Hund's Rules (L-S coupling scheme – how to fill up orbitals in atoms):

- Outer shell electrons of an atom in its ground state should assume:
  1. Max Value of S (spin momentum) allowed by exclusion principle.
  2. Maximum value of L (orbital momentum) compatible with (1).

3.  $J = |L - S|$  for less than half-filled shells.  
 $J = L + S$  for more than half-filled shells.

Causes:  $\begin{cases} \text{parallel spins have lower Coulomb energy.} \\ \text{e's meet less frequently if orbiting in same direction (parallel Ls).} \\ \text{Spin orbit coupling lowers energy for } +L * S < 0 \end{cases}$

- examples:

$$\begin{cases} \text{Mn}^{2+} : & 3d^5 & (1) \rightarrow S = 5/2 & \text{excl. princ.} \rightarrow L = 2 + 1 + 0 - 1 - 2 = 0 \\ \text{Ce}^{3+} : & 4f^1 & L = 3, S = \frac{1}{2} & (3) \rightarrow J = |3 - \frac{1}{2}| = 5/2 \\ \text{Pr}^{3+} : & 4f^2 & (1) \rightarrow S = 1 & (2) \rightarrow L = 3 + 2 = 5 \quad (3) \rightarrow J = |5 - 1| = 4 \end{cases}$$

- shell filling structure is important

### Paramagnetism (positive susceptibility):

- a paramagnet has a response that tends to enhance the applied field, i.e.,  $\chi > 0$ .
- This is usually due to the spin of the **unpaired electrons** fixed within the crystal.
- the simplest model for p.m. (known as **Currie Paramagnetism** after Pierre Curie, or Langevin Paramagnetism) is the result of considering a collection of non-interacting spin-1/2 particles.
- Occurrence of electronic paramagnetism:
  - Atoms, molecules, and lattice defects with **odd numbers of electrons** ( $S \neq 0$ ). E.g., Free sodium atoms, gaseous NO, F centers in alkali halides, organic free radicals such as  $C(C_6H_5)_3$
  - Free atoms and ions with **partly filled inner shell** (free or in solid), E.g., Transition elements, ions isoelectronic with transition elements, rare earth and actinide elements such as  $Mn^{2+}$ ,  $Gd^{3+}$ ,  $U^{4+}$ .
  - Only a few compounds with even number of electrons, E.g.  $O_2$ , organic biradicals.
  - metals**
- For a free spin-1/2 particle, the Hamiltonian is given by the so called the Zeeman Term:

$$H = g\mu_B \mathbf{B} \cdot \vec{\sigma}$$

where  $g = 2$  is the g-factor for the electron,  $\vec{\sigma}$  is an operator for the spin and  $\mu_B = e\hbar/(2m) \approx 0.67k_B$  Kelvin/Tesla is the Bohr Magneton.

- The single spin can be oriented either parallel or antiparallel to the field, so the energies for the two states of a single spin can be:

$$E = \pm\mu_B B$$

- Then we know that the probabilities of the two states are given by:

$$p_{\uparrow} = \frac{e^{-\beta\mu_B B}}{Z}, \quad p_{\downarrow} = \frac{e^{+\beta\mu_B B}}{Z}, \quad Z = e^{-\beta\mu_B B} + e^{+\beta\mu_B B}$$

where  $\beta = 1/(k_B T)$

- Zeeman Splitting

- 36:00min derivation to get susceptibility:

$$\chi = \frac{\mu_0 \mu_B^2}{k_B T}$$

and for a collection of spins with density  $n$  we then have

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

- Result: **Magnetization increases as you lower the temperature: Curie Law susceptibility is dependence on  $1/T$**

#### Paramagnetic Susceptibility of Conduction Electrons:

- Classical free electrons:  $M \approx \frac{N \mu^2 B}{k_B T} \sim$  Curie paramagnetism
- Experiments on normal non-ferromagnetic metals:  $M$  independent of  $T$
- Pauli's resolution: Electrons in Fermi sea cannot flip over due to exclusion principle. Only fraction  $T/T_f$  near Fermi level can flip.

#### Pauli Paramagnetism

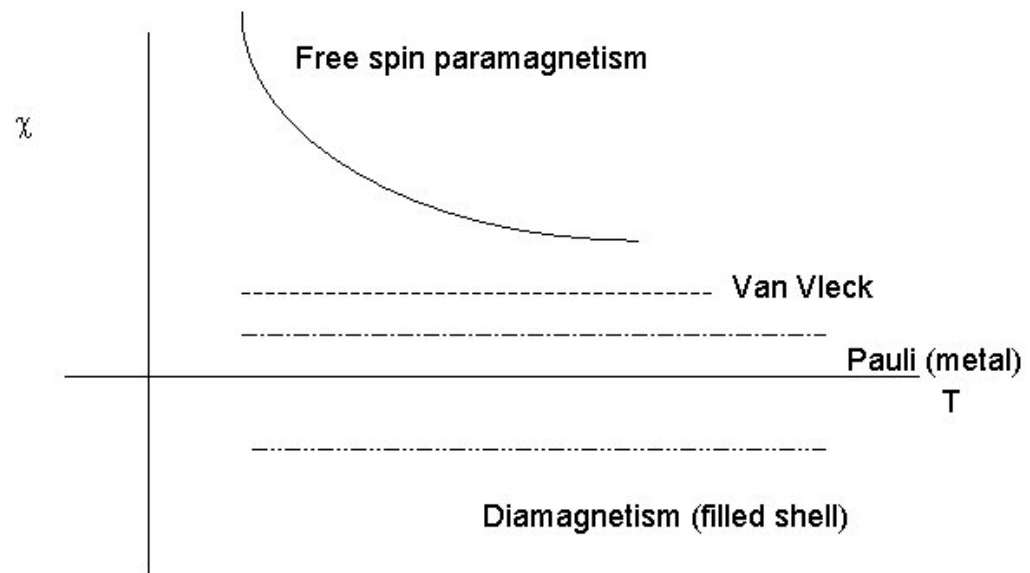
- For some alkali metals and noble metals, conduction electrons are weakly interacting and delocalized in space forming a Fermi gas. For these materials one contribution to the magnetic response comes from the interaction between the electron spins and the magnetic field known as Pauli paramagnetism.
- The Pauli paramagnetic susceptibility is a macroscopic effect and has to be contrasted with Landau diamagnetic susceptibility which is equal to minus one third of Pauli's and also comes from delocalized electrons. The Pauli susceptibility comes from the spin interaction with the magnetic field while the Landau susceptibility comes from the spatial motion of the electrons and it is independent of the spin. In doped semiconductors the ratio between Landau's and Pauli's susceptibilities changes as the effective mass of the charge carriers  $m^*$  can differ from the electron mass  $m_e$ .
- Before Pauli's theory, the lack of a strong Curie paramagnetism in metals was an open problem as the leading Drude model could not account for this contribution without the use of quantum statistics. Pauli paramagnetism and Landau diamagnetism are essentially applications of the spin and the free electron model, the first is due to intrinsic spin of electrons the second is due to their orbital motion.

#### Diamagnetism

- can come from orbital mechanism in a Free Electron Gas (not going to talk much about it)
- or from a fully filled shell
- famous example is frog floating in a magnetic field (diamagnetism)
- phenom characterized by negative susceptibility ( $\chi < 0$ ).
- appears in most materials but is often dominated by other effects
- superconductors tend to be good diamagnets
- main type is called Larmor diamagnetism (comes from Larmor Precession) when other magnetic effects are not present.

- Need  $J=0$  otherwise Curie Paramagnetism dominates
- relates in Lenz's Law
- you can also use paramagnets to make an adiabatic demagnetization refrigerators

## Magnetic susceptibility of different non ferromagnets



## 16 Magnetic Order

- spontaneous or under the infl of some **interactions**: all the spins line up in the same direction even without an external magnetic field
- ex. ferromagnet, antiferromagnet, and ferrimagnet.
- best ex of ferromagnet is Iron
- above a particular temp, spins tend to align randomly and there is a transition at the so called Curie Temperature to a paramagnetic behaviour.
- spin in the same direction reduces the energy and so is favourable for the system
- Spin-Spin interactions of localised spins we have the **Heisenberg Hamiltonian**

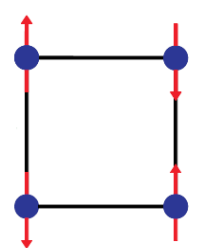
$$-J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J > 0$$

and  $\mathbf{S}_i$  is the spin operator for the  $i$ th spin and  $i, j$  denotes the sum over all neighbouring spins.

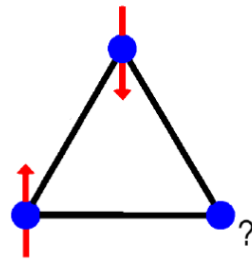
- Also **Antiferromagnet** ordered at low Temp, but with zero magnetisation.
- discovered by Louis Neel in the 1930s (thus we get Neel Order).
- **Heisenberg Hamiltonian** is very similar but without the negative sign:

$$J \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j, \quad J > 0$$

- i.e. alternating spins (up-down-up-down-...) results in minimizing the energy.
- if the lattice is triangular you get a **frustrated magnet** because there are lattice sites that you cannot







Square Lattice  
Unfrustrated



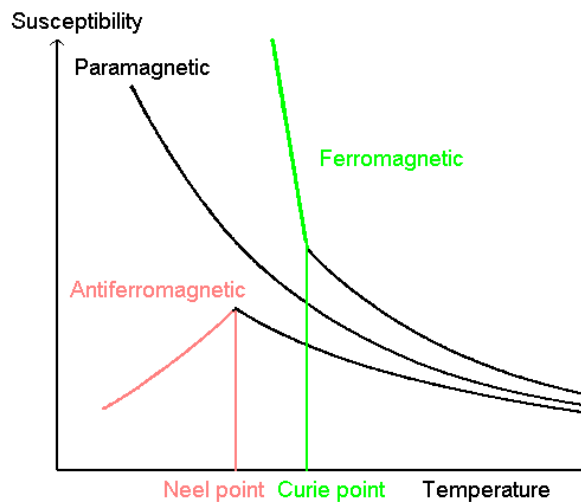
Triangular Lattice  
Frustrated

optimize the lowest energy very well. i.e. think of triangular lattice.

- **Ferrimagnetism**: 'weak form of ferromagnetism', spins allign within one sublattice but oppose each other on other sublattices. Normally a net magnetic field but typically weaker.

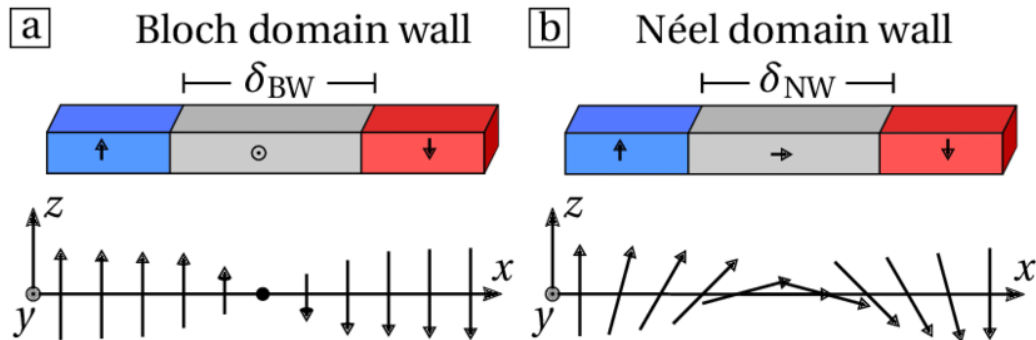
<b>Ferromagnetic</b> 	Below $T_C$ , spins are aligned parallel in magnetic domains
<b>Antiferromagnetic</b> 	Below $T_N$ , spins are aligned antiparallel in magnetic domains
<b>Ferrimagnetic</b> 	Below $T_C$ , spins are aligned antiparallel but do not cancel
<b>Paramagnetic</b> 	Spins are randomly oriented (any of the others above $T_C$ or $T_N$ )

- Also possible order called canted antiferromagnet and helical spin array.



- How to detect magnetic order?
- Measure how magnetic susceptibility changes as you decrease the temperature. Find possible critical temperatures to see deviant behaviour. At high temps they all behave like a paramagnet.
- Neutron Scattering Experiment (neutrons have spin): the moments of the neutrons will overlap with the atoms. Interactions with the spin up atoms will be different than the spin down atoms. So you can measure the lattice spacing between spin up or down atoms and see how it increases or decreases with decreasing temperatures. This can show you if it became antiferromagnetic (bigger lattice constant, that is between the atoms of the same spin) or ferromagnetic (smaller lattice constant).
- **Domains and Hysteresis:**
- **Annealing:** to make a ferromagnet, hold it at a high temperature and slowly lower the temperature while applying a strong magnetic field in one direction.
- **Magnetic domains** separated by **domain walls:** If it is cooled down too quickly or the field is too weak, then symmetry can be broken differently in different regions.

- **Quench:** Changing a parameter such as temperature quickly across a transition.
- Domain walls normally occur over a small region and involve the spin gradually rotating from the value of one domain to that of another (energy is minimized). We then have the bloch (rotation through the plane) and neel (rotation in the plane) walls:

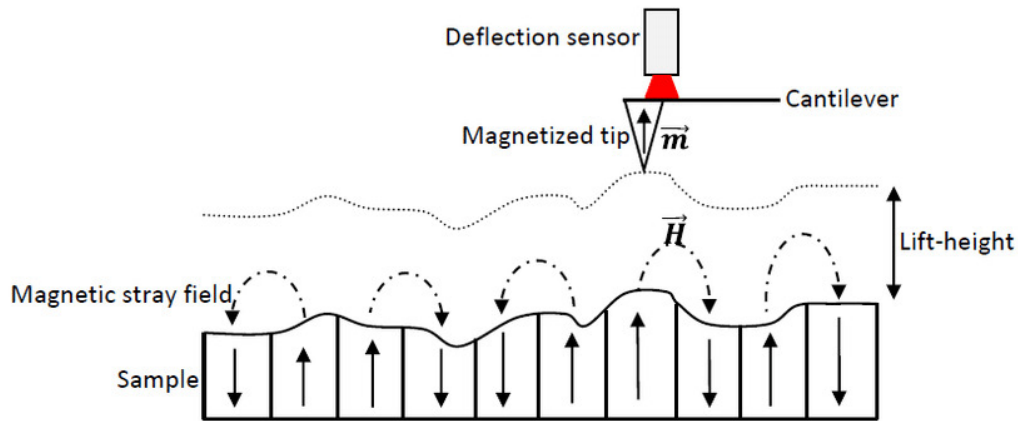


- For instant change we get an energy cost of:  $\Delta U = JS^2$
- For a domain wall of finite width we get:  $\Delta U = JS^2(1 - \cos \theta)$ ,  $\theta = \frac{\pi}{N}$  since the spins change by 180 degrees in N spin steps. If we only consider this it would seem the wall would extend to infinite. Therefore we find an extra anisotropy term:

$$\Delta U = +JS^2 \frac{N}{2} \left( \frac{\pi}{N} \right)^2 + KN$$

Where K = anisotropy term

- Average width of the wall is around 150 lattice constants for iron and other ferromagnets.
- Size of domains walls can be seen as a trade off between energy cost of spins not being aligned (worse if the interactions are stronger), and the preference of the crystal to have particular spin directions (not diagonal: the anisotropy energy).
- **Domain wall pinning:** tendency of domain walls to intersect where the defects are in the crystal to minimize the overall energy.
- **"Hard Ferromagnet" = Nonzero Hysteresis Loop.**  
We observe hysteresis in magnetic susceptibility – there is typically residual magnetisation when the field is changed.
- **Magnetic Force Microscopy (MFM):** Resolution 10-100 nm



- Also Atomic Force Microscope (AFM) used for non magnetic samples. Can identify individual atom lattice sites if tuned well. External vibration frequency from the cantilever removes noise (mechanical lock-in technique).
- Many Types of Resonance Phenomena/ Instruments
- **Information Gained:**
  - Fine structure of absorption: Electronic structure of individual defects.
  - Change in line width: Motion of the spin or its surroundings
  - Chemical or Knight shift: Internal Magnetic field felt by the spin.
  - Collective spin excitations.

#### Main Applications with Nuclear Magnetic Resonance:

- Identification and structure determination for organic / biochemical compounds
- Medical (MRI)
- **NMR:**  
Nucleus with a magnetic moment  $\mu$  and angular momentum  $I$ .

$$\mu = \gamma \hbar I, \quad \gamma = \text{gyromagnetic ratio}$$

Resonance at:

$$\omega_0 = \gamma B_0$$

- Signal Detection (via RF coil)



## 17 Mean Field Theories of Magnetism

The Ising Model Goal: Get Magnetization as a function of Temperature and Magnetic Field;  $M(T, B)$

- If we forget about spin interactions, Spins within a lattice will act as a paramagnet and try to align with an external field.

$$H_p = \sum_l g\mu_B \vec{B} \cdot \vec{\sigma}_l$$

And can be simplified if we consider a given field direction.

- We also can take into account the interactions between nearest neighbouring spins within a 2D lattice (summation will double counting, so divide by 2 on the outside):

$$H_{int} = -\frac{J}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

- if  $J > 0$  this is a ferromagnet and for  $J < 0$  this would be an antiferromagnet.
- Ising grad student solved it in 1D (1925). And in 2D by Onsager (1945). Only solvable in 3D with more approximations (mean field theory approach). The combination of the two interactions that the Ising Model considered is:

$$H_{Ising} = g\mu_B B \sum_l \sigma_l - \frac{J}{2} \sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

### Mean-field theory for the Ising Model:

- Single out a subset of the system and then treat interactions with all other parts of the system as some sort of potential. In a sense averaging out all the interactions will give you the mean field.
- Self-consistent result that is useful for a large number of particle systems.
- Focussing on one spin at site  $i$ , the Hamiltonian is:

$$H_i = g\mu_B B \sigma_i - J \sigma_i \sum_{j \in N_i} \sigma_j$$

summing over all  $j$  that are nearest neighbours of  $i$ .

- Next, we instead use the average over all the neighbours of  $i$ :

$$H_i \approx g\mu_B B \sigma_i - J \sigma_i \sum_{j \in N_i} \langle \sigma_j \rangle$$

- Solution gives us the transcendental equation which we can solve numerically or graphically:

$$\langle \sigma_i \rangle = \frac{1}{2} \tanh \left( \frac{\beta J z \langle \sigma_i \rangle}{2} \right)$$

- Solution shows that when  $T$  is large (small  $\beta$ ) the curves only intersect at  $\langle \sigma_i \rangle = 0$  so that there is no average magnetization.
- When  $T$  is small, we enter a regime where curves intersect at three points. This shows spontaneous magnetization.

- transition point between two behaviours happens when slopes are the same at small  $\langle \sigma_i \rangle$
- Make some simplifications and get a critical temperature:

$$T_c = \frac{J_z}{4k_B}$$

### (Spontaneous) Symmetry Breaking

- Free energy of the system as we pass through the  $T_c$ . Using  $F = -k_B T \log Z$ , we can compute this function as a function of  $\langle \sigma_i \rangle$  from the partition function.
- parabola (with min at 0) changes to camelback (with 2 mins on either side of 0, and a hump at 0) after going past  $T_c$ , the middle hump is an unstable point and system will lower energy by breaking symmetry and going to a non-zero magnetization – i.e. spontaneously polarize.
- Applying an external field explicitly breaks the symmetry and we can determine the directions in which the spins align.
- to Make Permanent Magnet from Iron: Heat above  $T_c$ , align with a strong field, then cool to a temperature below  $T_c$ .

### Itinerant Ferromagnetism

- Ising model said spins are fixed and can only interact; now this model spins can also hop (and still interact with each other).
- electrons tend to exhibit this behaviour
- The **Hubbard Model** describes electrons that hop through a tight-binding lattice, combined with interactions that occur if two electrons are on the same site of the lattice.
- Tunnelling amplitude  $J$  (not same as Ising), and interaction energy if 2 electrons are on the same lattice site,  $U$ .

$$H_{interaction} = \sum_i U n_{i\uparrow} n_{i\downarrow}$$

## 18 Superconductivity Experiments

- Interesting topic because we get neat phenomena like  $R=0$ , and also quantum mech application.
- Lecture is survey on superconductivity and why it is different
- Not just band theory (fails here), need to account for interactions between electrons.

### Heat capacity of Solids

- Heat capacities at constant volume are defined as the rate of change of energy with temperature.

$$C = \frac{dE}{dT}$$

- at high temperature,  $C = 3Nk$ , where  $N$  is the number of atoms in the solid and  $k$  is Boltzmann's constant (law of Dulong and Petit).
- Understood classically from the law of equipartition, which assigns a heat capacity of  $k/2$  to each degree of freedom in the material.

### Temperature dependence of Resistivity

- Metal: for a sufficiently narrow range of temperature, make a linear approximation:

$$\rho(T) = \rho_0[1 + \alpha(T - T_0)]$$

where  $\alpha$  is the temp coefficient of resistivity,  $T_0$  is a reference coefficient of resistivity, and  $\rho_0$  is the resistivity at temperature  $T_0$ .

- Standard resistivity of metal changes with temp.
- Electrons in fermi gas occupy metal.
-

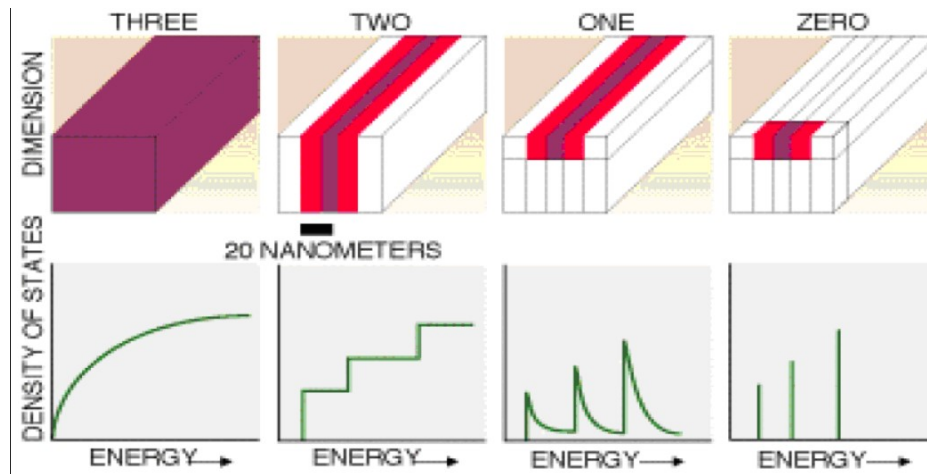


Figure 21.1: DOS

## 21 Physics of Low-Dimension Systems: 2D

- **Graphene:** is single layer of atoms. they are 2D in the sense that the wavefunction is so confined to the plane of graphene and does not stick out at all.
- **2D electron gas (2DEG):** useful cause of their large mean free paths (low impurities), and high electron mobilities.
  - For MOS structures, at the semiC-insulator interface.
  - For semiC heterostructures (remote dopants), 2DEG is formed at the interface between the 2 semiconductors.
- **Density of State (DOS)for Free Electrons:**
  - electrons not in a crystal (free in 3D) have a Fermi surface that is just a sphere. DOS is propto sqrt of E
  - and in 2D Fermi surface is a circle. DOS is constant as E increases.
  - in 1D Fermi surface is two points. DOS is propto 1/sqrt(E) as E increase. **van Hove singularity:** At energy E=0 electrons pile up (i.e. have a high DOS).
- **Bands vs Sub-bands:** Sub bands are based on excited states
- Sub-bands for 1D: van-Hove singularities for each sub-band with density of state:

$$g(E) = \frac{1}{\sqrt{E - E_n}} \quad (21.1)$$

- Summary for all dimensions:
- **Quantum Dots:** 0D systems where the wavefunction of the system is the same size as the system. (for semiCs it can be tens of nm or the size of one atom).
- **Drude Model with a Magnetic field: Hall Effect:** Integer Quantum Hall effect. Expected classical linear increase in Resistance xy as perpendicular Bz field increases.

- 2DEG in magnetic field at low temperatures so that QM effects can manifest nicely and instead we see linear increase only at small B increase but then we get a dramatically increasing staircase. Steps get bigger as we get to higher fields. Conductivity increases in equal steps.
- you expect resistance xx longitudinal to not change much. it starts out like this at low B field. But then everytime a jump happens in the hall resistance, a massive drop in Rxx occurs, going to 0 ohms where it flows without resistance looking like a superconductor and then peaks that show insulating behaviour.
- 2DEG gets cyclotron motion with B-field (classical). From **Lorentz Force**:

$$\vec{F} = \frac{d\vec{p}}{dt} = q(\vec{v} \times \vec{B}) \quad (21.2)$$

- Bohr-Sommerfeld quantization rule: number of wavelength along the trajectory must be integer. only discrete values of the trajectory radius are allowed. **Landau Levels**:

$$E_n = \hbar\omega_c(n + \frac{1}{2}) \quad (21.3)$$

- Wave functions are smeared around classical orbits with:

$$r_n = l_B \sqrt{n}, \quad l_B = \sqrt{\frac{\hbar}{m\omega_c}} \quad (21.4)$$

- where  $l_B$  : magnetic length
- difference in classical and quantum here is that quantum has many different landau levels of radial SHO. each level has an enormous degeneracy (and is allowed because they don't overlap).
- **Shubnikov-de Haas effect**: both Rxx and Rxy show oscillations at high magnetic field and low temp. each oscillation is a Fermi level pierced by a landau level. Oscillations allow to determine effective mass as well as scattering time. Efficient way to find parameters of 2DEG (magneto-transport studies).
- impurity may momentarily disrupt the forward propagation of the electron.
- Chiral edge channels: are these skipping electron edges
- composite picture of **FQHE**